FIVE-FOLD d-ELECTRON DEGENERACY IN THE HUBBARD MODEL OF TRANSITION METAL MAGNETISM

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ABSTRACT

FIVE-FOLD d-ELECTRON DEGENERACY IN THE HUBBARD MODEL OF TRANSITION METAL MAGNETISM

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The purpose of this inquiry is to elucidate the basic mechanisms and criteria for the formation of long range order magnetic phases in the Hubbard Model of transition metals. We include intrasite d-d electron interactions exactly, rather than in a simplified picture used by Penn (Phys. Rev., Vol. 142, Number 2, February, 1966). In this work Penn utilized s-band electrons in the tight binding approximation and solved the Heisenberg equation of motion for the energy of the system as a function of the direct coulomb coupling constant divided by the band energy. He plotted the total energy at T = 0 as a function of this ratio, and of the ratio of number of electrons to the total number of states in the system (the filling of the band). The result was a phase diagram for the various magnetic states, ferromagnetism, antiferromagnetism, and paramagnetism, in which

stability regions were chosen on the basis of minimization of the total energy as a function of the two parameters mentioned.

We have repeated Penn's calculation, but with inclusion of the full five-fold degeneracy of the d-band that exists in real transition metals. This treatment leads to a similar phase diagram, but with a third axis, that of exchange coupling constant divided by band energy. The reason for this is that in a s-band calculation, only an up spin and a down spin electron may interact in each Wigner-Seitz cell due to the Pauli principle. With five-fold degenerate d-electrons, there is an exchange energy contribution to the total energy. We also try to extend this calculation to non-zero temperatures and compare the evolution of our phase diagram as T varies with the 3d, 4d, and 5d transition metal Curie and Neel points. Lastly, a comparison with a t-matrix calculation by Kemeny and Caron will be attempted, in which we hope to show whether doing a many-body calculation on s-electrons or a one-body Hartree Fock calculation of five-fold degenerate d-electrons gives a more realistic fit to the real transition metals, both of these calculations being done in the Hubbard Model. This should allow a conclusion as to how one should proceed to improve the Hubbard Model, without including s-d electron interactions and s-d and d-d screening.

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By

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INTRODUCTION

In this thesis, we shall investigate the relative stability of ferromagnetic, antiferromagnetic, and paramagnetic phases of a Hubbard Model of the transition metals by numerically calculating the free energies of these three phases. We take into account the full five fold degeneracy of the d electrons which contribute to condensed magnetic phases in the transition metals, thus including d-d exchange energy, and base our calculation technique upon the general formulation of[1], and the explicit s electron Hubbard Model calculation of[2]. We do not take into account static nor dynamic d-d interactions nor s-d interactions explicitly, nor local correlations within any one Wigner-Seitz cell, although the minimization of local polarity energy would tend to produce a fairly uniform d electron or d hole density. Thus, we suppress polarity fluctuations, which would reduce the energy. Following Penn, we plot a phase diagram for a few values of temperature of direct Coulomb coupling constant, exchange Coulomb coupling constant and band filling. Emphasis throughout is on the Bloch ($\underline{k}$) space interpretation of condensed magnetic phase correlations between electrons as opposed to the Wannier (configuration) space interpretation of Hubbard.

The theory of the magnetic properties of transition metals has been divided up into two parts, the ferromagnetic-paramagnetic stability question and the paramagnetic-antiferromagnetic stability question. The ferromagnetic-antiferromagnetic transition is thus considered indirectly, through the intermediary of the paramagnetic state.

In the ferromagnetic-paramagnetic question, two schools of thought have arisen; the localized spin Heisenberg model[3] and the model of itinerant band theory of ferromagnetism[4]. For transition metals, experiments have shown that the d electron bands contribute to the possibility of large magnetic moments, and these d electrons are indeed in itinerant energy bands, and not localized[5,6,7,8]. On the theoretical side[9,10], a detailed itinerant band model has been developed in which a partially filled narrow d band is used as a basis for calculating and correlating electronic specific heats, Curie temperatures, magnetic moments, etc. of ferromagnetic and nonferromagnetic transition elements and alloys[11], by a more exact calculation than the Hartree-Fock technique of the itinerant d electron advocates, who argue that the "free" electron gas could not be ferromagnetic at any density. He was not concerned with Bloch electrons in a periodic potential so that there was some doubt of the applicability of his "free electron gas correlation energy" correction to real transition metals. An alternative

model for ferromagnetism utilizing polarity buildup on lattice sites was latter proposed[12,13]. A compromise theory involving competition between bands with itinerancy energy and quasi-localized polarity energy was arrived at[14]. In a coupled model for nickel, the d electrons were envisioned as distributed among atoms in states closely resembling d^{10} and d^9 states of the free nickel atom.

The holes (d^9 configuration) migrate through the lattice, avoiding one another owing to their electrostatic repulsion, producing minimum polarity contributions at each lattice site, lowering the energy of the system[15]. A major question in all of these theories was the effect of d band degeneracy certainly present in transition metals. This exchange contribution to the energy would be negative, enhancing the net magnetic susceptibility, and would even be present in an s band[16]. Whether this degeneracy, or Hund's rule of intra-atomic coupling, as for example between more than one 3d hole per atom in iron cobalt and nickel, dominated the enhancement of magnetic susceptibility at temperatures less than the Curie temperature was open to question[17].

One necessity in answering these questions is a knowledge of the band structure of transition metals which has been reviewed[18,19 20,21,22]. In addition to Hund's rule, coupling versus exchange (d electron degeneracy) as a criterion, the possibilities of s-d

and d-d screening to minimize polarity energy have to be considered[23,24]. In addition to these realistic considerations, a purely statistical mechanical model school, considering magnetic phase transitions as a symmetry breaking operation, just as other types of phase transitions, has been active[25]. Clearly, all of these approaches may be partially valid and one must pursue one or the other.

A fairly modern, semi-experimental review is available[26] as is an older one[27]. Herring[28] has reviewed the many and varied theories. The extent of polar fluctuations in d band metals has been summarized[29], with the s-d question being considered[30,31,32]. The correlation idea has been taken up by a large number of authors[33,34,35,36].

The antiferromagnetic-paramagnetic question seems to be quite a bit harder to handle because there arises in the electron dispersion relation a self consistent energy gap which must be calculated iteratively. The approach by way of spiral spin density[37] has been thoroughly summarized[38,39]. The basic idea that an exchange induced splitting of the energy band resulting in a self-consistent gap resembling the superconductivity B.C.S. gap equation[40], has been derived[41] based on the earlier ideas of Slater[42]. For the half-filled d band, this would produce an antiferromagnetic insulator since the Fermi energy would coincide

with the middle of the gap in the split d energy band[43]. This split d band model of antiferromagnetism is reviewed by Herring in great detail[44]. Herring points out that the usefulness of the Slater Hartree-Fock picture as developed by Slater[45] and des Cloizeaux[46] is tempered with the need for inclusion of a good deal of configuration interaction and polarity energy, which must be considered separately for different metals as their filling of the d band at a given temperature is different since their valences and ionic structures vary. Clearly, a general theory of antiferromagnetism must cut across the different atomic parameters of the various transition metals, lest we wind up with a completely separate theory for each metal. Des Cloizeaux showed that one could write Bloch functions as linear combinations of a $\underline{k}\sigma$, and a $\underline{k}+\underline{Q}$, σ state, and that such linear combination wave functions determined a gap Δ, the exchange field parameter, independent of $\underline{k}$. It is unclear what "exchange" means in this context since explicit five-fold d electron subband degeneracy was never included. His work is in agreement with that of Matsubara and Yokota[47] and of Kemeny and Caron[48] in regard to the description of the antiferromagnetic state.

The inclusion of exchange among electrons in narrow d bands is described[49] for Bloch electrons in a periodic potential in which semi-quantitative comparisons between the various transition metals are made for the negative exchange energy contribution.

The Hubbard Model[50,51] was proposed to satisfy the need for a simple, itinerant band theory of magnetism and magnetic phase transitions at zero temperature. Hubbard worked in configuration space and developed the configuration space Green's function for the one electron density matrix, and hence, the expectation values of all one-electron operators, the relevant quantities in his model. He did this only because he used the Gorkov factorization technique[52] to renormalize the constants in the potential energy part of the system Hamiltonian and express its two-body interaction, four operator product as an equivalent kinetic energy two operator product, making it identical in operator form to the kinetic band term in his Hamiltonian. He found that the poles of the Green's function play the role of quasi-particle energies, and that the Fermi surface volume was altered. Since the electron-electron interaction strength had been proven to be unchanged by electron interactions to all orders of perturbation theory[53], this lead Hubbard to conclude that as it was increased, the electrons could undergo a phase change leading to a superlattice antiferromagnetic order or ferromagnetic order[54]. Herring pointed out that Hubbard's conclusion destroys the implicit assumptions of his model, that of equal electron and spin densities on each lattice site, since an antiferromagnetic or ferromagnetic does not possess this property. Nevertheless, the Hubbard model is one of the best general methods of attacking the magnetic phase transition problem, and yields to an analysis

that could never be applied to the real transition metals with any hope of success. A shift of thinking of major importance occurred between Hubbard's work and that of des Cloizeaux, Matsubara, Yokota, Caron, Kemeny. Hubbard worked out his correlations completely in configuration space with Wannier functions for the electrons at each lattice site so that his Green's functions were configuration space expectation values. The latter authors all paired $\underline{k}$ states and completely worked in a Bloch space with Bloch functions for each electron state $\underline{k}$. They thus made the description of the antiferromagnetic state quite transparent and easy to deal with.

The treatment of the antiferromagnetic-paramagnetic question and the ferromagnetic-paramagnetic question, and thus indirectly, the ferromagnetic-antiferromagnetic question, was carried out simultaneously by Penn[55]. His work will be described extensively in the next chapter, but it is briefly summarized here to fit it into its historical perspective. Like des Cloizeaux, Matsubara, Yokoto, Caron, and Kemeny, he used a Bloch space description pairing states $\underline{k}\sigma$ with $\underline{k} + \underline{Q}$, σ in a simple cubic lattice ($Q = 1/2\underline{G} = 1/2\pi$) for the antiferromagnetic state. His basic Hamiltonian was that of Hubbard which he then Gorkov factorized to get an equivalent one-body form. This is thus a "Hartree-Fock" theory. Penn used correlation functions instead of Green's functions and calculated, for zero temperature, which magnetic phases would exist for various values of the interaction energy-band

energy ratio and filling of the d band. This was done for the simple magnetic phases by direct energy comparison in the parameter space of the phase diagram and by a susceptibility argument[56] for the more complicated ferrimagnetic and spiral spin density wave states. He arrived at a phase diagram for the three simple phases that illustrates a dominance of paramagnetism for an almost empty and an almost full d band. A dominance of antiferromagnetism for the half-filled band which disappears as the electron-electron interaction strength goes to zero, and disappears as the electron-electron interaction strength goes to infinity. The ferromagnetic state, which is sandwiched inbetween the paramagnetic and antiferromagnetic states, grows toward the half-filled band region[57].

A particularly illuminating general treatment of the theory of fermion phase transitions from a very general and unified point of view is the work of Mattuck and Johansson[58]. They use the spin correlation function $S'(\underline{r}-\underline{r}') = \langle S(\underline{r}) \cdot S(\underline{r}') \rangle$ to describe the correlation functions in configuration space of spins at sites $\underline{r}$ and $\underline{r}'$ in a lattice. For the short range ordered paramagnetic state, they require $S'(|\underline{r}-\underline{r}'|>0) \neq 0$ and $\lim_{|\underline{r}-\underline{r}'|\to\infty} S'(|\underline{r}-\underline{r}'|)=0$ and for the long range ordered ferromagnetic state they require $\lim_{|\underline{r}-\underline{r}'|\to\infty} S'(|\underline{r}-\underline{r}'|) \neq 0$. Their spin correlation functions in configuration space are equivalent to our Bloch space correlation

functions, to be introduced in the next chapter, by a simple Fourier transformation. An alternative way of viewing magnetic phases is by broken symmetry[59,60]. For the paramagnetic-ferromagnetic phase transition, the broken symmetry is "rotation" and the long range order parameter is "magnetization", as we shall see in the next chapter describing Penn's definitions of magnetizations for the various magnetic states. For the paramagnetic-antiferromagnetic phase transition, the broken symmetries are "rotation" and "translation" and the long range order parameter is "$S_{\underline{Q}}$ the amplitude of the $\underline{Q}$th Fourier component of spin density." This concept is also used by Penn and will be delved into in greater length in the next chapter, since $\underline{S}_{\underline{Q}}$ corresponds to the exact Fourier transformation to Bloch space we had mentioned before, being equivalent to our $(a^{+}_{\underline{k}+\underline{Q}}+a_{\underline{k}+\underline{Q}})$ type of terms we shall use throughout this work. When a source field is allowed to exist (a very weak magnetic field which breaks the 2^N fold rotational degeneracy (symmetry) of a randomly initiated ferromagnetic state in the atomic limit), we may describe the long range order of the magnetic state in a simpler way than by the spin correlation function description. Mattuck and Johanssen define the average value of spin density itself $\langle\underline{S}\rangle$ and write the relative magnetization (ratio of actual magnetization and magnetization) as (1.1) $M = \frac{2}{N}\langle\underline{S}\rangle$, N being the electron number. M is called the long range order parameter and is finite in the ferromagnetic state. A broken symmetry is needed to use M instead of S' since if all directions of total spin were equally likely,

the above $\langle \underline{S} \rangle = 0$, so that M would be zero even in the ferromagnetic phase. The spin correlation function S' is always nonzero in a ferromagnet since $\underline{S}(\underline{r}) \cdot \underline{S}(\underline{r}')$ is a scalar, and hence independent of total spin. Thus the spin correlation function is more generally utilized, but harder to apply. Actually one may calculate M from (1.2) $M = \lim_{\nu \to 0} \frac{2}{N} \langle \Psi_{o\nu} | \underline{S} | \Psi_{o\nu} \rangle$ where $\Psi_{o\nu}$ is the ground state for a given ν where the external source field is νH. This is the quasi-average method of Bogoliubov. For the general spiral spin density wave antiferromagnetic state (1.3) $S = \langle \Psi_o(\underline{s}) | \hat{\underline{S}}_{op} | \Psi_o(\underline{s}) \rangle = \sum_{\underline{Q}} \underline{S}_{\underline{Q}} e^{i\underline{Q} \cdot \underline{r}}$ where $|\underline{Q}|$ is one of the reciprocal lattice vectors of the spiral: $2\pi/R$, $4\pi/R$ . . ., and can include all harmonics of $\underline{Q}$ (whereas Overhauser's work[61] included only perfect spirals, with $|\underline{Q}| = 2\pi/R$), and $\underline{s}$ is the direction of the spiral axis. The particular $\underline{Q}$ dealt with in this thesis is $\underline{Q} = \frac{\pi}{2} = \frac{G}{2}$, one half of each component of the reciprocal lattice vector, which is explicitly defined only when we consider a specific lattice structure (simple cubic).

Mattuck and Johannson further discuss the general difference between a first order and a second order phase transition. In the second order phase transition the long range order parameter changes continuously from a nonmagnetic to a magnetic state (as in the paramagnetic-ferromagnetic phase transition) while in the first order phase transition, the long range order parameter changes discontinuously at the transition point. They emphasize

a very important result of Uhlenbeck, namely that in a finite system all dynamic variables (such as the long range order parameter) change continuously as a function of temperature, density, and interaction strength so that discontinuous changes of dynamic variables imply that only an infinitely large system can undergo a first order phase transition.

A contact is made with Heisenberg's effective internal field concept in the following way: A long range effective internal field is defined

$$(1.4) \quad F = F^{STATIC} + F^{DYNAMIC}$$

where the static field is due to all the other particles of the system considered as stationary, and the dynamic field is due to the motion of the other particles of the system which correllates with the motion of the particular particle being considered. The long range order parameter is related to the internal field by a self-consistent equation:

$$(1.5) \quad \theta = \theta(F(\theta))$$

where θ is the long range order parameter and F is the internal self-consistent field. They further show that the condensed phases in a Fermi system may be described field theoretically by a matrix propagator whose off diagonal elements are directly related to the long range order parameter (our spin correlation function in Bloch space). Equation (1.5) indicates that the

rest of the system produces an internal field which extends throughout the system and "produces" [or is "produced by", depending upon how one reads equation (1.5)] the condensed phase. It is of only limited range and "produces" (or is "produced by") the local, short range order. The field in a magnetic phase problem is called the spin aligning field or the spiral spin aligning field. It was introduced by Weiss in a theory of ferromagnetism, molecular field being a synonym for it. This molecular field acts somewhat like a magnetic field, but it is not a real magnetic field since the charged particle orbits are unbent by a Lorentz force.

They further assume that

$$\theta = \theta(Co, T, \rho) \tag{1.6}$$

where Co is the interparticle interaction strength, ρ is the particle density (equivalent to our band filling in chapter 3), and T is the absolute temperature. Thus

$$\theta(Co,T,\rho)=\theta\Big(F\big(\theta(Co,T,\rho)\big)\Big) = \theta\big(F(Co,T,\rho)\big) \tag{1.7}$$

The self-consistency is seen clearly in (1.7). θ must be found self-consistently, i.e. we assume a nonzero value for θ, find F from it, substitute into (1.5) to get a new value for θ, compare it with the initial θ value, etc., until our iterative cycles start reproducing the same values of θ and F on every cycle. This proceedure dominates our calculational flow charts

at the end of chapter 3. If the self-consistent values of θ is nonzero, the system is indeed in a condensed (magnetic) phase. There are inherent dangers in such a technique which will concern us very deeply in this work. There is no way to determine which magnetic phases exist for a particular set of ρ, Co, and T values and the number of magnetic phases one can study must be limited to a finite number. At a given ρ, Co, and T, the self-consistent equations for F and θ possess more than one solution. θ can be zero or nonzero for the same ρ, Co, and T values, so that a relative comparison of the free energies of the two phases must be used as a criterion for ascertaining which are the thermodynamically stable by virtue of a minimum free energy. We must make a guess, based on the experimental relevance of our analysis to the particular metals we desire to study, The transition metals. They then write a Hartree-Fock equation for $\varphi_{\underline{k}}$:

$$(1.8)\quad \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r}) + A(\varphi_1,\ldots,\varphi_N)\right]\varphi_{\underline{k}}(\underline{r}) = \epsilon_{\underline{k}}\varphi_{\underline{k}}(\underline{r})$$

where the $\varphi_{\underline{k}}$'s determine the trial wave function Ψ_o by a Slater determinant:

$$(1.9)\quad \Psi_0 = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_1(1) & \cdots & \varphi_1(N) \\ \vdots & & \\ \varphi_N(1) & \cdots & \varphi_N(N) \end{vmatrix}$$

Since a single Slater determinant best characterizes the anti-symmetry of one electron wave function, the single φ's give symmetry to Ψ_o, so that Ψ_o has the symmetry and long range order θ chosen. This is done by putting in the correct self-consistent A value appropriate to the particular phase studied, as A is an integral operator giving the potential felt by a particle in state $\varphi_{\underline{k}}$ due to its interaction with all the other particles; A is the self-consistent potential of the Weiss internal field. The long range order parameter can then be obtained from Ψ_o as seen in (1.1) and (1.2), and hence from the φ's. (1.8) and (1.9) have the same form as the ordinary Hartree-Fock theory, but here the trial wave function Ψ_o has the (less than perfect) symmetry of the condensed (magnetic) phase built into it; the normal phase has perfect symmetry included in Ψ_o. Thus in the condensed (magnetic) phase, operator A describes a long range internal field; in the normal phase it describes a short range field. The Hartree-Fock theory thus presented yields only the F^{STATIC}; the $F^{DYNAMIC}$ is due to correlations between the particle motions. This $F^{DYNAMIC}$ may possibly destroy the condensed (magnetic) phase.

Since particles, propagators in the normal system, directly proportional to the correlation functions, are defined as

$$(1.10) \quad G_{PARA}(\underline{k},\sigma,t'-t)=-i\langle\Psi_0\left|\hat{T}^{op.}\{a_{\underline{k},\sigma}(t')a^{+}_{\underline{k},\sigma}(t)\}\right|\Psi_0\rangle$$

or

$$(1.11)\quad G_{PARA}(\underline{r}'-\underline{r},\sigma,t'-t) = -i\langle\Psi_0\left|\hat{T}^{op}\cdot\{\Psi_\sigma^{op}(\underline{r}',t')\Psi_\sigma^{+op}(\underline{r},t)\}\right|\Psi_0\rangle$$

in configuration space, where $\hat{T}^{op}$ is a time ordering operator. These propagators describe the following experiment. At a time t a particle spin-orbital state $\varphi_{\underline{k},\sigma} = \Omega^{-1/2}e^{i\underline{k}\cdot\underline{r}}$ is added to the system in its exact ground state $\Psi_o\rangle$. The particle propagates in the system until time t' when a particle in $\varphi_{\underline{k},\sigma}$ is removed. Thus the propagator gives the probability amplitude of observing the system to have an added particle in $\varphi_{\underline{k},\sigma}$ at time t'; this amplitude is the sum of amplitudes for all processes in which a particle enters in $\varphi_{\underline{k},\sigma}$, interacts with the other particles of the system, and leaves in $\varphi_{\underline{k},\sigma}$. (We stress "a particle" since the occupied state is of interest; not which particle is in it. These propagators describe a quasi-particle in state $\underline{k},\sigma$ with energy.

$$(1.12)\quad E_{\underline{k}} = \epsilon_{\underline{k}} + \sum_{\ell<\underline{k}F}(V_{\underline{k},\sigma;\underline{\ell},\sigma'\underline{k}\sigma;\underline{\ell}\sigma'} - V_{\underline{k},\sigma;\underline{\ell},\sigma\underline{\ell},\sigma;\underline{k},\sigma}\delta_{\sigma\sigma'})$$

This is a static Hartree-Fock energy caused by a static Hartree-Fock internal field, F^{STATIC}, whose potential is seen in the second term of (1.12) to have an average direct coulomb part and a subtractive average exchange coulomb part. These propagators can be found from a diagrammatic perturbation series.

Mattuck and Johannson then define the anomalous propagators, directly proportional to the anomalous correlation function, in the condensed (magnetic) phase as the diagrammatic

perturbation series method breaks down then since they are not included in it. In the ferromagnetic phase the internal spin aligning field, F, may flip a spin. This results in an anomalous spin flipping propagator (with a similar meaning):

$$(1.13)\quad G_{\text{FERRO}}(\underline{k}_-,\underline{k}_+,t'-t) = -i\langle\Psi_0\left|T^{op.}\{a_{\underline{k}-}(t')a^+_{\underline{k}+}(t)\}\right|\Psi_0\rangle$$

or

$$(1.14)\quad G_{\text{FERRO}}(\underline{k}_+,\underline{k}_-,t'-t) = -i\langle\Psi_0\left|T^{op.}\{a_{\underline{k}+}(t')a^+_{\underline{k}-}(t)\}\right|\Psi_0\rangle$$

where "+" denotes an up spin electron and "-" a down spin electron, in addition to the normal propagator (1.10) and (1.11). These anomalous propagators are zero in the normal (paramagnetic) phase. They arise from multiple scatterings from the internal spin aligning potential, which depopulates state $|k,\sigma\rangle$ and repopulates $|k,\sigma'\rangle$. The difference in propagating spin up or spin down particles (with respect to the small, external source field) is given by:

$$(1.15)\quad \Delta G = G(\underline{k}_+,\underline{k}_-,t'-t) - G(\underline{k}_-,\underline{k}_+,t'-t)$$

This is zero in the normal (paramagnetic) phase since $F = 0$, but nonzero in the condensed (ferromagnetic) phase since $F \neq 0$. In the condensed (antiferromagnetic) phase the characteristic anomalous propagator is:

$$(1.16)\quad G_{\text{ANTIFERRO}} = -i\langle\Psi_0\left|\hat{T}\{a_{\underline{k}+\underline{Q}',\sigma'}a^+_{\underline{k}+\underline{Q},\sigma}\}\right|\Psi_0\rangle$$

This seemingly describes a particle picking up momentum $\underline{Q}-\underline{Q}'$ from scattering against the periodic structure of the spiral

internal field, and having its spin flipped from σ to σ' by the spin-aligning character of the internal field. What actually happens is neither a momentum pick up nor spin slip by the particle; Ψ_0 is a linear combination of Slater determinants, so that the aa^+ connect different Slater determinants, both of which occur in the linear combination with nonzero amplitude. In this paper, we will choose $\underline{Q} = 0$, $\underline{Q}'$ redefined as $\underline{Q}$ and $\sigma = \sigma'$; thus no spin flip takes place and only Bloch electrons with wave vector $\underline{k}$ are scattered off the spiral internal field.

Mattuck and Johannson further generalize their work by defining a general anomalous propagator:

$$(1.17)\quad G_{\text{ANOMALOUS}}(\underline{k}',\sigma',\alpha';\underline{k},\sigma,\alpha;t'-t) = -i\langle\Psi_0|\, T^{po}\cdot\{a^{\alpha'}_{\underline{k}',\sigma'}(t')\, a^{+\alpha}_{-,\sigma}(t)\}\,|\Psi_0\rangle$$

or

$$(1.18)\quad G_{\text{ANOMALOUS}}(\underline{r}',\sigma',\alpha';\underline{r},\sigma,\alpha;t'-t) = -i\langle\Psi_0|\, T^{op}\cdot\{\Psi^{op}_{\sigma'}(\underline{r}',t')\, \Psi^{+op\alpha}_{\sigma}(\underline{r},t)\}\,|\,\Psi_0\rangle$$

in configuration space, where α, $\alpha' = +$ or 1, so that the creation operator may or may not precede the annihilation operator. Generally G is a function of $\underline{r}-\underline{r}'$ since exact translational invariance does not hold in many condensed phases, as in the antiferromagnetic state. The major power of this technique is that it applied to all sorts of "condensed" phases: ferromagnets, antiferromagnets, superconductors, and solids. These authors

then derive the long range order parameters from the propagators: For the ferromagnetic phase:

$$(1.19)\quad M = \frac{1}{N}\sum_{\underline{k}} \langle \Psi_0 \left| a^{+}_{\underline{k},+} a_{\underline{k},+} + a^{+}_{\underline{k},-} a_{\underline{k},-} \right| \Psi_0 \rangle$$

and for the antiferromagnetic phase:

$$(1.20)\quad S_{\underline{Q}} = \sum_{\underline{k}} \langle \Psi_0 \left| a^{+}_{\underline{k}+\underline{Q},+} a_{\underline{k},+} + a^{+}_{\underline{k},-} a_{\underline{k}+\underline{Q},-} \right| \Psi_0 \rangle$$

The general relation is:

$$(1.21)\quad \theta = \text{CONSTANT} \times \sum_{\substack{\underline{k}',\sigma',\alpha' \\ \underline{k},\sigma,\alpha}} A_{\underline{k}',\sigma',\alpha';\underline{k},\sigma,\alpha} \langle \Psi_0 \left| a^{\alpha'}_{\underline{k}',\sigma'} a^{+a}_{\underline{k},\sigma} \right| \Psi_0 \rangle$$

In the ferromagnetic phase:

$$(1.22)\quad A_{\underline{k}',\sigma',\alpha';\underline{k},\sigma,\alpha} = \delta_{\underline{k}',\underline{k}} \delta_{\sigma',-\sigma} - \delta_{\alpha',+} \delta_{\alpha,+}$$

as an example. The general relation can be written directly in terms of the propagator as:

$$(1.23)\quad \theta = \sum_{\substack{\underline{k}',\sigma',\alpha' \\ \underline{k},\sigma,\alpha}} A_{\underline{k}',\sigma',\alpha';\underline{k},\sigma,\alpha} G_{\text{ANOMALOUS}} (\underline{k},\sigma',\alpha';\underline{k}',\sigma,\alpha;t'-t=\bar{0})$$

where $\bar{0}$ is a negative infinetesimal. Thus, in the normal phase when $G_{\text{ANOMALOUS}} = 0$, the long range order parameter, $\theta = 0$; a normal phase can only have short range order at best.

A detailed investigation of the mathematical structure of the condensed versus normal phase is given. As pointed out by them, the normal perturbation series for the normal propagator breaks down in the condensed phase since anomalous propagators cannot

be taken into account. The reason that this is so is that for the normal perturbation expansion of a propagator to be valid, the interacting groung state $|\Psi_0\rangle$ must have the same "structure" as the non-interacting ground state $|\Phi_0\rangle$; i.e. it must overlap $|\Phi_0\rangle$ so that:

$$\langle\Psi_0|\Phi_0\rangle \neq 0 \qquad \text{(nonorthogonality)} \tag{1.24}$$

Since at infinite volume the structure of the condensed phase differs markedly from that of the normal phase, we always have

$$\langle\Psi_0|\Phi_0\rangle \equiv 0 \qquad \text{(orthogonality)} \tag{1.25}$$

violating the criterion (1.24) for a normal perturbation expansion of the propagator to be valid. For example, in the condensed (ferromagnetic state in the Hartree-Fock approximation:

$$|\Psi_0\rangle = |1_{\underline{k}_1,+}, 1_{\underline{k}_2,+}\ldots 1_{\underline{k}_M,+}; 1_{\underline{k}_1,-}, 1_{\underline{k}_2,-}\ldots 1_{\underline{k}_P,-}, 000\ldots\rangle \tag{1.26}$$

where M>P, i.e. there are more up spins than down spins. This is clearly orthogonal to the normal non-interacting state $|\Phi_0\rangle$ (for free electrons) which has M ≡ P.

Mattuck and Johannson construct a perturbation expansion of the anomalous propagator, valid for the condensed phase, by replacing each normal propagator by a matrix propagator. Its diagonal elements are normal propagators and its off diagonal elements are anomalous propagators. For the ferromagnetic phase:

$$(1.27)\quad \underset{\text{FERRO}}{G(\underline{k},t'-t)} = -i \begin{bmatrix} \langle \Psi_0 | T^{op}\{a_{\underline{k},+}(t')a^{+}_{\underline{k},+}(t)\} | \Psi_0 \rangle \langle \Psi_0 | T^{op}\{a_{\underline{k},+}(t')a^{+}_{\underline{k},-}(t)\} | \Psi_0 \rangle \\ \langle \Psi_0 | T^{op}\{a_{\underline{k},-}(t')a^{+}_{\underline{k},+}(t)\} | \Psi_0 \rangle \langle \Psi_0 | T^{op}\{a_{\underline{k},-}(t')a^{+}_{\underline{k},-}(t)\} | \Psi_0 \rangle \end{bmatrix}$$

If the interaction between electrons was switched off, this would become:

$$(1.28)\quad \underset{\text{FERRO}}{G^{0}(\underline{k},\omega)} = -i \begin{bmatrix} [\omega-(\epsilon_{\underline{k}}-\mu)+i\delta^{\mu}_{\underline{k}}]^{-1} & 0 \\ 0 & [\omega-(\epsilon_{\underline{k}}-\mu)+i\delta^{\mu}_{\underline{k}}]^{-1} \end{bmatrix}$$

the free electron propagators are on the diagonal and the anomalous propagators vanish; the system reverts to a normal (paramagnetic) state.

The antiferromagnetic general spiral spin density wave state has an infinite matrix propagator since the $\underline{Q}$ that an electron can absorb or emit to the spiral spin structure is unspecified and can be $n\underline{Q}$, n being any integer; and $\underline{Q}$ being unspecified itself:

$$(1.29)\quad \underset{\text{ANTIFERRO}}{G(\underline{k},t'=t)} = -i \begin{bmatrix} \langle a_{\underline{k},+}\, a^{+}_{\underline{k},+} \rangle \langle a_{\underline{k},+}\, a^{+}_{\underline{k}+\underline{Q},-} \rangle \langle a_{\underline{k},+}\, a^{+}_{\underline{k}+\underline{Q},+} \rangle \cdots \\ \langle a_{\underline{k}+\underline{Q},-}\, a^{+}_{\underline{k},-} \rangle \langle a_{\underline{k}+\underline{Q},-}\, a^{+}_{\underline{k}+\underline{Q},-} \rangle \langle a_{\underline{k}+\underline{Q},-}\, a^{+}_{\underline{k}+\underline{Q},+} \rangle \cdots \\ \langle a_{\underline{k}+\underline{Q},+}\, a^{+}_{\underline{k},+} \rangle \quad \cdots \\ \langle a_{\underline{k}+2\underline{Q},-}\, a^{+}_{\underline{k},+} \rangle \quad \cdots \end{bmatrix}$$

In this work, we shall put $\underline{Q} = \pi/a = \underline{G}/2$, as before, and n = 1, so that we reduce (1.29) to a 2 x 2 matrix propagator (for spins

up or spins down):

$$(1.30)\quad G^{(\pm)}_{\text{ANTIFERRO}}(\underline{k},t'-t) = -i\begin{bmatrix} \langle a_{\underline{k},\pm}\ a^{+}_{\underline{k},\pm}\rangle\langle a_{\underline{k},\pm}\ a^{+}_{\underline{k}+\underline{Q},\pm}\rangle \\ \langle a_{\underline{k}+\underline{Q},\pm}a^{+}_{\underline{k},\pm}\rangle\langle a_{\underline{k}+\underline{Q},\pm}a^{+}_{\underline{k}+\underline{Q},\pm}\rangle \end{bmatrix}$$

No spin flipping occurs and only one wavevector exchange of crystal momentum, $\underline{Q}$, is allowed.

Finally, Mattuck and Johannson note that the long range order parameter is directly related to the source term in the Hamiltonian (i.e. to the source field since $F = -\partial H_{SOURCE}/\partial space$):
variable

$$(1.31)\quad \theta = \text{CONSTANT} \times \frac{1}{\nu}\langle \Psi_0 | H_{SOURCE} | \Psi_0 \rangle$$

For the ferromagnetic phase:

$$(1.32)\quad H^{FERRO}_{SOURCE} = \nu g\beta H_x S_x = \text{external magnetic potential}$$
$$= \nu g\beta H_x \sum_{\underline{k}} (a^{+}_{\underline{k},-}a_{\underline{k},+} + a^{+}_{\underline{k},+}a_{\underline{k},-})$$

where β is the Bohr magneton number of an electron and g is the electron g-factor, and the ν's in (1.31) and (1.32) cancel.
For the spin density wave antiferromagnetic phase:

$$(1.33)\quad H^{S.D.W.\ ANTIFERRO}_{SOURCE} = \nu g\beta H \sum_{\underline{k}\underline{Q}} (a^{+}_{\underline{k},+}a_{\underline{k}+\underline{Q},+} + a^{+}_{\underline{k}+\underline{Q},-}a_{\underline{k},-})$$

where the constants are defined as before and the ν's cancel.
For our chose of $\underline{Q} = \pi/a = \underline{G}/2$ and n = 1, we drop the $\sum_{\underline{Q}}$ and get:

$$(1.34)\quad H^{ANTIFERRO}_{SOURCE} = \nu g\beta H \sum_{\underline{k}} (a^{+}_{k,+}a_{\underline{k}+\underline{Q},+} + a^{+}_{\underline{k}+\underline{Q},-}a_{\underline{k},-})$$

We have thoroughly emphasized the Mattuck and Johannson approach since it seems to be a general, unified description of phase transitions, being based on Brout's work quoted earlier. In subsequent chapters we will not utilize the propagator approach, but rather the correlation function approach, and all relations will differ from those of this chapter by constants, i.e. factors of i. We will not delve into perturbation theoretic series calculation of propagators as we will be able to find them exactly by expressing them in terms of known coefficients in the condensed state wave functions. However, Mattuck and Johannson's development is a general basis for all of the calculations that we shall undertake and should be kept in mind throughout.

NON-DEGENERATE MODEL AND RESULTS

Penn[62] treated the Hubbard Model at zero temperature in solving for the phase stability of model transition metals by neglecting intersite interaction and treating the tight binding narrow d band.

$$(2.1) \quad \epsilon_{\underline{k}} = -E''(\cos k_x a + \cos k_y a + \cos k_z a)$$

as a tight binding s band in a simple cubic lattice. His treatment was not explicitly worked out, so that this chapter had to be derived by us.

The effect of the non-inclusion of intersite interaction between electrons, the basic simplicity of the Hubbard Model, is that one can treat the lattice of isolated Wigner-Seitz cells in configuration space as a geometric point lattice so that the electrons hop only from site to site. The region within the Wigner-Seitz cell surrounding the lattice point has no meaning in this problem, being suppressed by integrals extending over its volume which are associated with the lattice point, so that electrons can be found at the lattice point. The electron wave functions are thus modified by:

$$(2.2) \quad \delta(\underline{r}-\underline{R}_j), \ \underline{R}_j = \text{lattice sites}$$

Tight binding energy bands nearly accomplish this, and still allow a hopping term in the Hubbard Hamiltonian, the band being

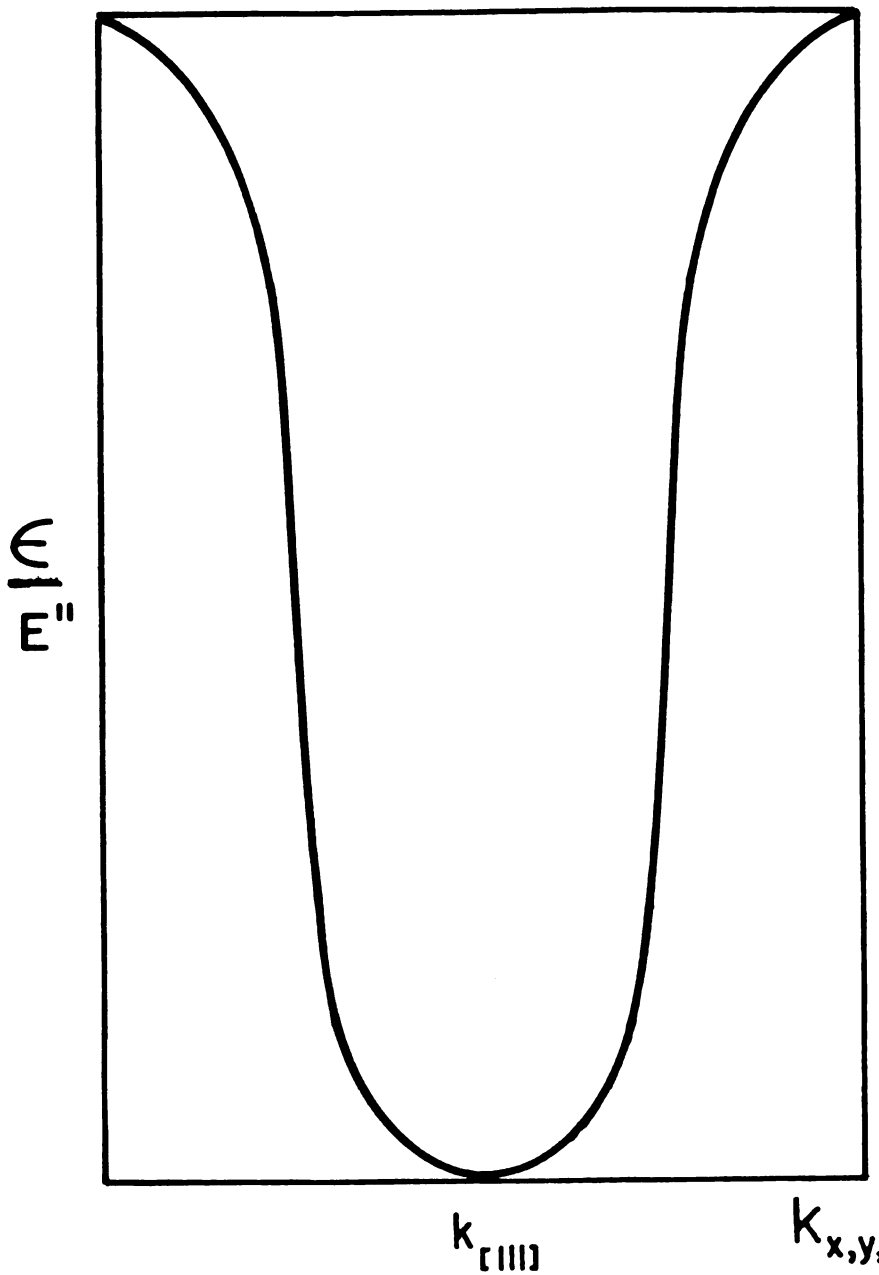


Figure 1. s-Electron Tight Binding Band.

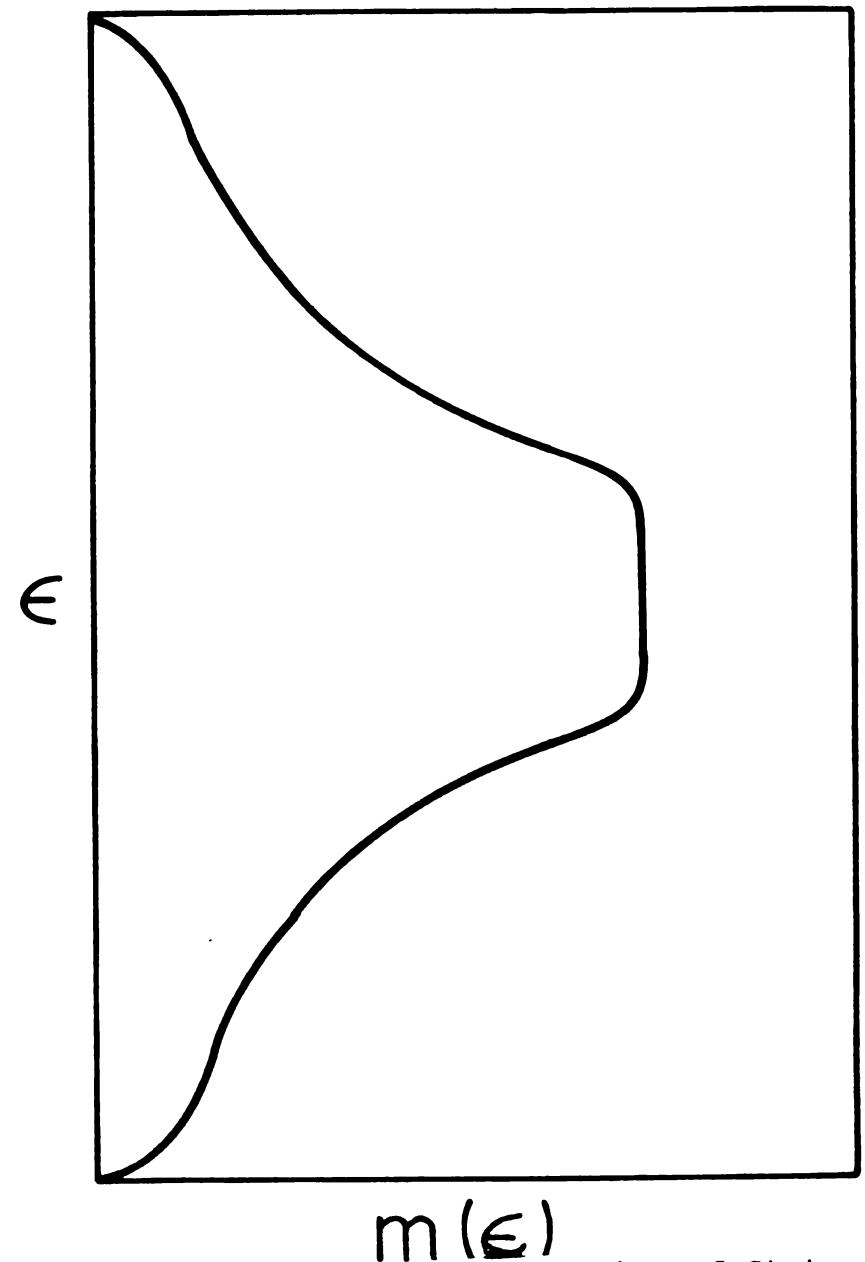


Figure 2. s-Electron Density of States.

extremely narrow in energy. A simple cubic Brillouin zone is definable:

$$(2.3) \quad -\frac{\pi}{a} < k_i < \frac{\pi}{a}, \quad i = x,y,z$$

with a being the nearest neighbor distance in the crystal.

Figures 1 and 2 indicate the [111] direction energy band dispersion relation in $\underline{k}$ space and the associated density of states. Penn correctly pointed out that these curves are not exactly equal to the band form and density of states of real transition metal d bands.

There are basically three reasons for this nonequivalence. Firstly, there may be actually a different d band form owing to the non-tight binding of d electrons to the degree implied here; the d band tight binding form differs from that of the s band. This fault will not be corrected in this paper as it involves some use of empirical results for the dispersion relation and density of states, an approach we want to avoid.

Secondly, Penn has not actually treated a d band, but only an s band. The crucial question of band degeneracy has been ignored as it is very difficult to include. We will correct this fault as much as possible, the extent of our being able to take into account all five degenerate states of each $\underline{k}$

state in the d band being governed by computational difficulties. We decide on this correction because it is of inherent physical interest in real transition metals.

Thirdly, the crystal symmetry makes Figures 1 and 2 idealizations because it is not simple cubic.

In Penn's non-degenerate treatment, the Pauli principle forces each site to have no more than two electrons on it, and those to be of antiparallel spin. As site-site interaction is neglected (except for the trivial hopping kinetic energy in the Hubbard Hamiltonian), no parallel spin interactions can exist. Thus the all important exchange energy is not included in the model and the resultant energies of the various magnetic phases considered are thus lacking in a large, negative interaction contribution. If this exchange energy were the same for all states, it would only shift the energy origin on Penn's final magnetic phase diagram uniformly for all states, making his results correct for real d bands as well as the d bands modeled as s bands that he actually used. All evidence would indicate that in states of different magnetic ordering there is no a priori reason why this exchange energy should be the same, and if so, it would only be fortuitous, since the number of parallel spins varies from state to state.

Starting with the Hubbard Hamiltonian in Wannier (configuration) space:

$$(2.4)\quad H^{\text{Wannier}}_{\text{Hubbard}} = \sum_{i,j,\sigma} Tij\ C^{+}_{i\sigma}\ C_{j\sigma} + J \sum_{i\ \sigma\neq\sigma'} n_{i\sigma}\ n_{i\sigma'}$$

he transforms the operators into their equivalent in Bloch space ($\underline{k}$ space) which operate on states of a definite $\underline{k}$:

$$(2.5)\quad C_{i,\sigma} = \frac{1}{\sqrt{N}} \sum_{\underline{k}} \ell^{i\underline{k}\cdot\underline{R}i}\ a_{\underline{k},\sigma}$$

$$(2.6)\quad C^{+}_{i,\sigma} = \frac{1}{\sqrt{N}} \sum_{\underline{k}} \ell^{i\underline{k}\cdot\underline{R}i}\ a^{+}_{\underline{k},\sigma}$$

where N is the number of sites. Thus, the Hubbard Hamiltonian becomes:

$$(2.7)\quad H_{\text{Hubbard}} = \sum_{i,j,\sigma} Tij\ \frac{1}{N} \sum_{\underline{k}} \ell^{i\underline{k}\cdot\underline{R}i}\ a_{\underline{k},\sigma} \sum_{\underline{k}} \ell^{i\underline{k}\cdot Rj}\ a_{\underline{k},\sigma}$$

$$+\frac{J}{N} \sum_{i\ \sigma\neq\sigma'} a^{+}_{\underline{k}_3,\sigma} a^{+}_{\underline{k}_4,\sigma'} a_{\underline{k}_1,\sigma} a_{\underline{k}_2,\sigma'} \frac{1}{N} \sum_{\substack{\underline{k}_1,\underline{k}_2\\ \underline{k}_3,\underline{k}_4}} \ell^{i(\underline{k}_1+\underline{k}_2-\underline{k}_3-\underline{k}_4)\cdot\underline{R}_i}$$

Now

$$(2.8)\quad \frac{1}{N} \sum_{i} \ell^{i(\underline{k}_1+\underline{k}_2-\underline{k}_3-\underline{k}_4)\cdot\underline{R}i} = \delta(\underline{k}_1+\underline{k}_2-\underline{k}_3-\underline{k}_4)$$

$$(2.9)\quad \sum_{j} Tij\ell^{i\underline{k}\cdot\underline{R}j} \equiv \epsilon(\underline{k})$$

$$(2.10)\quad \frac{1}{N} \sum_{j} \ell^{i(\underline{k}-\underline{k}')\cdot Rj} = \delta(\underline{k}-\underline{k}')$$

so that

$$(2.11)\quad H^{\text{Bloch}}_{\text{Hubbard}} = \sum_{\underline{k}\sigma} \epsilon(\underline{k}) M_{\underline{k},\sigma} + \frac{J}{N} \sum_{\substack{\underline{k}_1,\underline{k}_2\\ \underline{k}_3,\underline{k}_4}} \delta(\underline{k}_1+\underline{k}_2-\underline{k}_3-\underline{k}_4)\, a^{+}_{\underline{k}_3,+}$$

$$a_{\underline{k}_4,-} a_{\underline{k}_1,+} a_{\underline{k}_2,-}$$

where + means σ and - means σ'.

Penn first transformed the Wannier space form of this Hamiltonian, which contains products of four creation and annihilation operators (and is thus an explicit two-body Hamiltonian) into an effective quasi-particle Hamiltonian containing products of two of these operators multiplied by the expectation value of the other two.

$$(2.12)\quad H^{\text{Interaction}}_{\text{Bloch Hubbard}} = Co \sum_{l\sigma,\bar{\sigma}} [\langle c^{+}_{l,\sigma} c_{l,\sigma}\rangle c^{+}_{l,\bar{\sigma}} c_{l,\bar{\sigma}} - \langle c_{l,\sigma} c_{l,\bar{\sigma}}\rangle c^{+}_{l,\bar{\sigma}} c_{l,\sigma}]$$

This Govkov factorization 58 is of a Hartree form and $H^{\text{Interaction}}$ is now formally equivalent to a one-body kinetic energy for the quasi-particles. Co is a constant representing the particle-particle interaction strength.

This model forces the Hamiltonian to be specified by two parameters, the total particle number n and the quasi-particle-quasi-particle interaction strength Co (Measured relative to E"). Thus the phase diagram can be represented in the versus plane. Penn notes that actually Co and E" should depend on the magnetic state of the system, but neglects it since including this dependence would be a hard computational problem. To do so, one would choose a Ψ magnetic, compute Co and E" from it, use Co and E" to determine a Ψ magnetic at a certain line in

the Co/E"-n/2N plane, and then iteratively correct Co and E" to approach self-consistency. This would be an arduous task since the dependence of Co and E" upon Ψ magnetic could only be guessed at roughly.

Thus, all Penn could do was to compute relative state energies and compare them, absolute cohesive energies of the system in various magnetic states being out of the question.

In general, one can imagine an infinite number of magnetic states, and handling them all is a difficult task. Penn could only calculate the energy of a few of the magnetic states that he chose to consider, the rest being compared by a magnetic susceptibility calculation which we will avoid because the comparison of energy (or free energy) slopes as a function of band filling uniquely defines state stability. Penn chooses six magnetic states defined by an operator $\gamma_{\underline{k}}$, a wave function $\Psi_{\underline{k}}$, and equivalently by their correlations, defined as the sum over-occupied $\underline{k}$ states of the expectation values of 2-operator products taken in the magnetic states of each electron with wave vector $\underline{k}$:

$$(2.13)\quad A_{mn} = \pm Co \sum_{\underline{k}} \langle \Psi_{MAG}^{\underline{k}} | a_m^+ a_n | \Psi_{MAG}^{\underline{k}} \rangle$$

these wave functions combining to form Ψ magnetic by summing over all filled $\underline{k}$ states.

The other two types of definitions are generally, in operator form:

$$(2.14)\quad \gamma_{\underline{k}} = B_1 a_{\underline{k},+} + B_2 a_{\underline{k},-} + B_3 a_{\underline{k}+\underline{q},+} + B_4 a_{\underline{k}+\underline{q},-}$$

being composed of Bloch function operators, and in wave function form:

$$(2.15)\quad \Psi_{\underline{k}} = B_1 \Psi_{\underline{k},+} + B_2 \Psi_{\underline{k},-} + B_3 \Psi_{\underline{k}+\underline{q},+} + B_4 \Psi_{\underline{k}+\underline{q},-}$$

being composed of Bloch functions proper.

Penn chooses $\underline{q} = \underline{Q} = \underline{G}/2 = \underline{\pi}$, where $\underline{G}$ is a reciprocal lattice vector equal to $2\pi/a$ (i, j or k) with a equal to unity being a unit lattice constant in configuration space, so that the magnetic state function component contributed by the electron in Bloch state $\underline{k},+$ is paired with a component from Bloch state $\underline{k},-$, and $\underline{k}+\underline{Q},+$ and $\underline{k}+\underline{Q},-$ components also interfere generally.

Clearly a simple group of states must be singled out for comparison, and Penn chooses:

ferromagnetic ≡ $|FM\rangle$
paramagnetic ≡ $|PM\rangle$
antiferromagnetic ≡ $|AFM\rangle$
ferrimagnetic ≡ $|FIM\rangle$
spiral spin density wave ≡ $|SSDW\rangle$

(the two that he chooses are equivalent under a coordinate axis rotation)

which are defined as:

$$(2.16)\quad \Psi_{\underline{k}}^{PM} = |PM> = B_1\Psi_{\underline{k},+} \text{ or } B_2\Psi_{\underline{k},-}$$

$$(2.17)\quad \Psi_{\underline{k}}^{FM} = |FM> = B_1\Psi_{\underline{k},+} \text{ or } B_2\Psi_{\underline{k},-}$$

$$(2.18)\quad \Psi_{\underline{k}}^{AFM} = |AFM> = B_1\Psi_{\underline{k},+} + B_3\Psi_{\underline{k}+\underline{Q},+}$$

$$\text{or} \qquad B_2\Psi_{\underline{k},-} + B_4\Psi_{\underline{k}+\underline{Q},-}$$

$$(2.19)\quad \Psi_{\underline{k}}^{FIM} = |FIM> = B_1\Psi_{\underline{k},+} + B_2\Psi_{\underline{k},-} + B_3\Psi_{\underline{k}+\underline{Q},+} + B_4\Psi_{\underline{k}+\underline{Q},-}$$

$$(2.20)\quad \Psi_{\underline{k}}^{SSDW} = |SSDW> = B_1\Psi_{\underline{k},+} + B_4\Psi_{\underline{k}+\underline{Q},-} \text{ or } B_2\Psi_{\underline{k},-} + B_3\Psi_{\underline{k}+\underline{Q},+}$$

The correlation function language for describing these states involves the sums over matrix elements:

$$(2.21)\quad A_{o+-} = -Co \sum_{\underline{k}} < a^{+}_{\underline{k},+} \quad a_{\underline{k},-} >$$

$$(2.22)\quad A_{o++} = Co \sum_{\underline{k}} < a^{+}_{\underline{k},+} \quad a_{\underline{k},+} >$$

$$(2.23)\quad A_{o--} = Co \sum_{\underline{k}} < a^{+}_{\underline{k},-} \quad a_{\underline{k},-} >$$

$$(2.24)\quad A_{\underline{Q}+-} = -Co \sum_{\underline{k}} < a^{+}_{\underline{k}+\underline{Q},-} \quad a_{\underline{k},+} >$$

$$(2.25)\quad A_{\underline{Q}++} = Co \sum_{\underline{k}} < a^{+}_{\underline{k}+\underline{Q},-} \quad a_{\underline{k},-} >$$

$$(2.26)\quad A_{\underline{Q}--} = Co \sum_{\underline{k}} < a^{+}_{\underline{k}+\underline{Q},+} \quad a_{\underline{k},+} >$$

where $\sum_{\underline{k}}$ is over the whole Brillouin zone.

When the various Ψ magnetic states are put into the matrix elements to measure the correlations in those states, certain A's become equal or vanish:

(2.27) 1PM>: $A_{o++}=A_{o,--};A_{o,+-}=o;A_{\underline{Q},+-}=o;A_{\underline{Q},++}=o;A_{\underline{Q},--}=o$
Five Relations

(2.28) 1FM>: $A_{o,++};A_{o,--};A_{o,+-}=o;A_{\underline{Q},+o}=o;A_{\underline{Q},++}=o;A_{\underline{Q},+-}=o$
Four Relations

(2.29) 1AFM>: $A_{o,++}=A_{o,--};A_{\underline{Q},++}=A_{\underline{Q},--};A_{o,+-}=o;A_{\underline{Q},+-}=o$
Four Relations

(2.30) 1SSDW>: $A_{o,++};A_{o,--};A_{\underline{Q},+-};A_{\underline{Q},++}=o;A_{o,+-}=o;A_{\underline{Q},--}=o$
Three Relations

(2.31) 1FIM>: $A_{o,++};A_{o,--};A_{\underline{Q},++};A_{\underline{Q},--};A_{\underline{Q},+-}=o;A_{o,+-}=o$
Two Relations

These are derived as follows: We assume all coefficients B are real and independent of $\underline{k}$.

(2.32) 1PM> For ℓ=1,2 or 3,4 by translation of all indices by $\underline{Q}$: $\langle B_\ell \Psi_{\underline{k},\sigma} \mid a^+_{\underline{p},\sigma''} a_{\underline{q},\sigma'} \mid B_\ell \Psi_{\underline{k},\sigma} \rangle = B_\ell{}^2 \delta_{\underline{q},\underline{k}} \delta_{\underline{p},\underline{k}} \delta_{\sigma\sigma'} \delta_{\sigma\sigma''}$
with $B_1=B_2$

Thus there is only one correlation, that of a sum of exptectation values of a number operator,

(2.33) because: $a_{q,\sigma} \mid B_\ell \Psi_{k,\sigma'} \rangle = o$ if $\underline{q} \neq \underline{k}$, $\sigma \neq \sigma'$

(2.34) 1FM>: For ℓ = 1,2 or 3,4 by translation of all indices by $\underline{Q}$: $\langle B_\ell \Psi_{k,\sigma} \mid a^+_{p,\sigma''} a_{q,\sigma'} \mid B_\ell \Psi_{k,\sigma} \rangle =$
$B_\ell{}^2 \delta_{\underline{p},\underline{k}} \delta_{\underline{q},\underline{k}} \delta_{\sigma\sigma'} \delta_{\sigma\sigma''}$

Here $B_1 \neq B_2$, and we have <u>two</u> non-zero correlations, sums of expectation values of the spin up and spin down number operators.

|AFM>: Here we cannot see by inspection which A's are non-zero, so we must work them all out, the vanishing of certain A's being a result of the properties of Fermion annihilation operator:

$$(2.35)\quad \langle B_1\Psi_{\underline{k},+}+B_3\Psi_{\underline{k}+\underline{Q},+}\; a^+_{\underline{k},+}a_{\underline{k},+}\; B_1\Psi_{\underline{k}+\underline{Q},+}\rangle = B_1^2, \text{ a number operator}$$

Using abbreviated notation for the magnetic states and dropping commas in the subscripts.

$$(2.36)\quad \langle 1,3|a^+_{\underline{k}-}\; a_{\underline{k}-}\;|1,3\rangle = 0$$

$$(2.37)\quad \langle 1,3|a^+_{\underline{k}+\underline{Q}+}a_{\underline{k}+\underline{Q}+}|1,3\rangle = B_3{}^2, \text{ number operator}$$

$$(2.38)\quad \langle 1,3|a^+_{\underline{k}+\underline{Q}-}a_{\underline{k}+\underline{Q}-}|1,3\rangle = 0$$

$$(2.39)\quad \langle 1,3|a^+_{\underline{k}-}\; a_{\underline{k}+}\;|1,3\rangle = 0$$

$$(2.40)\quad \langle 1,3|a^+_{\underline{k}+}\; a_{\underline{k}-}\;|1,3\rangle = 0$$

$$(2.41)\quad \langle 1,3|a^+_{\underline{k}+\underline{Q}+}a_{\underline{k}+}\;|1,3\rangle = B_1B_3, \text{ anomalous operator}$$

$$(2.42)\quad \langle 1,3|a^+_{\underline{k}+\underline{Q}-}a_{\underline{k}-}\;|1,3\rangle = 0$$

$$(2.43)\quad \langle 1,3|a^+_{\underline{k}+}\; a_{\underline{k}+\underline{Q}-}|1,3\rangle = 0$$

(2.44) $\langle 1,3 | a^{+}_{\underline{k}+} \; a_{\underline{k}+\underline{Q}+} | 1,3 \rangle = B_3 B_1$, anomalous operator

(2.45) $\langle 1,3 | a^{+}_{\underline{k}-} \; a_{\underline{k}+\underline{Q}-} | 1,3 \rangle = 0$

(2.46) $\langle 1,3 | a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+} \; | 1,3 \rangle = 0$

(2.47) $\langle 1,3 | a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+} \; | 1,3 \rangle = 0$

(2.48) $\langle 1,3 | a^{+}_{\underline{k}-} \; a_{\underline{k}+\underline{Q}+} | 1,3 \rangle = 0$

(2.49) $\langle 2,4 | a^{+}_{\underline{k}+} \; a_{\underline{k}+} \; | 2,4 \rangle = 0$

(2.50) $\langle 2,4 | a^{+}_{\underline{k}-} \; a_{\underline{k}-} \; | 2,4 \rangle = B_2{}^2$, number operator

(2.51) $\langle 2,4 | a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+} | 2,4 \rangle = 0$

(2.52) $\langle 2,4 | a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} | 2,4 \rangle = B_4{}^2$, number operator

(2.53) $\langle 2,4 | a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+} \; | 2,4 \rangle = 0$

(2.54) $\langle 2,4 | a^{+}_{\underline{k}-} \; a_{\underline{k}+} \; | 2,4 \rangle = 0$

(2.55) $\langle 2,4 | a^{+}_{\underline{k}+} \; a_{\underline{k}-} \; | 2,4 \rangle = 0$

(2.56) $\langle 2,4 | a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}-} \; | 2,4 \rangle = B_2 B_4$, anomalous operator

(2.57) $\langle 2,4 | a^{+}_{\underline{k}+} \; a_{\underline{k}+\underline{Q}-} | 2,4 \rangle = 0$

(2.58) $\langle 2,4 | a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+} \; | 2,4 \rangle = 0$

(2.59) $\langle 2,4 | a^{+}_{\underline{k}-} \; a_{\underline{k}+\underline{Q}-} | 2,4 \rangle = B_4 B_2$, anomalous operator

(2.60) $\langle 2,4 | a^{+}_{\underline{k}-} \; a_{\underline{k}+\underline{Q}+} | 2,4 \rangle = 0$

$$(2.61)\quad \langle 2,4|a^{+}_{\underline{k}+}\ a_{\underline{k}+\underline{Q}-}|2,4\rangle=0$$

$$(2.62)\quad \langle 2,4|a^{+}_{\underline{k}+\underline{Q}-}a_{\underline{k}+}\ |2,4\rangle=0$$

There are four nonzero number operator matrix elements and four nonzero anomalous operator matrix elements. We note that the physically relevant quantities are still sums of these nonzero matrix elements multiplied by occupation number $F_{\underline{k}}$ between zero and one, so that the unfilled $\underline{k}$ states cannot contribute to these sums:

$|SSDW\rangle$:

$$(2.63)\quad \langle B_1\Psi_{\underline{k}+}+B_4\Psi_{\underline{k}+\underline{Q}-}|a^{+}_{\underline{k}+}a_{\underline{k}+}|\ B_1\Psi_{\underline{k}+}+B_4\Psi_{\underline{k}+\underline{Q}-}\rangle=B_1{}^2,\ \text{number operator}$$

$$(2.64)\quad \langle 1,4|a^{+}_{\underline{k}+}\ a_{\underline{k}+}\ |1,4\rangle=0$$

$$(2.65)\quad \langle 1,4|a^{+}_{\underline{k}-}\ a_{\underline{k}-}\ |1,4\rangle=0$$

$$(2.66)\quad \langle 1,4|a^{+}_{\underline{k}+\underline{Q}-}a_{\underline{k}+\underline{Q}-}|\ 1,4\rangle=B_4{}^2,\ \text{number operator}$$

$$(2.67)\quad \langle 1,4|a^{+}_{\underline{k}-}\ a_{\underline{k}+}\ |1,4\rangle=0$$

$$(2.68)\quad \langle 1,4|a^{+}_{k+}\ a_{\underline{k}-}\ |1,4\rangle=0$$

$$(2.69)\quad \langle 1,4|a^{+}_{\underline{k}+\underline{Q}+}a_{\underline{k}+}\ |1,4\rangle=0$$

$$(2.70)\quad \langle 1,4|a^{+}_{\underline{k}+\underline{Q}-}a_{\underline{k}-}\ |1,4\rangle=0$$

$$(2.71)\quad \langle 1,4|a^{+}_{\underline{k}+\underline{Q}-}a_{\underline{k}+}\ |1,4\rangle=B_1B_4,\ \text{anomalous operator}$$

(2.72) $\langle 1,4 | a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}-} | 1,4 \rangle = 0$

(2.73) $\langle 1,4 | a^{+}_{\underline{k}+} a_{\underline{k}+\underline{Q}+} | 1,4 \rangle = 0$

(2.74) $\langle 1,4 | a^{+}_{\underline{k}-} a_{\underline{k}+\underline{Q}-} | 1,4 \rangle = 0$

(2.75) $\langle 1,4 | a^{+}_{\underline{k}+} a_{\underline{k}+\underline{Q}-} | 1,4 \rangle = B_4 B_1$, anomalous operator

(2.76) $\langle 1,4 | a^{+}_{\underline{k}-} a_{\underline{k}+\underline{Q}+} | 1,4 \rangle = 0$

(2.77) $\langle B_2 \Psi_{\underline{k}-} + B_3 \Psi_{\underline{k}+\underline{Q}+} | a^{+}_{\underline{k}+} a_{\underline{k}-} | B_2 \Psi_{\underline{k}-} + B_3 \Psi_{\underline{k}+\underline{Q}+} \rangle = 0$

(2.78) $\langle 2,3 | a^{+}_{\underline{k}-} a_{\underline{k}+} | 2,3 \rangle = B_2^{\,2}$, number operator

(2.79) $\langle 2,3 | a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+} | 2,3 \rangle = B_3^{\,2}$, number operator

(2.80) $\langle 2,3 | a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} | 2,3 \rangle = 0$

(2.81) $\langle 2,3 | a^{+}_{\underline{k}-} a_{\underline{k}+} | 2,3 \rangle = 0$

(2.82) $\langle 2,3 | a^{+}_{\underline{k}+} a_{\underline{k}-} | 2,3 \rangle = 0$

(2.83) $\langle 2,3 | a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+} | 2,3 \rangle = 0$

(2.84) $\langle 2,3 | a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}-} | 2,3 \rangle = 0$

(2.85) $\langle 2,3 | a^{+}_{\underline{k}+} a_{\underline{k}+\underline{Q}+} | 2,3 \rangle = 0$

(2.86) $\langle 2,3 | a^{+}_{\underline{k}-} a_{\underline{k}+\underline{Q}-} | 2,3 \rangle = 0$

(2.87) $\langle 2,3 | a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+} | 2,3 \rangle = 0$

(2.88) $\langle 2,3 | a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}-} | 2,3 \rangle = B_2 B_3$, anomalous operator

(2.89) $\langle 2,3 | a^{+}_{\underline{k}-} a_{\underline{k}+\underline{Q}+} | 2,3 \rangle = B_3 B_2$, anomalous operator

(2.90) $\langle 2,3 | a^{+}_{\underline{k}-} a_{\underline{k}+\underline{Q}-} | 2,3 \rangle = 0$

There are again four nonzero anomalous operator matrix elements and four nonzero number operator matrix elements.

$|FIM\rangle$:

In general, all four B's in each wave function are nonzero so that <u>every</u> correlation exists and is nonzero.

We now seek the relations between the A's and the coefficients B in a general way. Penn finds:

$$(2.91) \quad A_{o+-} = -\frac{Co}{N} \sum_{\underline{k}} F_{\underline{k}} (B_1 B_2 + B_3 B_4)$$

$$(2.92) \quad A_{o++} = \frac{Co}{N} \sum_{\underline{k}\,\underline{k}} F (B_2^2 + B_4^2)$$

$$(2.93) \quad A_{o--} = \frac{Co}{N} \sum_{\underline{k}} F_{\underline{k}} (B_1^2 + B_3^2)$$

$$(2.94) \quad A_{\underline{Q}+-} = -\frac{Co}{N} \sum_{\underline{k}} F_{\underline{k}} (B_1 B_4 + B_2 B_3)$$

$$(2.95) \quad A_{\underline{Q}++} = \frac{Co}{N} \sum_{\underline{k}} F_{\underline{k}} B_2 B_4$$

$$(2.96) \quad A_{\underline{Q}--} = \frac{Co}{N} \sum_{\underline{k}} F_{\underline{k}} B_1 B_3$$

Now we choose a wave function for a state, i.e., we find which B's in the general four term linear combination of states that is Ψ magnetic, are zero.

For a given state we wrote down the relations among the A's and which A's were zero. Utilizing the definitions of the A's in terms of the B's directly above, we see that we will obtain relations among the B's with the $\underset{k}{\Sigma}F_{\underline{k}}$ multiplier being needed only when we discuss which states are filled and which are empty, but not their structure. Explicitly:

Table 1. Magnetic Wave Function Coefficient Relations.

State	Correlation Function Relation	State Structure	State Structure and Filling	Conclusions
PM	$A_{\underline{Q}+-}=0$	$B_1B_4=-B_2B_3$	$\underset{k}{\Sigma}F_{\underline{k}}B_1B_4=\underset{k}{\Sigma}F_{\underline{k}}(-B_2B_3)$	$B_1=B_2$
	$A_{\underline{Q}++}=0$	$B_1B_3=0$	$\underset{k}{\Sigma}F_{\underline{k}}B_1B_3=0$	
	$A_{\underline{Q}--}=0$	$B_2B_4=0$	$\underset{k}{\Sigma}F_{\underline{k}}B_2B_4=0$	
	$A_{o+-}=0$	$B_1B_2=-B_3B_4$	$\underset{k}{\Sigma}F_{\underline{k}}B_1B_2=\underset{k}{\Sigma}F_{\underline{k}}(-B_3B_4)$	$B_3=B_4=0$
	$A_{o++}=A_{0--}$	$B_2^2+B_4^2=B_1^2+B_3^2$	$\underset{k}{\Sigma}F_{\underline{k}}(B_2^2+B_4^2)=$ $\underset{k}{\Sigma}F_{\underline{k}}(B_1^2+B_3^2)$	
FM	$A_{\underline{Q}++}=0$	$B_1B_3=0$	$\underset{k}{\Sigma}F_{\underline{k}}B_1B_3=0$	$B_2\neq B_1$
	$A_{\underline{Q}--}=0$	$B_2B_4=0$	$\underset{k}{\Sigma}F_{\underline{k}}B_2B_4=0$	
	$A_{\underline{Q}+-}=0$	$B_1B_4=-B_2B_3$	$\underset{k}{\Sigma}F_{\underline{k}}B_1B_4=\underset{k}{\Sigma}F_{\underline{k}}(-B_2B_3)$	$B_4=B_3=0$
	$A_{o+-}=0$	$B_1B_2=-B_3B_4$	$\underset{k}{\Sigma}F_{\underline{k}}B_1B_2=\underset{k}{\Sigma}F_{\underline{k}}(-B_3B_4)$	

Table 1 (cont'd.)

State	Correlation Function Relation	State Structure	State Structures and Filling	Conclusions
AFM	$A_{o++}=A_{o--}$	$B_2^2+B_4^2=B_1^2+B_3^2$	$\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2) = \sum_{\underline{k}} F_{\underline{k}}(B_1^2+B_3^2)$	$B_1=B_2$
	$A_{\underline{Q}++}=A_{\underline{Q}--}$	$B_1B_3=B_2B_4$	$\sum_{\underline{k}} F_{\underline{k}}B_1B_3=\sum_{\underline{k}} F_{\underline{k}}B_2B_4$	$B_3=B_4, B_2=B_4$
	$A_{\underline{Q}+-}=0$	$B_1B_4=-B_2B_3$	$\sum_{\underline{k}} F_{\underline{k}}B_1B_4=\sum_{\underline{k}} F_{\underline{k}}(B_2B_3)$	$B_1=B_3$ and B_1, B_3 or B_2, B_4 pairs are zero when the other pair is not
	$A_{o+-}=0$	$B_1B_2=-B_3B_4$	$\sum_{\underline{k}} F_{\underline{k}}B_1B_2=\sum_{\underline{k}} F_{\underline{k}}(-B_3B_4)$	
SSDW	$A_{\underline{Q}++}=0$	$B_1B_3=0$	$\sum_{\underline{k}} F_{\underline{k}}B_1B_3=0$	$B_1\neq 0$, $B_2\neq 0$ or
	$A_{\underline{Q}--}=0$	$B_2B_4=0$	$\sum_{\underline{k}} F_{\underline{k}}B_2B_4=0$	$B_2\neq 0$, $B_3\neq 0$
	$A_{o+-}=0$	$B_1B_2=-B_3B_4$	$\sum_{\underline{k}} F_{\underline{k}}B_1B_2=\sum_{\underline{k}} F_{\underline{k}}(-B_3B_4)$	
FIM	$A_{\underline{Q}+-}=0$	$B_1B_4=-B_2B_3$	$\sum_{\underline{k}} F_{\underline{k}}B_1B_4=\sum_{\underline{k}} F_{\underline{k}}(-B_2B_3)$	$B_4=-B_2B_3/B_1$ }] $B_4=-B_1B_2/B_3$ }] $B_1=B_3$ or $B_2=B_4$] thus $B_1^2=B_3^2$
	$A_{o+-}=0$	$B_1B_2=-B_3B_4$	$\sum_{\underline{k}} F_{\underline{k}}B_1B_2=\sum_{\underline{k}} F_{\underline{k}}(-B_3B_4)$	

Thus, from the correlations, he concludes:

(2.97) $\Psi^{PM} = B_1\Psi_{\underline{k}+}$ or $B_2\Psi_{\underline{k}-}$, equally populated

(2.98) $\Psi^{FM} = B_1\Psi_{\underline{k}+}$ or $B_2\Psi_{\underline{k}-}$, unequally populated

(2.99) $\Psi^{AFM} = B_1\Psi_{\underline{k}+} + B_3\Psi_{\underline{k}+\underline{Q}+}$ or $B_2\Psi_{\underline{k}-}+B_4\Psi_{\underline{k}+\underline{Q}-}$

$$(2.100)\quad \Psi^{SSDW} = B_1\Psi_{\underline{k}+}+B_4\Psi_{\underline{k}+\underline{Q}-} \text{ or } B_2\Psi_{\underline{k}-}+B_3\Psi_{\underline{k}+\underline{Q}+}$$

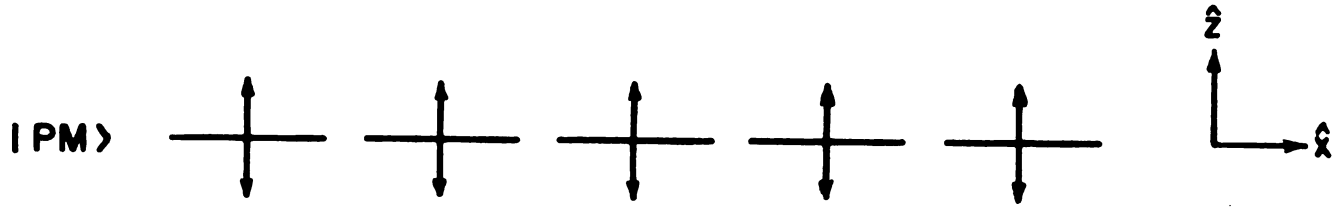
$$(2.101)\quad \Psi^{FIM} = B_1\Psi_{\underline{k}+}+B_2\Psi_{\underline{k}-}+B_3\Psi_{\underline{k}+\underline{Q}+}+B_2\Psi_{\underline{k}+\underline{Q}-} \text{ or}$$

$$B_1\Psi_{k+}+B_2\Psi_{\underline{k}-}+B_1\Psi_{\underline{k}+\underline{Q}+}B_4\Psi_{\underline{k}+\underline{Q}-}$$

as written earlier.

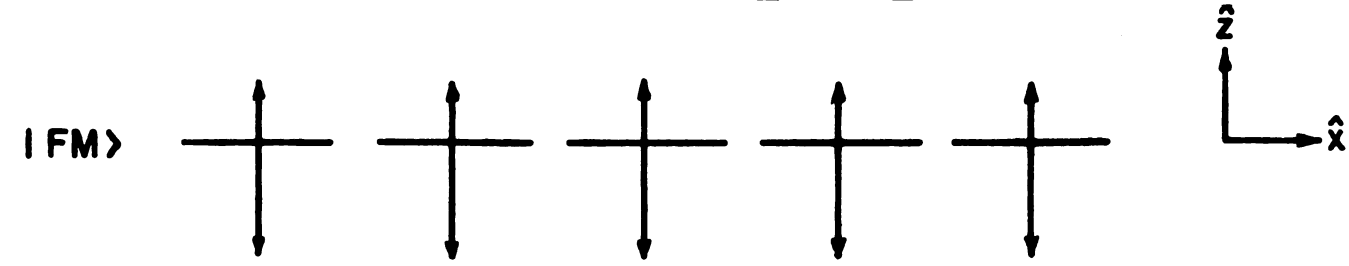
We now seek to graphically illustrate the spatial spin structure of these states using a plane wave basis set for the Ψ's:

$|PM\rangle$: $\Psi^{PM}=B_1\ell_+^{i\underline{k}\cdot\underline{r}}$ and $B_2\ell_-^{i\underline{k}\cdot\underline{r}}$ and $\sum_{\underline{k}} F_{\underline{k}}B_1^{\,2} = \sum_{\underline{k}} F_{\underline{k}}{}^{1}B_2^{\,2}$:



$F_{\underline{k}}=1$ or 0, $F_{\underline{k}'}=1$ or 0, but when $F_{\underline{k}}=1, F_{\underline{k}'}=1$ (is occupied) also.

$|FM\rangle$: $\Psi^{FM}=B_1\ell_+^{i\underline{k}\cdot\underline{r}}$ and $B_3\ell_-^{i\underline{k}\cdot\underline{r}}$ and $\sum_{\underline{k}} F_{\underline{k}}B_1^{\,2} \neq \sum_{\underline{k}} F_{\underline{k}}, B_2^{\,2}$:

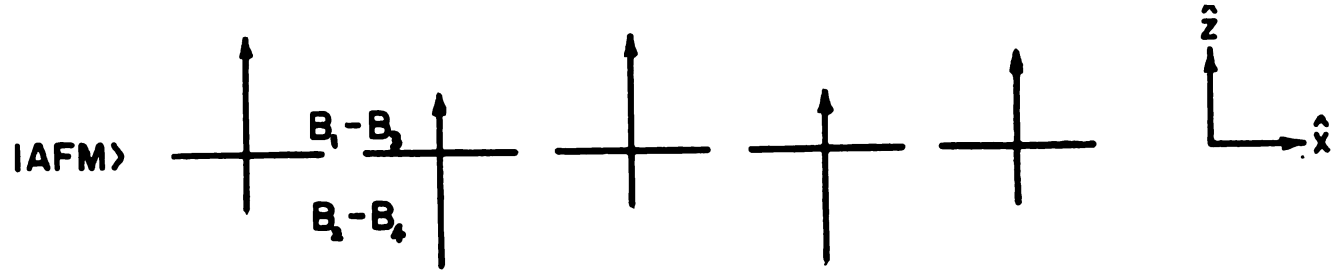


Here $F_{\underline{k}}\neq F_{\underline{k}'}$, so we have unequal occupation of spin up state and spin down state on each site.

$|AFM\rangle$: $\psi^{AFM} = B_1 \ell_+^{i\underline{k}\cdot\underline{r}} + B_3 \ell_+^{i\underline{k}\cdot\underline{r}} \ell^{i\underline{Q}\cdot\underline{r}}$

and $B_2 \ell_-^{i\underline{k}\cdot\underline{r}} + B_4 \ell_-^{i\underline{k}\cdot\underline{r}} \ell^{i\underline{Q}\cdot\underline{r}}$

the $\ell^{i\underline{Q}\cdot\underline{r}}$ term oscillating in sign from site to site.

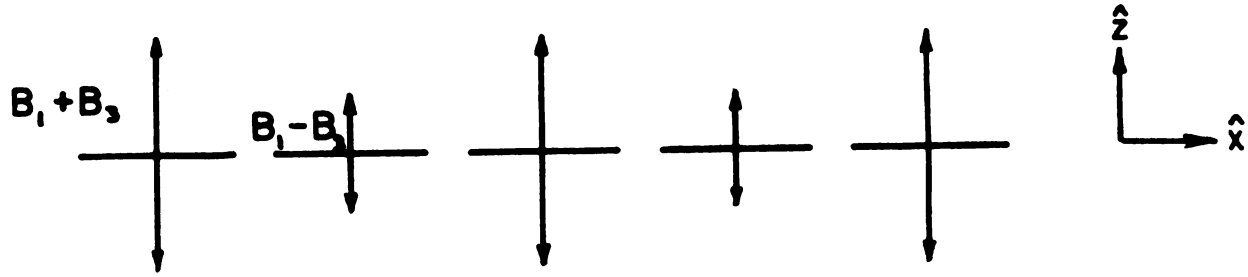


We note that if our wave function is:

$$\psi^{AFM} = B_1 \ell_+^{i\underline{k}\cdot\underline{r}} + B_3 \ell_+^{i\underline{k}\cdot\underline{r}} \ell^{i\underline{Q}\cdot\underline{r}}$$

$$\text{and } B_2 \ell_-^{i\underline{k}\cdot\underline{r}} - B_4 \ell_-^{i\underline{k}\cdot\underline{r}} \ell^{i\underline{Q}\cdot\underline{r}}$$

we get:

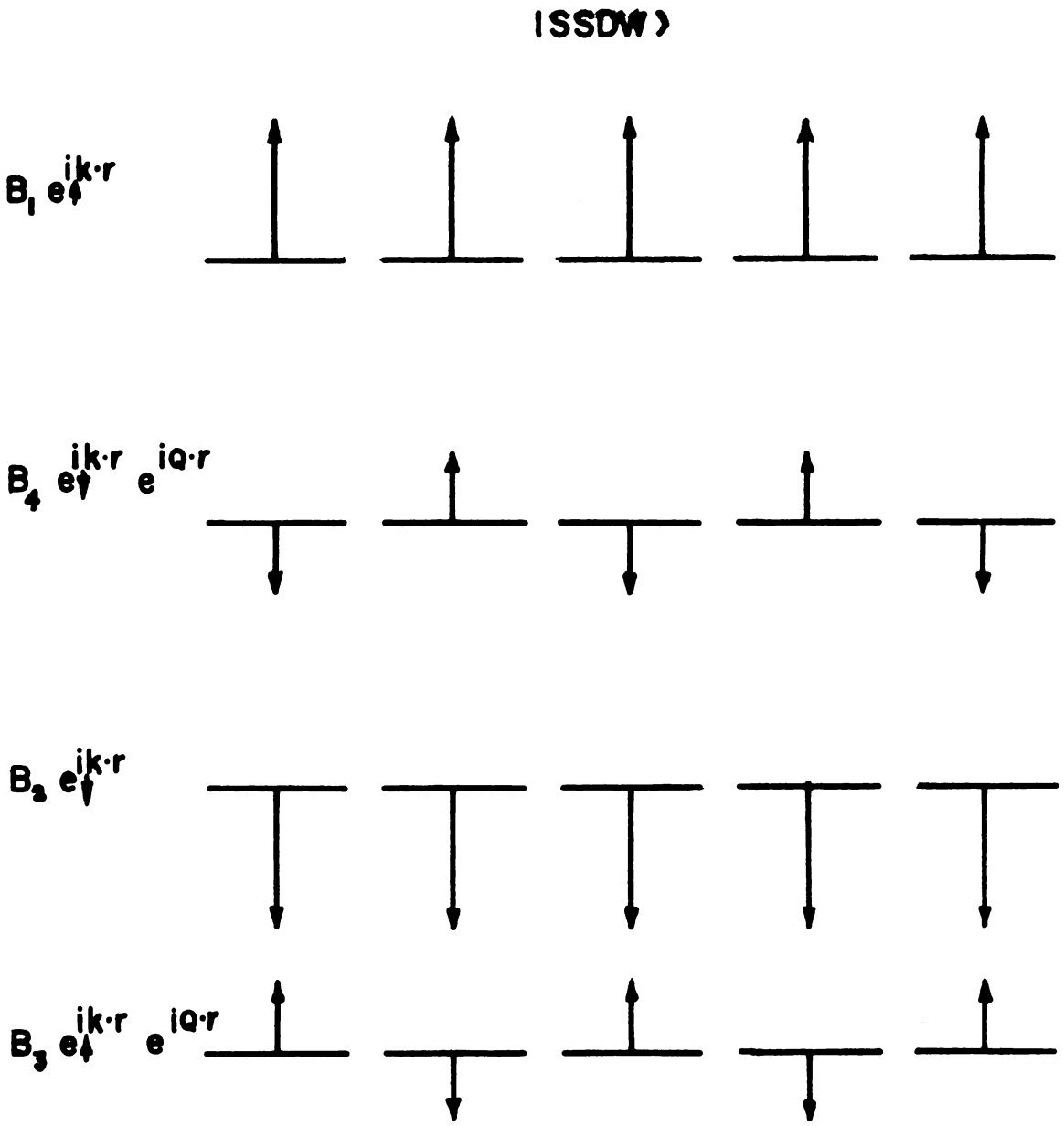


We get a one site phase shift of the lower AFM wave with respect to the upper, leading to a new spin density cancellation of each lattice site, but a net charge density fluctuation from site to site, a charge density wave.

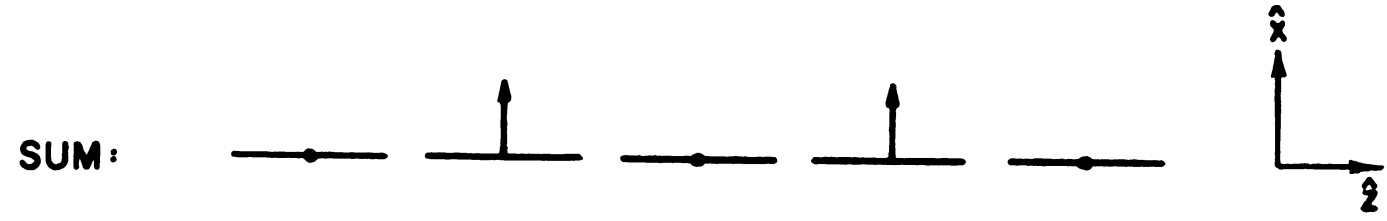
$|SSDW\rangle$: $\psi^{SSEW} = B_1 \ell_+^{i\underline{k}\cdot\underline{r}} + B_4 \ell_-^{i\underline{k}\cdot\underline{r}} \ell^{i\underline{Q}\cdot\underline{r}}$

$$\text{and } B_2 \ell_-^{i\underline{k}\cdot\underline{r}} + B_3 \ell_+^{i\underline{k}\cdot\underline{r}} \ell^{i\underline{Q}\cdot\underline{r}}$$

which is the site by site sum of the following waveforms:



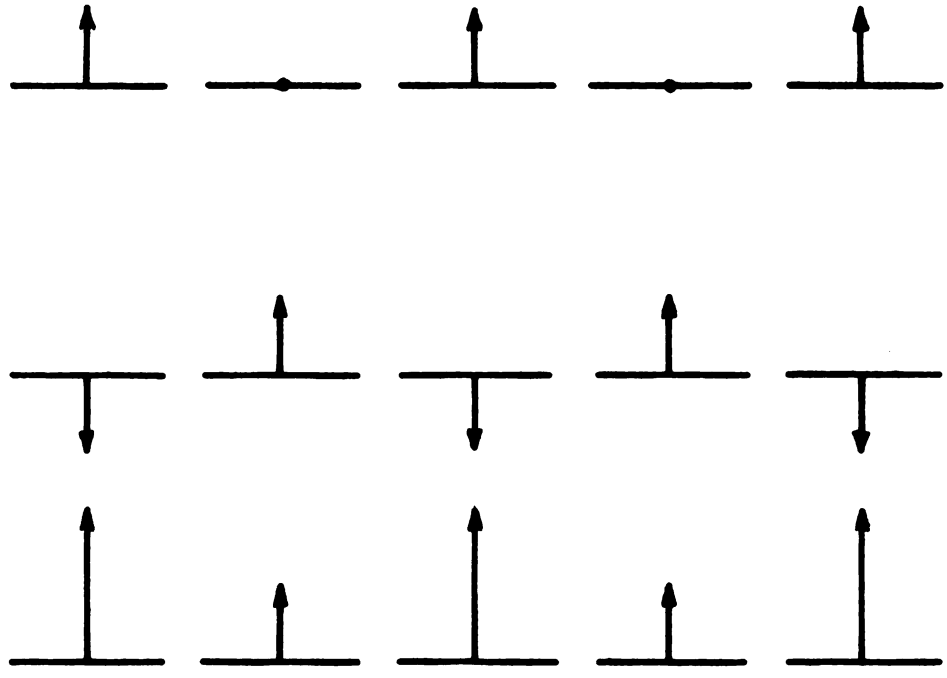
Their site by site sum is a Spiral Spin Density Wave:

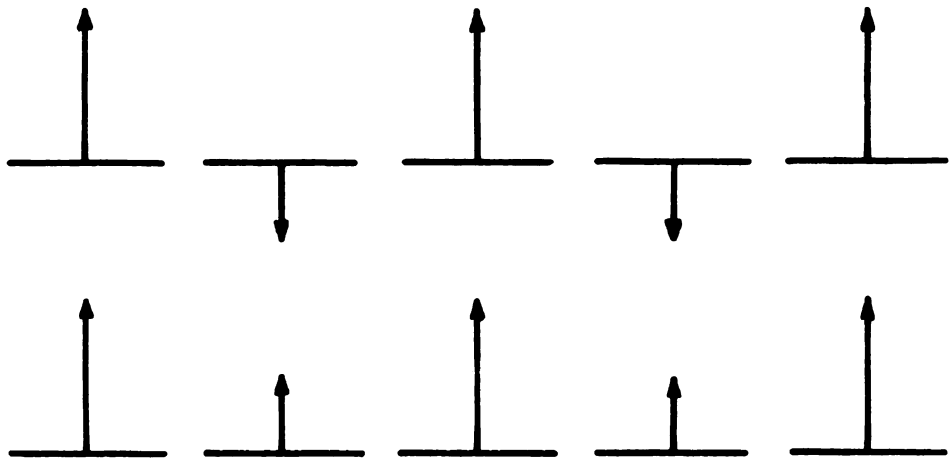


We note the change in axis orientation. The SSDW spirals along the $\hat{Z}$, not the $\hat{X}$ axis. We have graphed the SSDW for a particular choice of coefficient magnitudes: $B_1 > B_2 > B_4 > B_3$. The SSDW will look different if a different relation among the B's is chosen, but will still spiral along the $\hat{Z}$ axis.

Some of these other SSDW states are:

Other |SSDW⟩ States





with varying relative amplitudes, phases with respect to the four components that were added to arrive at each of these spin structures. These are only a special case of the general SSDW, that for $A_{o+-}=0$ and $\underline{Q} = \underline{G}/2 = \pi$. The above SSDW spin structures differ only in pitch angle along the $\hat{Z}$ axis.

There are again, as in the SSDW case, a few possible FIM structures, depending on relative B magnitudes. These are the same as the SSDW spin structures in form, but directed along the $\hat{X}$ axis, making the spins point parallel or antiparallel to $\hat{Z}$.

The meaning of these states in terms of the nonzero correlation functions can best be seen by writing out the magnetization and numbers of electrons in terms of them.

Penn defines these as: (in terms of the Bohr Magneton, μ_B)

$$(2.102)\quad M_X(0) \equiv \frac{-2\mu_B}{Co} A_{o+-}$$

$$(2.103)\quad M_X(\underline{Q}) \equiv \frac{-2\mu_B}{Co} A_{\underline{Q}+-}$$

$$(2.104)\quad M_Z(\underline{Q}) \equiv \frac{\mu_B}{Co} (A_{\underline{Q}++} - A_{\underline{Q}--})$$

$$(2.105)\quad M_Z(0) \equiv \frac{\mu_B}{Co} (A_{o++} - A_{o--})$$

$$(2.106)\quad n(0) \equiv \frac{1}{Co} (A_{o++} + A_{o--})$$

$$(2.107)\quad n(\underline{Q}) \equiv \frac{1}{Co} (A_{\underline{Q}++} + A_{\underline{Q}--})$$

For all the states he considered $A_{o+-} \equiv 0$ so that $M_X(0) = 0$. The states are seen to possess the following properties:

$\underline{|PM>:}$

$$(2.108)\quad M_X(0) = 0$$

$$(2.109)\quad M_X(\underline{Q}) = 0$$

$$(2.110)\quad M_Z(0) = 0$$

$$(2.111)\quad M_Z(\underline{Q}) = 0$$

$$(2.112)\quad n(0) = \sum_{\underline{k}} F_{\underline{k}} (B_1^2 + B_2^2) = \sum_{\underline{k}} F_{\underline{k}} (2B_1^2)$$

$$(2.113)\quad n(\underline{Q}) = 0$$

$\underline{|FM>:}$

(2.114) $M_X(0) = 0$

(2.115) $M_X(Q) = 0$

(2.116) $M_Z(0) = \frac{\mu_B}{Co} \sum_{\underline{k}} F_{\underline{k}} \ (B_1^2 - B_2^2)$

(2.117) $M_Z(Q) = 0$

(2.118) $n(0) = \sum_{\underline{k}} F_{\underline{k}} (B_1^2 + B_2^2)$

(2.119) $n(Q) = 0$

$|AFM>$:

(2.120) $M_X(0) = 0$

(2.121) $M_X(Q) = 0$

(2.122) $M_Z(0) = 0$

(2.123) $M_Z(Q) = 0$

(2.124) $n(0) = \frac{1}{Co} \sum_{\underline{k}} F_{\underline{k}} (B_1^2+B_2^2+B_3^2+B_4^2) = \frac{2}{Co} \sum_{\underline{k}} F_{\underline{k}} (B_1^2+B_2^2)$

(2.125) $n(Q) = \frac{1}{Co} \sum_{\underline{k}} F_{\underline{k}} (B_1B_3+B_3B_1+B_2B_4+B_4B_2) = \frac{2}{Co} \sum_{\underline{k}} F_{\underline{k}} (B_1B_3+B_2B_4)$

$|SSDW>$:

(2.126) $M_X(0) = 0$

(2.127) $M_X(Q) = \frac{-2\mu_B}{Co} \sum_{\underline{k}} F_{\underline{k}} (2B_1B_4)$

(2.128) $M_Z(0) = \frac{\mu_B}{Co} \sum_{\underline{k}} F_{\underline{k}} (-B_1^2+B_2^2-B_3^2+B_4^2)$

(2.129) $M_Z(Q) = 0$

(2.130) $n(0) = \frac{1}{Co} \sum_{\underline{k}} F_{\underline{k}} (B_1^2+B_2^2+B_3^2+B_4^2)$

(2.131) $n(Q) = 0$

$|FIM>$:

(2.132) $M_X(0) = 0$

(2.133) $M_X(Q) = 0$

(2.134) $M_Z(0) = \frac{\mu_B}{Co} \sum_{\underline{k}} F_{\underline{k}} (B_1^2+B_2B_3-B_2^2-B_2B_4)$ where $B_1=B_3$, $B_2=B_4$

(2.135) $M_Z(Q) = \frac{\mu_B}{Co} \sum_{\underline{k}} F_{\underline{k}} (B_2B_4+B_2^2-B_3B_2-B_1^2)$

(2.136) $n(0) = \frac{1}{Co} \sum_{\underline{k}} F_{\underline{k}} (B_1^2+B_2B_3+B_2^2 + B_2B_4)$

(2.137) $n(Q) = \frac{1}{Co} \sum_{\underline{k}} F_{\underline{k}} (B_2B_4+B_2^2+B_2B_3+B_1^2)$

Penn utilized the correlation function, A, to derive the energy of a magnetic state at some point of the phase diagram $(\frac{Co}{E''} - \frac{n}{2N})$, and compared this with that of another state whose energy is calculated with the same value of those two parameters in order to see which states are stable for that particular point on the magnetic phase diagram (considering the five states previously mentioned as the only possible magnetic states of the system in the Hubbard Model). We note that his SSDW and FIM states are special cases since generally $A_{o+-} \neq 0$, so that, especially in the

FIM case, all four coefficients B are not related at all, while in Penn's FIM state, $A_{o+-} = 0$ forces one B to be related to the other three. Also, the special chose of $\underline{q} = \underline{Q} = \underline{G}/2 = \underline{\pi}$ only brings out SSDW and FIM states with a certain pitch, while in general, the pitch or phase is arbitrary for both spin structures.

He computes the energy by solving the Heisenberg equation of motion for the state operator $\gamma_{\underline{k}}$.

$$(2.138) \quad [H, \gamma_{\underline{k}}] = \gamma_{\underline{k}} E_{\underline{k}}$$

or equivalently:

$$(2.139) \quad [H, \gamma^{+}_{\underline{k}}] = \gamma^{+}_{\underline{k}} E_{\underline{k}}$$

for its adjoint.

We first write H out in the Bloch representation and in quasi-particle form where the Gorkov factorization has been done, as before, to the two-body (four operator) potential term to make it an effective one-body (two operator) quasi-particle term.

$$(2.140) \quad H^{\text{Bloch}} = \sum_{\underline{k}} \epsilon_{\underline{k}} a^{+}_{\underline{k}} a_{\underline{k}} + \frac{\text{Co}\mathcal{N}}{2\mathcal{N}^2} \sum_{\underline{k}}^{\text{whole Brillouin zone}} \delta_{\underline{k}\underline{k}"} \sum_{\sigma,\sigma' \atop \sigma \neq \sigma'} \Big[\langle a^{+}_{\underline{k}"\sigma} a_{\underline{k}"\sigma} \rangle a^{+}_{\underline{k}"\sigma'} a_{\underline{k}"\sigma'} - \langle a^{+}_{\underline{k}"\sigma} a_{\underline{k}"\sigma'} \rangle a^{+}_{\underline{k}"\sigma'} a_{\underline{k}"\sigma} \Big]$$

where the $\delta_{\underline{k}\underline{k}}$, comes from the Fourier transformation of H^{Wannier}.

We rewrite this as:

$$(2.141)\quad H^{Bloch} = \sum_{\underline{k}} \epsilon_{\underline{k}} a^{+}_{\underline{k}} + \frac{Co}{2N} \sum_{\underline{k}_1,\underline{k}_2,\underline{k}_3,\underline{k}_4} \delta(\underline{k}_1+\underline{k}_2-\underline{k}_3-\underline{k}_4)$$
$$\sum_{\substack{\sigma,\sigma' \\ \sigma\neq\sigma'}} \left[\langle a^{+}_{\underline{k}_3\sigma} a_{\underline{k}_2\sigma} \rangle a_{\underline{k}_4\sigma'} a_{\underline{k}_1\sigma'} - \langle a^{+}_{\underline{k}_3\sigma} a_{\underline{k}_1\sigma'} \rangle a_{\underline{k}_4\sigma'} a_{\underline{k}_2\sigma} \right]$$

Summing over $\underline{k}'' = \underline{k}$ and $\underline{k} + \underline{Q}$

$$(2.142)\quad H^{Bloch} = \sum_{\underline{k}} \epsilon_{\underline{k}} a^{+}_{\underline{k}} a_{\underline{k}} + \frac{Co}{2N} \sum_{\substack{\underline{k} \\ \text{whole} \\ \text{Brillouin} \\ \text{zone}}} \sum_{\substack{\sigma,\sigma' \\ \sigma\neq\sigma'}} \frac{1}{2} \Big[\langle a^{+}_{\underline{k}\sigma} a_{\underline{k}\sigma} \rangle$$

$$a^{+}_{\underline{k}\sigma'} a_{\underline{k}\sigma'} + \langle a^{+}_{\underline{k}+\underline{Q},\sigma} a_{\underline{k}+\underline{Q},\sigma} \rangle a^{+}_{\underline{k}+\underline{Q},\sigma} a_{\underline{k}+\underline{Q},\sigma'} +$$

$$- \langle a^{+}_{\underline{k}\sigma} a_{\underline{k}\sigma'} \rangle a^{+}_{\underline{k}\sigma'} a_{\underline{k}\sigma} - \langle a^{+}_{\underline{k}+\underline{Q}\sigma} a_{\underline{k}+\underline{Q}\sigma'} \rangle a^{+}_{\underline{k}+\underline{Q}\sigma'} a_{\underline{k}+\underline{Q}\sigma}$$

$$+ \langle a^{+}_{\underline{k}\sigma} a_{\underline{k}\sigma} \rangle a^{+}_{\underline{k}\sigma'} a_{\underline{k}\sigma'} + \langle a^{+}_{\underline{k}+\underline{Q}\sigma} a_{\underline{k}+\underline{Q}\sigma} \rangle a^{+}_{\underline{k}\sigma'} a_{\underline{k}\sigma'}$$

$$+ \langle a^{+}_{\underline{k}\sigma} a_{\underline{k}+\underline{Q}\sigma} \rangle a^{+}_{\underline{k}+\underline{Q}\sigma'} a_{\underline{k}\sigma'} + \langle a^{+}_{\underline{k}+\underline{Q}\sigma} a_{\underline{k}\sigma} \rangle a^{+}_{\underline{k}\sigma'} a_{\underline{k}+\underline{Q}\sigma'}$$

$$+ \langle a^{+}_{\underline{k}\sigma} a_{\underline{k}\sigma} \rangle a^{+}_{\underline{k}+\underline{Q}\sigma'} a_{\underline{k}+\underline{Q}\sigma'} + \langle a^{+}_{\underline{k}+\underline{Q}\sigma} a_{\underline{k}+\underline{Q}\sigma} \rangle a^{+}_{\underline{k}\sigma'} a_{\underline{k}\sigma'}$$

$$- \langle a^{+}_{\underline{k}\sigma} a_{\underline{k}\sigma'} \rangle a^{+}_{\underline{k}+\underline{Q}\sigma'} a_{\underline{k}+\underline{Q}\sigma} - \langle a_{\underline{k}+\underline{Q}\sigma} a_{\underline{k}+\underline{Q}\sigma'} \rangle a^{+}_{\underline{k}\sigma'} a_{\underline{k}\sigma}$$

$$- \langle a^{+}_{\underline{k}\sigma} a_{\underline{k}+\underline{Q}\sigma} \rangle a^{+}_{\underline{k}+\underline{Q}\sigma'} a_{\underline{k}+\underline{Q}\sigma} - \langle a^{+}_{\underline{k}+\underline{Q}\sigma} a_{\underline{k}\sigma} \rangle a^{+}_{\underline{k}\sigma'} a_{\underline{k}+\underline{Q}\sigma}$$

$$- \langle a^{+}_{\underline{k}\sigma} a_{\underline{k}\sigma'} \rangle a^{+}_{\underline{k}+\underline{Q}\sigma'} a_{\underline{k}+\underline{Q}\sigma} - \langle a^{+}_{\underline{k}+\underline{Q}\sigma} a_{\underline{k}+\underline{Q}\sigma'} \rangle a^{+}_{\underline{k}\sigma'} a_{\underline{k}\sigma} \Big]$$

where the extra 1/2 factor is put into account for double counting, i.e., the fact that, for example, the second and third terms are

equivalent by the translation of $-\underline{Q}$ in the Brillouin zone. Summing over σ and σ' we find:

$$(2.143)\quad H^{\text{Bloch}} = \sum_{\underline{k}} \epsilon_{\underline{k}} a^{+}_{\underline{k}} a_{\underline{k}} + \frac{1}{2}\frac{Co}{2N} \sum_{\substack{\underline{k} \\ \text{whole} \\ \text{Brillouin} \\ \text{zone}}} \Big[\langle a^{+}_{\underline{k}+} a_{\underline{k}+} \rangle a^{+}_{\underline{k}-} a_{\underline{k}-} + \langle a^{+}_{\underline{k}-} a_{\underline{k}-} \rangle a^{+}_{\underline{k}+} a_{\underline{k}+}$$

$$+ \langle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+} \rangle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} + \langle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} \rangle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+}$$

$$- \langle a^{+}_{\underline{k}+} a_{\underline{k}+} \rangle a^{+}_{\underline{k}-} a_{\underline{k}-} - \langle a^{+}_{\underline{k}-} a_{\underline{k}-} \rangle a^{+}_{\underline{k}+} a_{\underline{k}+}$$

$$- \langle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+} \rangle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} - \langle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} \rangle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+}$$

$$+ \langle a^{+}_{\underline{k}+} a_{\underline{k}+} \rangle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} + \langle a^{+}_{\underline{k}-} a_{\underline{k}-} \rangle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+}$$

$$+ \langle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+} \rangle a^{+}_{\underline{k}-} a_{\underline{k}-} + \langle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} \rangle a^{+}_{\underline{k}+} a_{\underline{k}+}$$

$$+ \langle a^{+}_{\underline{k}+} a_{\underline{k}+\underline{Q}+} \rangle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}-} + \langle a^{+}_{\underline{k}-} a_{\underline{k}+\underline{Q}-} \rangle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+}$$

$$+ \langle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+} \rangle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} + \langle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}-} \rangle a^{+}_{\underline{k}+} a_{\underline{k}+\underline{Q}+}$$

$$+ \langle a^{+}_{\underline{k}+} a_{\underline{k}+} \rangle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} + \langle a^{+}_{\underline{k}-} a_{\underline{k}-} \rangle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+}$$

$$+ \langle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+} \rangle a^{+}_{\underline{k}-} a_{\underline{k}-} + \langle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} \rangle a^{+}_{\underline{k}+} a_{\underline{k}+}$$

$$- \langle a^{+}_{\underline{k}+} a_{\underline{k}-} \rangle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}-} - \langle a^{+}_{\underline{k}-} a_{\underline{k}+} \rangle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}-}$$

$$- \langle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}-} \rangle a^{+}_{\underline{k}-} a_{\underline{k}+} - \langle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}\pm} \rangle a^{+}_{\underline{k}+} a_{\underline{k}-}$$

$$- \langle a^{+}_{\underline{k}+} a_{\underline{k}+\underline{Q}-} \rangle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+} - \langle a^{+}_{\underline{k}-} a_{\underline{k}+\underline{Q}+} \rangle a^{+}_{\underline{k}\pm\underline{Q}+} a_{\underline{k}-}$$

$$- \langle a^{+}_{\underline{k}+\underline{Q}+} a_{\underline{k}-} \rangle a^{+}_{\underline{k}-} a_{\underline{k}+\underline{Q}+} - \langle a^{+}_{\underline{k}+\underline{Q}-} a_{\underline{k}+} \rangle a^{+}_{\underline{k}+} a_{\underline{k}+\underline{Q}-}$$

$$-\langle a^+_{\underline{k}+} a_{\underline{k}-} \rangle a^+_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}+} - \langle a^+_{\underline{k}-} a_{\underline{k}+} \rangle a^+_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}-}$$

$$-\langle a^+_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}-} \rangle a^+_{\underline{k}-} a_{\underline{k}+} - \langle a^+_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}+} \rangle a^+_{\underline{k}+} a_{\underline{k}-} \Big]$$

Now, we put in our correlation function definitions (2.21 - 2.26) and find:

$$(2.144)\quad H^{Bloch} = \sum_{\underline{k}} \epsilon_{\underline{k}} a^+_{\underline{k}} a_{\underline{k}} + \frac{1}{2} \Big[A_{o--} \sum_{\underline{k}} a^+_{\underline{k}-} a_{\underline{k}-} + A_{o++} \sum_{\underline{k}} a^+_{\underline{k}+} a_{\underline{k}+}$$

$$+A_{o+-} \sum_{\underline{k}} a^+_{\underline{k}+} a_{\underline{k}-} + A_{\underline{Q}+-} \sum_{\underline{k}} a^+_{\underline{k}-} a_{\underline{k}+\underline{Q}+} + A_{\underline{Q}+-} \sum_{\underline{k}} a^+_{\underline{k}+} a_{\underline{k}+\underline{Q}-}$$

$$+A_{\underline{Q}--} \sum_{\underline{k}} a^+_{\underline{k}+\underline{Q}-} a_{\underline{k}-} + A_{\underline{Q}++} \sum_{\underline{k}} a^+_{\underline{k}+\underline{Q}+} a_{\underline{k}-} + A_{\underline{Q}+-} \sum_{\underline{k}} a^+_{\underline{k}+\underline{Q}-} a_{\underline{k}+}$$

$$+A_{\underline{Q}+-} \sum_{\underline{k}} a^+_{\underline{k}+\underline{Q}+} a_{\underline{k}+} + A_{\underline{Q}++} \sum_{\underline{k}} a^+_{\underline{k}+} a_{\underline{k}+\underline{Q}+} + A_{\underline{Q}--} \sum_{\underline{k}} a^+_{\underline{k}-} a_{\underline{k}+\underline{Q}-}$$

$$+A_{o+-} \sum_{\underline{k}} a^+_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}-} + A_{o+-} \sum_{\underline{k}} a^+_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}+} + A_{o++} \sum_{\underline{k}} a^+_{\underline{k}+\underline{Q}+} a_{\underline{k}+\underline{Q}+}$$

$$+A_{o--} \sum_{\underline{k}} a^+_{\underline{k}+\underline{Q}-} a_{\underline{k}+\underline{Q}-} + A_{o+-} \sum_{\underline{k}} a^+_{\underline{k}-} a_{\underline{k}+} \Big]$$

Now:

$$(2.145)\quad \gamma^+_{\underline{k}} = B_1 a^+_{k+} + B_2 a^+_{\underline{k}-} + B_3 a^+_{\underline{k}+\underline{Q}+} + B_4 a^+_{\underline{k}+\underline{Q}-}$$

So that:

$$(2.146)\quad \gamma^+_{\underline{k}} H - H \gamma^+_{\underline{k}} = \gamma^+_{\underline{k}} (T+V) - (T+V) \gamma^+_{\underline{k}} = [\gamma^+_{\underline{k}}, T] + [\gamma^+_{\underline{k}}, V]$$

and substituting in $\gamma^+_{\underline{k}}$ from (2.145) yields:

$$(2.147)\quad [\gamma^+_{\underline{k}}, H] = B_1 [(a^+_{\underline{k}+} T - T a^+_{\underline{k}+}) + (a^+_{\underline{k}+} V - V a^+_{k+})]$$

$$+B_2 [(a^+_{\underline{k}-} T - T a^+_{k-}) + (a^+_{k-} V - V a^+_{k-})]$$

$$+B_3 \quad [(a^+_{\underline{k}+\underline{Q}+}T - T\, a^+_{\underline{k}+\underline{Q}+}) + (a^+_{\underline{k}+\underline{Q}+}V - Va^+_{\underline{k}+\underline{Q}+})]$$

$$+B_4 \quad [(a^+_{\underline{k}+\underline{Q}-}T - T\, a^+_{\underline{k}+\underline{Q}-}) + (a^+_{\underline{k}+\underline{Q}-}V - Va^+_{\underline{k}+\underline{Q}-})]$$

Now, the kinetic energy commutator is composed of:

$$(2.148) \quad [a^+_{\underline{k}+},T] = a^+_{\underline{k}+}\sum_{\underline{k}'}\epsilon_{\underline{k}'}a^+_{\underline{k}'}a_{\underline{k}'} - \sum_{\underline{k}'}\epsilon_{\underline{k}'}a^+_{\underline{k}'}a_{\underline{k}'}a^+_{\underline{k}+}$$

$$= \sum_{\underline{k}'}\epsilon_{\underline{k}'}(a^+_{\underline{k}+}a^+_{\underline{k}'}a_{\underline{k}'} - a^+_{\underline{k}'}a_{\underline{k}'}a^+_{\underline{k}+})$$

$$= \sum_{\underline{k}'}\epsilon_{\underline{k}'}(-1)a^+_{\underline{k}'}(a^+_{\underline{k}+}a_{\underline{k}'} - a_{\underline{k}'}a^+_{\underline{k}+}) = \sum_{\underline{k}'}\epsilon_{\underline{k}'}(-1)\delta_{+o}\delta_{\underline{k}\underline{k}'}a^+_{\underline{k}'} =$$

$$-\epsilon_{\underline{k}}a^+_{\underline{k}+}$$

$$(2.149) \quad [a^+_{\underline{k}-},T] = -\epsilon_{\underline{k}}\, a^+_{\underline{k}-}$$

$$(2.150) \quad [a^+_{\underline{k}+\underline{Q}+},T] \quad -\epsilon_{\underline{k}+\underline{Q}}\, a^+_{\underline{k}+\underline{Q}+}$$

$$(2.151) \quad [a^+_{\underline{k}+\underline{Q}-},T] \quad -\epsilon_{\underline{k}+\underline{Q}}\, a^+_{\underline{k}+\underline{Q}-}$$

and the potential energy commutator is:

$$(2.152) \quad [a^+_{k+},V] = \sum_{\underline{k}'}A_{o--}\,[a^+_{\underline{k}+},a^+_{\underline{k}'-}a_{\underline{k}'-}] \qquad (1)$$

$$+ \sum_{\underline{k}'}A_{o++}\,[a^+_{\underline{k}+},a^+_{\underline{k}'+}a_{\underline{k}'+}] \qquad (2)$$

$$+ \sum_{\underline{k}'}A_{o+-}\,[a^+_{\underline{k}+},a^+_{\underline{k}'-}a_{\underline{k}'+}] \qquad (3)$$

$$+ \sum_{\underline{k}'}A_{o+-}\,[a^+_{\underline{k}+},a^+_{\underline{k}'+}a_{\underline{k}'+}] \qquad (4)$$

$$+ \sum_{\underline{k}'}A_{\underline{Q}+-}\,[a^+_{\underline{k}+},a^+_{\underline{k}'-}a_{\underline{k}'+\underline{Q}+}] \qquad (5)$$

$$+ \sum_{\underline{k}'} A_{\underline{Q}+-} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'+} \; a_{\underline{k}'+\underline{Q}-}\right] \qquad (6)$$

$$+ \sum_{\underline{k}'} A_{\underline{Q}--} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}-} a_{\underline{k}'-} \; \right] \qquad (7)$$

$$+ \sum_{\underline{k}'} A_{\underline{Q}++} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}+} a_{\underline{k}'+} \; \right] \qquad (8)$$

$$+ \sum_{\underline{k}'} A_{\underline{Q}+-} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}-} a_{\underline{k}'+} \; \right] \qquad (9)$$

$$+ \sum_{\underline{k}'} A_{\underline{Q}+-} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}+} a_{\underline{k}'-} \; \right] \qquad (10)$$

$$+ \sum_{\underline{k}'} A_{\underline{Q}++} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'+} \; a_{\underline{k}'+\underline{Q}+} \; \right] \qquad (11)$$

$$+ \sum_{\underline{k}'} A_{\underline{Q}--} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'-} \; a_{\underline{k}'+\underline{Q}-}\right] \qquad (12)$$

$$+ \sum_{\underline{k}'} A_{o+-} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}+} a_{\underline{k}'+\underline{Q}-}\right] \qquad (13)$$

$$+ \sum_{\underline{k}'} A_{o+-} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}-} a_{\underline{k}'+\underline{Q}+}\right] \qquad (14)$$

$$+ \sum_{\underline{k}'} A_{o++} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}+} a_{\underline{k}'+\underline{Q}+}\right] \qquad (15)$$

$$+ \sum_{\underline{k}'} A_{o--} \left[a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}-} a_{\underline{k}'+\underline{Q}-}\right] \qquad (16)$$

There are eight types of commutators in $[a^+_{k+}, V]$:

<u>Type A</u>: $\sum_{\underline{k}'} [a^+_{\underline{k}+}, a^+_{\underline{k}'-} a_{\underline{k}'-}] = \sum_{\underline{k}'} (a^+_{\underline{k}+} a^+_{\underline{k}'-} a_{\underline{k}'-} - a^+_{\underline{k}'-} a_{\underline{k}'-} a^+_{\underline{k}+}$

$= - \sum_{\underline{k}'} a^+_{\underline{k}'-} \delta_{\underline{k}\underline{k}'} \delta_{+-} = 0$

and a similar commutator equal to zero. These are old Hartree type terms, numbers (1) and (16).

Type B: $\sum_{\underline{k}'} [a^+_{\underline{k}+}, a^+_{\underline{k}'+} a_{\underline{k}'+}] = \sum_{\underline{k}'} (a^+_{\underline{k}+} a^+_{\underline{k}'+} a_{\underline{k}'+} - a^+_{\underline{k}'+} a_{\underline{k}'+} a^+_{\underline{k}+})$

$= - \sum_{\underline{k}'} a^+_{\underline{k}'+} \delta_{\underline{k}\underline{k}'} \delta_{++} = (-a^+_{\underline{k}+})$

and a similar sort of commutator yields $(-a^+_{\underline{k}+\underline{Q}+})$. These are old Hartree type terms, numbers (2) and (15).

Type C: $\sum_{\underline{k}'} [a^+_{\underline{k}+}, a^+_{\underline{k}'-} a_{\underline{k}'+}] = \sum_{\underline{k}'} (a^+_{\underline{k}+} a^+_{\underline{k}'-} a_{\underline{k}'+} - a^+_{\underline{k}'-} a_{\underline{k}'+} a^+_{\underline{k}+})$

$= - \sum_{\underline{k}'} a^+_{\underline{k}'-} \delta_{\underline{k}\underline{k}'} \delta_{++} = (-a^+_{\underline{k}-})$

and a similar sort of commutator yields $(-a^+_{\underline{k}+\underline{Q}-})$. These are terms (3) and (14).

Type D: $\sum_{\underline{k}'} [a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}-} a_{\underline{k}'+}] = \sum_{\underline{k}'} (a^+_{\underline{k}+} a^+_{\underline{k}'+\underline{Q}-} a_{\underline{k}'+} - a^+_{\underline{k}'+\underline{Q}-} a_{\underline{k}'+} a^+_{\underline{k}+})$

$= - \sum_{\underline{k}'} a^+_{\underline{k}'+\underline{Q}-} \delta_{\underline{k}\underline{k}'} \delta_{++} = (-a^+_{\underline{k}+\underline{Q}-})$

and a similar commutator yields $(-a^+_{\underline{k}-\underline{Q}-}) = (-a^+_{\underline{k}+\underline{Q},-})$ by translational symmetry. These are terms (5) and (9).

Type E: $\sum_{\underline{k}'} [a^+_{\underline{k}+}, a^+_{\underline{k}'+} a_{\underline{k}'-}] = \sum_{\underline{k}'} (a^+_{\underline{k}+} a^+_{\underline{k}'+} a_{\underline{k}'-} - a^+_{\underline{k}'+} a_{\underline{k}'-} a^+_{\underline{k}+})$

$= - \sum_{\underline{k}'} a^+_{\underline{k}'+} \delta_{\underline{k}\underline{k}'} \delta_{+-} = 0$

and a similar commutator = 0. These are numbers (4) and (10).

Type F: $\sum_{\underline{k}'} [a^+_{\underline{k}+}, a^+_{\underline{k}'+} a_{\underline{k}'+\underline{Q}-}] = \sum_{\underline{k}'} (a^+_{\underline{k}+} a^+_{\underline{k}'+} a_{\underline{k}'+\underline{Q}-} - a^+_{\underline{k}'+} a_{\underline{k}'+\underline{Q}-} a^+_{\underline{k}+})$

$= - \sum_{\underline{k}'} a^+_{\underline{k}'+} \delta_{\underline{k},\underline{k}+\underline{Q}} \delta_{+-} = 0$

and a similar commutator = 0. These are numbers (6) and (13).

Type G: $\sum_{\underline{k}'}[a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}-}a_{\underline{k}'}] = \sum_{\underline{k}'}(a^+_{\underline{k}+}a^+_{\underline{k}'+\underline{Q}-}a_{\underline{k}'} - a^+_{\underline{k}'+\underline{Q}-}a_{\underline{k}'} - a^+_{\underline{k}+})$

$= -\sum_{\underline{k}'} a^+_{\underline{k}'} - \delta_{\underline{k},\underline{k}+\underline{Q}}\delta_{+-} = 0$

and a similar commutator = 0. These are numbers (7) and (12)

Type H: $\sum_{\underline{k}'}[a^+_{\underline{k}+}, a^+_{\underline{k}'+\underline{Q}+}a_{\underline{k}'+}] = \sum_{\underline{k}'}(a^+_{\underline{k}+}a^+_{\underline{k}'+\underline{Q}+}a_{\underline{k}'} - -a^+_{\underline{k}'+\underline{Q}+}a_{\underline{k}'+} + a^+_{\underline{k}+})$

$= -\sum_{\underline{k}'} a^+_{\underline{k}'+\underline{Q}+}\delta_{\underline{k}\underline{k}'}\delta_{++} = (-a^+_{k+Q+})$

but a similar commutator has a δ_{+-} and hence equals zero. These are numbers (8) and (11).

Thus:

(2.153) $[a^+_{\underline{k}+}, V] = -[A_{o++}a^+_{\underline{k}+} + A_{o+-}a^+_{\underline{k}-} + A_{\underline{Q}+-}a^+_{\underline{k}+\underline{Q}-} + A_{\underline{Q}--}a^+_{\underline{k}+\underline{Q}+}$

$+A_{\underline{Q}+-}a^+_{\underline{k}+\underline{Q}-} + A_{\underline{Q}++}a^+_{\underline{k}+\underline{Q}+}A_{o+-}a^+_{\underline{k}+\underline{Q}-} + A^+_{o++}a^+_{\underline{k}+\underline{Q}+}] = -[a^+_{\underline{k}+}(A_{o++})$

$+a^+_{\underline{k}-}(A_{o+-}) + a^+_{\underline{k}+\underline{Q}+}(A_{\underline{Q}--} + A_{\underline{Q}++}) + a^+_{\underline{k}+\underline{Q}-}(A_{\underline{Q}+-} + A_{o+-})]$

Similarly:

(2.154) $[a^+_{\underline{k}-}, V] = -[(A_{o+-})a^+_{\underline{k}-} + (A_{o+-})a^+_{\underline{k}+} + (A_{\underline{Q}+-})a^+_{\underline{k}+\underline{Q}+} +$

$(A_{\underline{Q}--} + A_{\underline{Q}+-})a^+_{\underline{k}+\underline{Q}-}]$

Similarly:

(2.155) $[a^+_{\underline{k}+\underline{Q}+}, V] = -[(A_{\underline{Q}++})a^+_{\underline{k}+} + (A_{\underline{Q}+-})a^+_{\underline{k}-} + (A_{o++} + A_{o+-})$

$+(A_{o++} + A_{o+-})a^+_{\underline{k}+\underline{Q}+} + (A_{o+-})a^+_{\underline{k}+\underline{Q}-}]$

Similarly:

$$(2.156)\quad [a^{+}_{\underline{k}+\underline{Q}-}, V] = -[(A_{\underline{Q}+-})a^{+}_{\underline{k}+} + (A_{\underline{Q}--})a^{+}_{\underline{k}-} + (A_{o+-})$$

$$a^{+}_{\underline{k}+\underline{Q}+} + (A_{o--} + A_{o+-})a^{+}_{\underline{k}+\underline{Q}-}]$$

These yield the following four simultaneous equations:

$$(2.157)\quad -a^{+}_{\underline{k}+}[-B_1\epsilon_{\underline{k}} - B_1A_{o++} - B_2A_{o+-} - B_3A_{\underline{Q}++} - B_4A_{\underline{Q}+-}]$$

$$= B_1E_{\underline{k}}a^{+}_{\underline{k}+}$$

$$(2.158)\quad -a^{+}_{\underline{k}-}[-B_2\epsilon_{\underline{k}} - B_4A_{o+-} - B_3A_{\underline{Q}+-} - B_2A_{\underline{Q}--}] = B_2E_{\underline{k}}a^{+}_{\underline{k}-}$$

$$(2.159)\quad -a^{+}_{\underline{k}+\underline{Q}+}[-B_3\epsilon_{\underline{k}+\underline{Q}} - B_1A_{\underline{Q}++} - B_3A_{o++} - B_2A_{\underline{Q}+-} - B_4A_{o+-}] =$$

$$B_3E_{\underline{k}}a^{+}_{\underline{k}+\underline{Q}+}$$

$$(2.160)\quad -a^{+}_{\underline{k}+\underline{Q}-}[-B_4\epsilon_{\underline{k}+\underline{Q}} - B_1A_{\underline{Q}+-} - B_3A_{o+-} - B_2A_{\underline{Q}--} - B_4A_{o--}] =$$

$$B_4E_{\underline{k}}a^{+}_{\underline{k}+\underline{Q}-}$$

The condition for simultaneous solubility of these four homogeneous equations is that the determinant of their coefficients vanish. Their equation will be solved for the pseudo-eigenvalues $E_{\underline{k}}$, in terms of the $B(\underline{k})$'s (although Penn drops the B dependence on $(\underline{k})$ that the correlation functions (the A's) are composed of), and the three parameters: $\epsilon_{\underline{k}}$, the band energy; Co, the interaction strength and $\frac{n}{2N}$, the band filling:

(2.161)

$\epsilon_{\underline{k}}-E_{\underline{k}}+A_{o++}$	A_{o+-}	$A_{\underline{Q}++}$	$A_{\underline{Q}+-}$
A_{o+-}	$\epsilon_{\underline{k}}-E_{\underline{k}}+A_{o--}$	$A_{\underline{Q}+-}$	$A_{\underline{Q}--}$
$A_{\underline{Q}++}$	$A_{\underline{Q}+-}$	$\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}+A_{o++}$	A_{o+-}
$A_{\underline{Q}+-}$	$A_{\underline{Q}--}$	A_{o+-}	$\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}+A_{o--}$

$= 0$

We note that in all the states Penn considers $A_{o+-}=0$, and for each state certain other correlations are zero, and others are equal. We write out this energy secular equation for each of the states Penn considers:

PM: $A_{\underline{Q}+-}=A_{\underline{Q}++}=A_{\underline{Q}--}=0$, $A_{o++}+A_{o--}$:

(2.162)

$\epsilon_{\underline{k}}-E_{\underline{k}}+A_{o++}$	0	0	0
0	$\epsilon_{\underline{k}}-E_{\underline{k}}+A_{o++}$	0	0
0	0	$\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}+A_{o++}$	0
0	0	0	$\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}+A_{o++}$

$= 0$

FM: $A_{\underline{Q}++}=A_{\underline{Q}--}=A_{\underline{Q}+-}=A_{o+-}=0$:

(2.163)

$\epsilon_{\underline{k}}-E_{\underline{k}}+A_{o++}$	0	0	0
0	$\epsilon_{\underline{k}}-E_{\underline{k}}+A_{o--}$	0	0
0	0	$\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}+A_{o++}$	0
0	0	0	$\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}+A_{o--}$

$=0$

AFM: $A_{o++}=A_{o--}, A_{\underline{Q}++}=A_{\underline{Q}--}, A_{o+-}=A_{\underline{Q}+-}=0$:

(2.164)

$\epsilon_{\underline{k}}-E_{\underline{k}}+A_{o++}$	0	$A_{\underline{Q}++}$	0
0	$\epsilon_{\underline{k}}-E_{\underline{k}}+A_{o++}$	0	$A_{\underline{Q}++}$
$A_{\underline{Q}++}$	0	$\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}+A_{o++}$	0
0	$A_{\underline{Q}++}$	0	$\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}+A_{o++}$

$=0$

SSDW: $A_{\underline{Q}++}=A_{\underline{Q}--}=A_{o+-}=0$:

(2.165

$\epsilon_{\underline{k}}-E_{\underline{k}}+A_{o++}$	0	$A_{\underline{Q}++}$	$A_{\underline{Q}+-}$
0	$\epsilon_{\underline{k}}-E_{\underline{k}}+A_{o--}$	$A_{\underline{Q}+-}$	$A_{\underline{Q}++}$

A_{Q++}	A_{Q+-}	$\epsilon_{k+Q}-E_k$ $+A_{o++}$	0
A_{Q+-}	A_{Q++}	0	$\epsilon_{k+Q}-E_k$ $+A_{o++}$

$=0$

FIM: $A_{Q+-}=A_{o+-}=0$:

(2.166)

$\epsilon_k-E_k+A_{o++}$	0	A_{Q++}	0
0	$\epsilon_k-E_k+A_{o--}$	0	A_{Q++}
A_{Q++}	0	$\epsilon_{k+Q}-E_k$ $+A_{o++}$	0
0	A_{Q++}	0	$\epsilon_{k+Q}-E_k$ $+A_{o--}$

$=0$

We note that the secular equation has an already diagonal form in the FM and PM cases so that it reduces to:

$$(2.167)\quad (\epsilon_k-E_k+A_{o++})^2(\epsilon_{k+Q}-E_k+A_{o++})^2 = 0$$

for the PM case and

$$(2.168)\quad (\epsilon_k-E_k+A_{o++})(\epsilon_k-E_k+A_{o--})(\epsilon_{k+Q}-E_k+A_{o++})(\epsilon_{k+Q}-E_k+A_{o--}) = 0$$

for the FM case.

Penn solved these and the AFM determinant exactly to get:

$$(2.169) \quad E_{\underline{k}} = E_{\underline{k}}(\epsilon_{\underline{k}}, A(B)'s)$$

with the band energy $\epsilon_{\underline{k}}$ and the interaction strength (in the A definition) as parameters.

We rewrite the five secular equations putting in the definitions for the correlation functions, A, in terms of the coefficients of the linearly combined terms in the wave functions for the five magnetic states, B: with the aid of relations (2.91) to (2.96):

PM:

(2.170)

$\epsilon_{\underline{k}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2)$	0	0	0
0	$\epsilon_{\underline{k}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2)$	0	0
0	0	$\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2)$	0
0	0	0	$\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2)$

$=0$

FM:

(2.171)

$$\begin{vmatrix} \epsilon_{\underline{k}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2) & 0 & 0 & 0 \\ 0 & \epsilon_{\underline{k}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1^2+B_3^2) & 0 & 0 \\ 0 & 0 & \epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2) & 0 \\ 0 & 0 & 0 & \epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1^2+B_3^2) \end{vmatrix} = 0$$

AFM:

(2.172)

$$\begin{vmatrix} \epsilon_{\underline{k}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2) & 0 & \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4 & 0 \\ 0 & \epsilon_{\underline{k}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2) & 0 & \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4 \\ \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4 & 0 & \epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2) & 0 \\ 0 & \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4 & 0 & \epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2) \end{vmatrix} = 0$$

SSDW:

(2.173)

$\epsilon_{\underline{k}}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2)$	0	$\frac{Co}{N}F_k B_2 B_4$	$-\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_1B_4+B_2B_3)$
0	$\epsilon_{\underline{k}}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_1^2+B_3^2)$	$-\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_1B_4+B_2B_3)$	$\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}B_2B_4$
$\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}B_2B_4$	$-\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_1B_4+B_2B_3)$	$\epsilon_{\underline{k}+Q}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2)$	0
$-\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_1B_4+B_2B_3)$	$\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}B_2B_4$	0	$\epsilon_{\underline{k}+Q}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_1^2B_3^2)$

FIM:

(2.174)

$\epsilon_{\underline{k}}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2)$	0	$\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}B_2B_4$	0
0	$\epsilon_{\underline{k}}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_1^2+B_3^2)$	0	$\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}B_2B_4$
$\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}B_2B_4$	0	$\epsilon_{\underline{k}+Q}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2)$	0
0	$\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}B_2B_4$	0	$\epsilon_{\underline{k}+Q}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_1^2+B_3^2)$

$=0$

We see $\frac{\Sigma F_{\underline{k}}}{N}$ (goes to $\frac{n}{2N}$), the fraction of the lower energy band that is filled (in the case of band splitting) and $\frac{Co}{E''}$, the fraction of the Wannier space kinetic energy that is potential energy, emerge naturally as the two parameters of our problem for phase diagram construction, as we have mentioned intuitively before.

We now solve these secular equations for the five simple magnetic states chosen:

For PM case, equation (2.167) has two sets of double roots:

$$(2.175)\quad E_{\underline{k}}^{(1)} = \epsilon_{\underline{k}} + A_{o++}$$

$$(2.176)\quad E_{\underline{k}}^{(2)} = \epsilon_{\underline{k}} + A_{o++}$$

and

$$(2.177)\quad E_{\underline{k}}^{(3)} = \epsilon_{\underline{k}+\underline{Q}} + A_{o++}$$

$$(2.178)\quad E_{\underline{k}}^{(4)} = \epsilon_{\underline{k}+\underline{Q}} + A_{o++}$$

Putting in the B coefficients from (2.91) - (2.96) we find:

$$(2.179)\quad E_{\underline{k}}^{(1)} = \epsilon_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2)$$

$$(2.180)\quad E_{\underline{k}}^{(2)} = \epsilon_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2) = E_{\underline{k}}^{(1)}$$

$$(2.181)\quad E_{\underline{k}}^{(3)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2)$$

$$(2.182)\quad E_{\underline{k}}^{(4)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2) = E_{\underline{k}}^{(3)}$$

For the FM case, (2.168) has four distinct roots:

$$(2.183)\quad E_{\underline{k}}^{(1)} = \epsilon_{\underline{k}} + A_{o++}$$

$$(2.184)\quad E_{\underline{k}}^{(2)} = \epsilon_{\underline{k}} + A_{o--}$$

$$(2.185)\quad E_{\underline{k}}^{(3)} = \epsilon_{\underline{k}+\underline{Q}} + A_{o++}$$

$$(2.186)\quad E_{\underline{k}}^{(4)} = \epsilon_{\underline{k}+\underline{Q}} + A_{o--}$$

Again, substituting in the B coefficients from (2.91) - (2.96) we find:

$$(2.187)\quad E_{\underline{k}}^{(1)} = \epsilon_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2)$$

$$(2.188)\quad E_{\underline{k}}^{(2)} = \epsilon_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}\ (B_1^2+B_3^2)$$

$$(2.189)\quad E_{\underline{k}}^{(3)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2)$$

$$(2.190)\quad E_{\underline{k}}^{(4)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1^2+B_3^2)$$

For the AFM case, we can bring the determinant (2.164) or (2.172) into diagonal form as follows:

$$(2.191)\quad \begin{vmatrix} A & O & B & O \\ O & C & O & D \\ E & O & F & O \\ O & G & O & H \end{vmatrix} \rightarrow \begin{vmatrix} A & O & B & O \\ E & O & F & O \\ O & C & O & D \\ O & G & O & H \end{vmatrix} \rightarrow \begin{vmatrix} A & B & O & O \\ E & F & O & O \\ O & O & C & D \\ O & O & G & H \end{vmatrix}$$

Thus: (2.164) or (2.172) become:

(2.192)

$$\begin{vmatrix} \epsilon_{\underline{k}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4 & \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4 & 0 & 0 \\ \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4 & \epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2) & 0 & 0 \\ 0 & 0 & \epsilon_{\underline{k}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2) & \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4 \\ 0 & 0 & \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4 & \epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}} + \frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2) \end{vmatrix} = 0$$

From this we find the AFM eigenvalues. Subblock 1 becomes:

$$(2.193) \quad [\epsilon_{\underline{k}}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2)][\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2)] - (\frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4)^2 = 0$$

which yields:

$$(2.194) \quad \epsilon_{\underline{k}}\epsilon_{\underline{k}+\underline{Q}}+\epsilon_{\underline{k}}(-E_{\underline{k}})+\epsilon_{\underline{k}}(\frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2))-E_{\underline{k}}(\epsilon_{\underline{k}+\underline{Q}})+E_{\underline{k}}^2 - E_{\underline{k}}(\frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2))+(\frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} (B_2+B_4))\epsilon_{\underline{k}+\underline{Q}}+(\frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2)) (-E_{\underline{k}})+(\frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2))^2-(\frac{Co}{N}\sum_{\underline{k}} F_{\underline{k}} B_2 B_4)^2 = 0$$

Subblock 2 becomes:

$$(2.195)\quad [\epsilon_{\underline{k}}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2+B_4)][\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2)]$$
$$-(\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}B_2B_4)^2 = 0$$

exactly the same as equation (2.193) for the first subblock.

Expanding (2.193) yields:

$$(2.196)\quad E_{\underline{k}}^2+E_{\underline{k}}(\epsilon_{\underline{k}}-\epsilon_{\underline{k}+\underline{Q}}-\frac{2Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2))+\{\epsilon_{\underline{k}}\epsilon_{\underline{k}+\underline{Q}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2)$$
$$+(\epsilon_{\underline{k}}+\epsilon_{\underline{k}+\underline{Q}})(\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2))+(\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2))^2$$
$$-(\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}B_2B_4)^2\} = 0$$

which is solved as:

$$(2.197)\quad E_{\underline{k}} = 1/2[\epsilon_{\underline{k}}+\epsilon_{\underline{k}+\underline{Q}}+\frac{2Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2)$$
$$\pm\sqrt{\begin{array}{l}[\epsilon_{\underline{k}}+\epsilon_{\underline{k}+\underline{Q}}+\frac{2Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2)]^2-4[\epsilon_{\underline{k}}\epsilon_{\underline{k}+\underline{Q}}+\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2)\\ +(\epsilon_{\underline{k}}+\epsilon_{\underline{k}+\underline{Q}})(\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2))+(\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}(B_2^2+B_4^2))^2\\ -(\frac{Co}{N}\sum_{\underline{k}}F_{\underline{k}}B_2B_4)^2\end{array}}$$

Thus:

$$(2.198)\quad E_{\underline{k}}^{\text{upper band}} = E_{\underline{k}}(1) = E_{\underline{k}}(3) = 1/2[\epsilon_{\underline{k}}+\epsilon_{\underline{k}+\underline{Q}}+\frac{2Co}{N}\sum_{\underline{k}}F_{\underline{k}}$$
$$(B_2^2+B_4^2)+\sqrt{\text{square root above}}\ ]$$

$$(2.199)\quad E_{\underline{k}}^{\text{lower band}} = E_{\underline{k}}(2) = E_{\underline{k}}(4) = 1/2[\epsilon_{\underline{k}}+\epsilon_{\underline{k}+\underline{Q}}+\frac{2Co}{N}\sum_{\underline{k}}F_{\underline{k}}$$
$$(B_2^2+B_4^2)-\sqrt{\text{square root above}}\ ]$$

Finally, the total energies for the three states we choose to work on in the next chapter, the PM, FM and AFM, Penn finds to be:

$$(2.200)\quad E^{PM}_{total} = \sum_{\underline{k}} F_{\underline{k}} E^{PM}_{\underline{k}} - \frac{N}{Co} A_{o++}$$

where:

$$(2.201)\quad E^{PM}_{\underline{k}} = 2E^{PM}_{\underline{k}}(1) + 2E^{PM}_{\underline{k}}(3)$$

is expressed in terms of our PM secular equation eigenvalues, and the correlations are subtracted off to prevent double counting of them in the total energy.

Similarly:

$$(2.202)\quad E^{FM}_{total} = \sum_{k} F_k E^{FM}_k - \frac{N}{Co} A_{o--} A_{o++}$$

where:

$$(2.203)\quad E^{FM}_k = E^{FM}_k(1) + E^{FM}_k(2) + E^{FM}_k(3) + E^{FM}_k(4)$$

is expressed in terms of our FM secular equation eigenvalues, the correlation subtraction again occurring.

Similarly:

$$(2.204)\quad F^{AFM}_{total} = \sum_{\underline{k}} F_{\underline{k}} E_{\underline{k}} - \frac{N}{Co}(A^2_{o++} + A^2_{\underline{Q}++})$$

where:

$$(2.205)\quad E^{AFM}_{\underline{k}} = 2E^{AFM}_{\underline{k}}(1) + 2E^{AFM}_{\underline{k}}(2)$$

as in the other two cases.

We note generally that Penn's expression (4.10) for the total energy contains all correlations in a subtractive manner:

$$(2.206)\quad E_{\text{total}}^{\text{Penn}} = \sum_{\underline{k}} F_{\underline{k}} E_{\underline{k}} - (A_{o++} A_{o--} + A_{\underline{Q}++} A_{\underline{Q}--} - A_{o+-}^2 - A_{\underline{Q}+-}^2)$$

We note further that for the AFM state, due to preferential filling of the lower band, we must split up (2.204) into:

$$(2.207)\quad E_{\text{total}}^{\text{AFM}} = \sum_{\underline{k}=0}^{\substack{\text{upper edge of} \\ \text{lower band}}} F_{\underline{k}} \cdot 2 \cdot E_{\underline{k}}^{\text{AFM}}(1) + \sum_{\substack{\text{lower edge of} \\ \text{upper band}}}^{\underline{k}_F} F_{\underline{k}} \cdot 2 \cdot E_{\underline{k}}^{\text{AFM}}(2)$$

for $\underline{k}_F$ in the upper band (see Fig. 3 and 4). If $\underline{k}_F$ is in the lower band, $F_{\underline{k}'}$, $\underline{k}' > \underline{k}_F$ is zero and the second term drops out. We also could put the upper limit on the second sum as infinite, since $F_{\underline{k}}$ for $\underline{k} > \underline{k}_F$ equals zero automatically. Temperature can be included, as we shall do, by noting its inclusion in $F_{\underline{k}}$:

$$(2.208)\quad F_{\underline{k}} = [1 + e^{E_{\underline{k}}/k_B T}]^{-1}$$

but then we would have to find the total free energy, which we shall do.

Penn's final phase diagram for PM, FM and AFM states at T = 0°K is shown (Figure 5a) which Kemeny and Caron have amended by showing that the AFM cusp near $\frac{Co}{E''} \to 0$ does not touch the $\frac{Co}{E''} = 0$ axis, so that antiferromagnetism in the half-filled band case cannot occur for arbitrarily small interaction strengths. This is shown in Figures 5b and 5c.

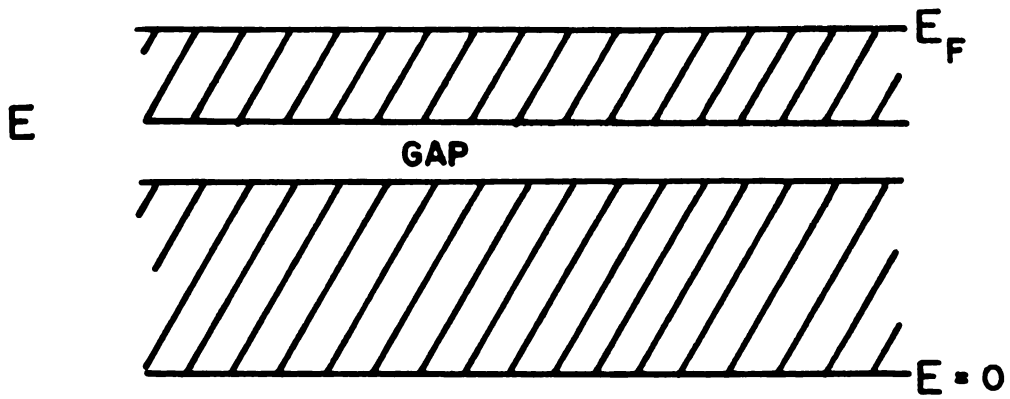


Figure 3. AFM Energy Gap.

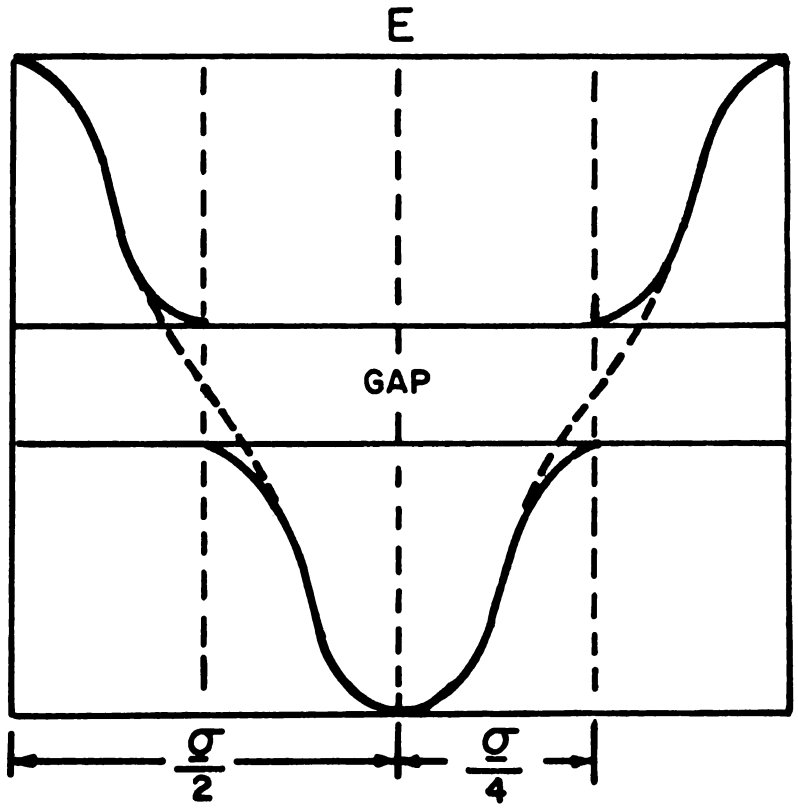


Figure 4. AFM Energy Gap on Dispersion Relation.

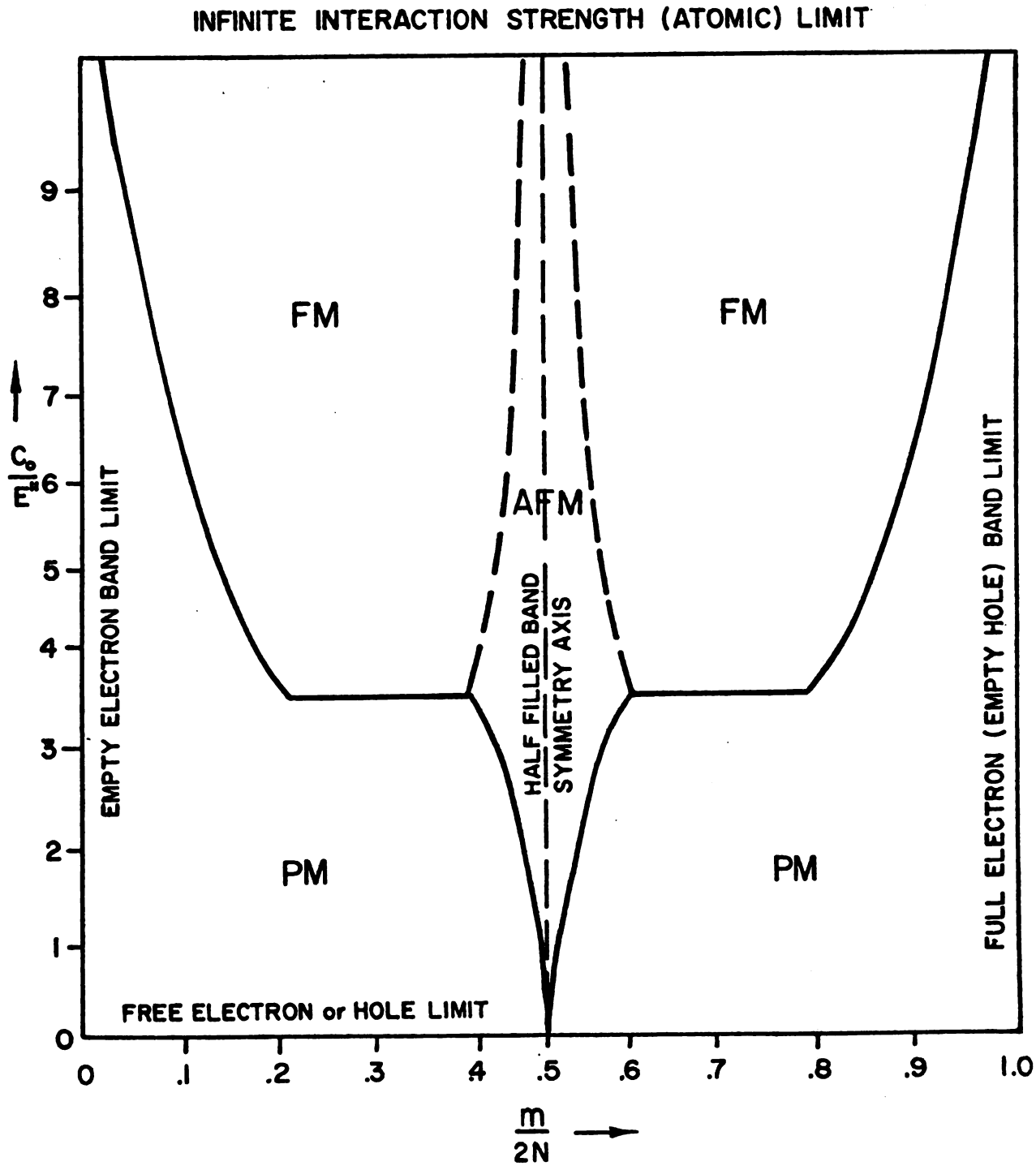


Figure 5a. Penn's Phase Diagram.

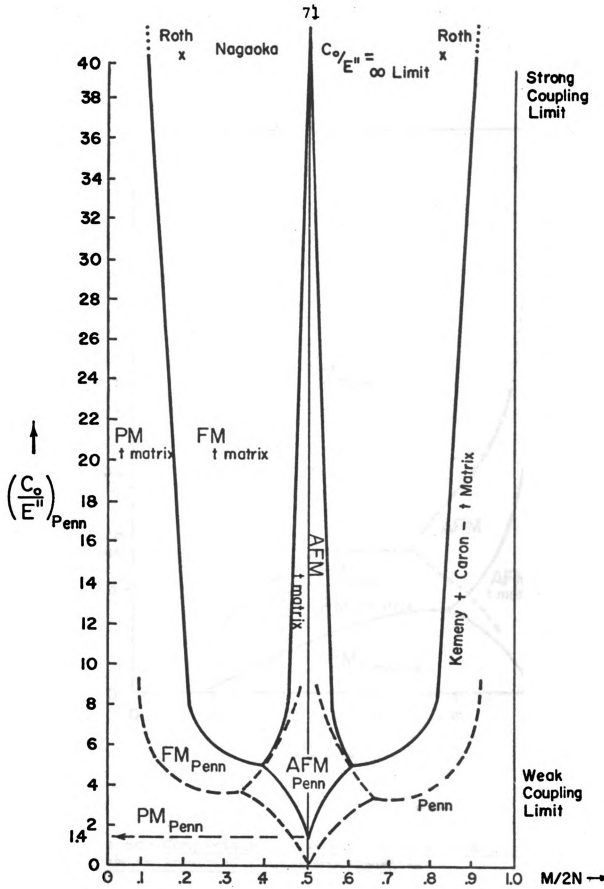


Figure 5b. Comparison of Penn's and the t-matrix Phase Diagram.

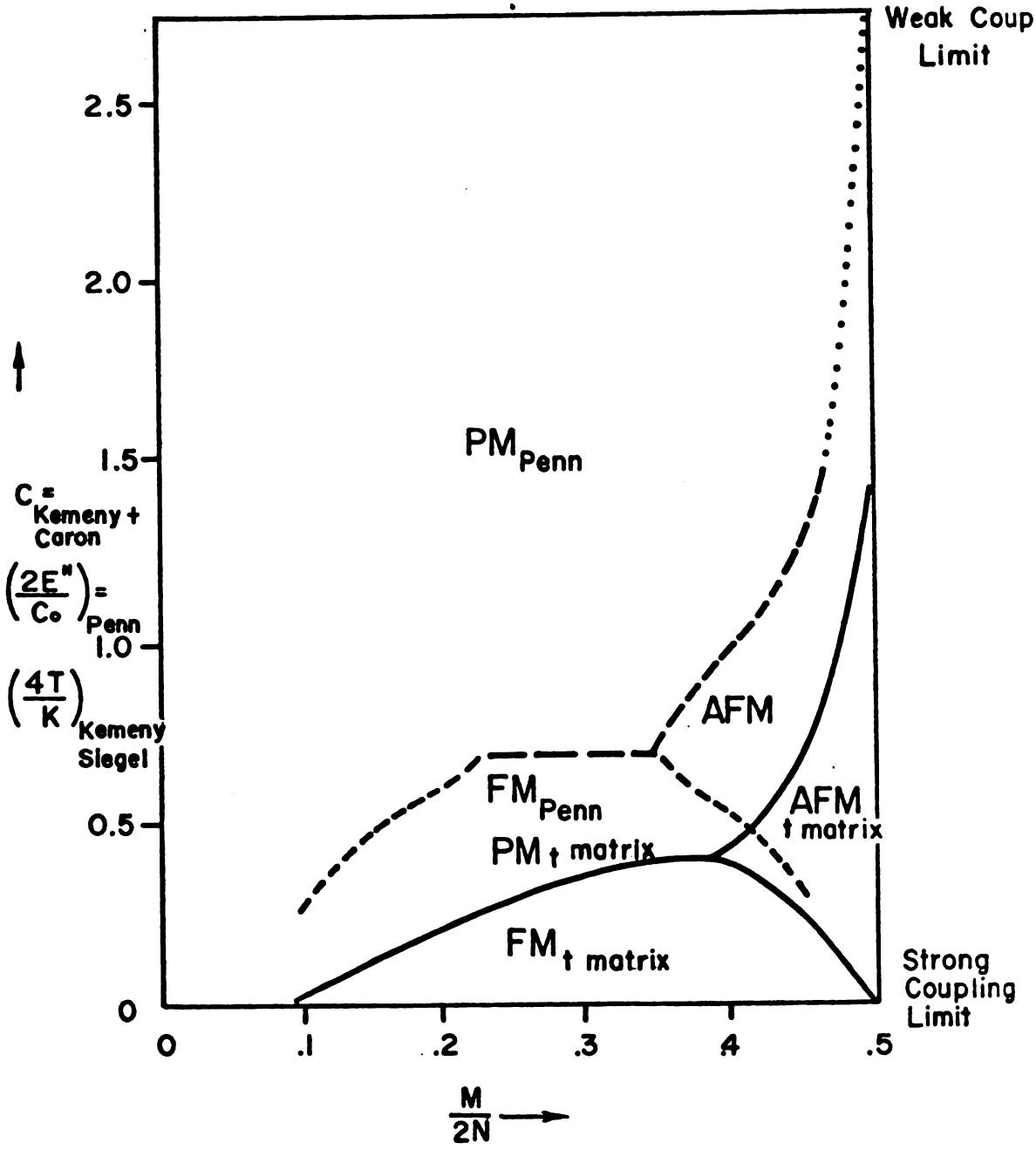


Figure 5c. Comparison of Penn's and the t-matrix Phase Diagram in Inverted Coordinate System.

THE TWO-FOLD AND FIVE-FOLD DEGENERATE PROBLEMS

We first must derive the energy of state by solving:

$$(3.1)\quad [\gamma_{\underline{k}}^{+(2)},\ H_{\text{Bloch}}^{(2\text{ fold})}] = E_{\underline{k}}\gamma_{\underline{k}}^{+(2)}$$

where

$$(3.2)\quad \gamma_{k}^{+(2)} = B_1 a_{\underline{k}1+}^{+} + B_2 a_{\underline{k}1-}^{+} + b_3 a_{\underline{k}+\underline{Q}1+}^{+} + B_4 a_{\underline{k}+\underline{Q}1-}^{+} + B_5 a_{\underline{k}2+}^{+} + B_6 a_{\underline{k}2-}^{+} + B_7 a_{\underline{k}+\underline{Q}2+}^{+} + B_8 a_{\underline{k}+\underline{Q}2-}^{+}$$

Here we use "+" to denot spin up and "-" to denote spin down. (3.2) is just like the adjoint of four term linear combination (2.14), but with eight terms. This corresponds to an eight term general magnetic state wave function:

$$(3.3)\quad \Psi_{\text{MAG}}^{(2)} = B_1 \Psi_{\underline{k}1+} + B_2 \Psi_{\underline{k}1-} + B_3 \Psi_{\underline{k}+\underline{Q}1+} + B_4 \Psi_{\underline{k}+\underline{Q}1-} + B_5 \Psi_{\underline{k}2+} + B_6 \Psi_{\underline{k}2-} + B_7 \Psi_{\underline{k}+\underline{Q}2+} + B_8 \Psi_{\underline{k}+\underline{Q}2-}$$

As in Penn's work, we must commute:

$$(3.4)\quad [\gamma_{\underline{k}}^{+(2)},\ H^{(2)}] = [\gamma_{\underline{k}}^{+(2)},\ T^{(2)} + V^{(2)}]$$

$$= [\gamma_{k}^{+(2)},\ T^{(2)}] + [\gamma_{k}^{+(2)},\ V^{(2)}] \text{ (by linearity)}$$

$$= [\sum_{i=1}^{8} B_i a_i^{+}, T^{(2)}] + [\sum_{i=1}^{8} B_i a_i^{+}, V^{(2)}]$$

Now

$$(3.5)\quad T^{(2)} = \sum_{\ell=1,2} \sum_{\sigma\underline{k}} \epsilon_{\underline{k}} a_{\underline{k}\ell\sigma}^{+} a_{\underline{k}\ell\sigma} = \sum_{\ell=1,2} [\sum_{\underline{k}} \epsilon_{\underline{k}} a_{\underline{k}\ell+}^{+} a_{\underline{k}\ell+} + \sum_{\underline{k}} \epsilon_{\underline{k}} a_{\underline{k}\ell-}^{+} a_{\underline{k}\ell-}]$$

where ℓ is the intra-atomic orbital index.

We assume the B's are independent of $\underline{k}$ for the moment. Thus:

$$
\begin{aligned}
(3.6)\quad [\gamma^{+(2)}, T^{(2)}] = \sum_{\ell=1,2} \Big\{ & B_1[a^+_{\underline{k}1+}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell+} a_{\underline{k}'\ell+}] \\
& + B_1[a^+_{\underline{k}1+}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell-} a_{\underline{k}'\ell-}] + B_2[a^+_{\underline{k}1-}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell+} a_{\underline{k}'\ell+}] \\
& + B_2[a^+_{\underline{k}1-}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell-} a_{\underline{k}'\ell-}] + B_3[a^+_{\underline{k}+\underline{Q}1+}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell+} a_{\underline{k}'\ell+}] \\
& + B_3[a^+_{\underline{k}+\underline{Q}1+}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell-} a_{\underline{k}'\ell-}] + B_4[a^+_{\underline{k}+\underline{Q}1-}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell+} a_{\underline{k}'\ell+}] \\
& + B_4[a^+_{\underline{k}+\underline{Q}1-}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell-} a_{\underline{k}'\ell-}] + B_5[a^+_{\underline{k}2+}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell+} a_{\underline{k}'\ell+}] \\
& + B_5[a^+_{\underline{k}2+}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell-} a_{\underline{k}'\ell-}] + B_6[a^+_{\underline{k}2-}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell+} a_{\underline{k}'\ell+}] \\
& + B_6[a^+_{\underline{k}2-}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell-} a_{\underline{k}'\ell-}] + B_7[a^+_{\underline{k}+\underline{Q}2+}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell+} a_{\underline{k}'\ell+}] \\
& + B_7[a^+_{\underline{k}+\underline{Q}2+}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell-} a_{\underline{k}'\ell-}] + B_8[a^+_{\underline{k}+\underline{Q}2-}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell+} a_{\underline{k}'\ell+}] \\
& + B_8[a^+_{\underline{k}+\underline{Q}2-}, \sum_{\underline{k}}, \epsilon_{\underline{k}}, a^+_{\underline{k}'\ell-} a_{\underline{k}'\ell-}] \Big\}
\end{aligned}
$$

If we label the term of (3.6) from 1 to 16 in order, we find, as done in chapter 2 (nut now where each term is summer over ℓ):

$$
\begin{aligned}
(1) &= -B_1 \epsilon_{\underline{k}} a^+_{\underline{k}} & (2) &= -B_2 \epsilon_{\underline{k}} a^+_{\underline{k}1-} \\
(3) &= -B_3 \epsilon_{\underline{k}+\underline{Q}} a^+_{\underline{k}+\underline{Q}1+} & (4) &= -B_4 \epsilon_{\underline{k}+\underline{Q}} a^+_{\underline{k}+\underline{Q}1-} \\
(5) &= -B_5 \epsilon_{\underline{k}} a^+_{\underline{k}2+} & (6) &= -B_6 \epsilon_{\underline{k}} a^+_{\underline{k}2-} \\
(7) &= -B_7 '_{\underline{k}+\underline{Q}} a^+_{\underline{k}+\underline{Q}2+} & (8) &= -B_8 \epsilon_{\underline{k}+\underline{Q}} a^+_{\underline{k}+\underline{Q}2-}
\end{aligned}
$$

and (9) and (16) are zero.

Summarizing:

$$(3.7)\quad [\gamma_{\underline{k}}^{+(2)}, T^{(2)}] = -\epsilon_{\underline{k}}[B_1 a_{\underline{k}1+}^{+} + B_2 a_{\underline{k}1-}^{+} + \epsilon_{\underline{k}+\underline{Q}}[B_3 a_{\underline{k}+\underline{Q}1+}^{+} + B_4 a_{\underline{k}+\underline{Q}1-}^{+}] + \epsilon_{\underline{k}}[B_5 a_{\underline{k}2+}^{+} + B_6 a_{\underline{k}2-}^{+}] + \epsilon_{\underline{k}+\underline{Q}}[B_7 a_{\underline{k}+\underline{Q}2+}^{+} + B_8 a_{\underline{k}+\underline{Q}2-}^{+}]$$

much as in Penn's s-band calculation.

In working out $[\gamma_{k}^{+(2)}, V^{(2)}]$, we need $V^{(2)}$

$$(3.8)\quad V_{\text{Wannier}}^{(2)} \equiv J \sum_{i} \sum_{\sigma \neq \sigma'} n_{i\sigma} n_{i\sigma'}$$

as in equation (2.4) of the review of Penn's calculation. We derive $V_{\text{Bloch}}^{(2)}$ by Fourier transforming $V_{\text{Wannier}}^{(2)}$ exactly as Penn has done and we have reviewed in equations (2.4) to (2.11).

Tabulated lists of terms in $V_{\text{Bloch}}^{(2)}$ are given in Table 3, and it is fully written out in equation (3.11).

We will derive the total energy of the Hubbard Model for the two-fold degeneracy of the d subband and show how it is immediately generalizable to the five-fold degeneracy of the d subband, the true degeneracy of d subbands in transition metals.

The $V_{\text{Bloch}}^{(2)}$ part of the Hamiltonian has, in $\underline{k}$ space, the following number operator combinations as its terms:

Table 2. Number Operator Combinations in $V^{(2)}_{Bloch}$.

n1+	n1-
n1+	n2+
n1+	n2-
n1-	n2+
n1-	n2-
n2+	n2-

We write these out explicitly in tabular form. There are twelve K/N type terms and six (K-J)/N type terms where K is the coulomb-coupling constant (Penn's Co) and J is the exchange coupling constant not present in his work. The table was arrived at by having:

$$(3.10)\quad \frac{1}{N} \sum_{\substack{\underline{k}_1,\underline{k}_2 \\ \underline{k}_3,\underline{k}_4}} \delta(\underline{k}_1+\underline{k}_2-\underline{k}_3-\underline{k}_4) = \sum_{\underline{k},\underline{k}'}$$

each over the whole Brillouin zone

and $\underline{k}' = \underline{k}+\underline{Q}$ with $\underline{Q} = \underline{G}/2 = \underline{\pi}$ by choice, as in Penn's work.

Table 3. Decomposition of Number Operator Combinations.

Coefficient	a^+ Subscript	a Subscript	a^+ Subscript	a Subscript
$\frac{K}{N}$	$\underline{k}1+$	$\underline{k}1+$	$\underline{k}1-$	$\underline{k}1-$
	$\underline{k}1+$	$\underline{k}+\underline{Q}1+$	$\underline{k}+\underline{Q}1-$	$\underline{k}1-$
	$\underline{k}1+$	$\underline{k}1+$	$\underline{k}+\underline{Q}1-$	$\underline{k}+\underline{Q}1-$

Table 3 (cont'd)

Coefficient	a+ Subscript	a Subscript	a+ Subscript	a Subscript
$\frac{K-J}{N}$	$\underline{k}1+$ $\underline{k}1+$ $\underline{k}1+$	$\underline{k}1+$ $\underline{k}+\underline{Q}1+$ $\underline{k}1+$	$\underline{k}2+$ $\underline{k}+\underline{Q}2+$ $\underline{k}+\underline{Q}2+$	$\underline{k}2+$ $\underline{k}2+$ $\underline{k}+\underline{Q}2+$
$\frac{K}{N}$	$\underline{k}1+$ $\underline{k}1+$ $\underline{k}1+$	$\underline{k}1+$ $\underline{k}+\underline{Q}1+$ $\underline{k}1+$	$\underline{k}2-$ $\underline{k}+\underline{Q}2-$ $\underline{k}+\underline{Q}2-$	$\underline{k}2-$ $\underline{k}2-$ $\underline{k}+\underline{Q}2-$
$\frac{K}{N}$	$\underline{k}1-$ $\underline{k}1-$ $\underline{k}1-$	$\underline{k}1-$ $\underline{k}+\underline{Q}1-$ $\underline{k}1-$	$\underline{k}2+$ $\underline{k}+\underline{Q}2+$ $\underline{k}+\underline{Q}2+$	$\underline{k}2+$ $\underline{k}2+$ $\underline{k}+\underline{Q}2+$
$\frac{K-J}{N}$	$\underline{k}1-$ $\underline{k}1-$ $\underline{k}1-$	$\underline{k}1-$ $\underline{k}+\underline{Q}1-$ $\underline{k}1-$	$\underline{k}2-$ $\underline{k}+\underline{Q}2-$ $\underline{k}+\underline{Q}2-$	$\underline{k}2-$ $\underline{k}2-$ $\underline{k}+\underline{Q}2+$
$\frac{K}{N}$	$\underline{k}2+$ $\underline{k}2+$ $\underline{k}2+$	$\underline{k}2+$ $\underline{k}+\underline{Q}2+$ $\underline{k}2+$	$\underline{k}2-$ $\underline{k}+\underline{Q}2-$ $\underline{k}+\underline{Q}2-$	$\underline{k}2-$ $\underline{k}2-$ $\underline{k}+\underline{Q}2-$

Thus:

$$(3.11)\quad V^{(2)}_{Bloch} = \sum_{\substack{\underline{k} \\ \text{entire Brillouin zone}}} \left\{ \frac{K}{N} \left[(a^{+}_{\underline{k}1+} a_{\underline{k}1+} a^{+}_{\underline{k}1-} a_{\underline{k}1-} + a^{+}_{\underline{k}1+} a_{\underline{k}+\underline{Q}1+} a^{+}_{\underline{k}+\underline{Q}1-} a_{\underline{k}1-} + a^{+}_{\underline{k}1+} a_{\underline{k}1+} a^{+}_{\underline{k}+\underline{Q}1-} a_{\underline{k}1-}) + (a^{+}_{\underline{k}2+} a_{\underline{k}2+} a^{+}_{\underline{k}2-} a_{\underline{k}2-} + a^{+}_{\underline{k}2+} a_{\underline{k}2+} a^{+}_{\underline{k}+\underline{Q}2-} a_{\underline{k}+\underline{Q}2-} + a^{+}_{\underline{k}2+} a_{\underline{k}+\underline{Q}2+} a^{+}_{\underline{k}2-} a_{\underline{k}+\underline{Q}2-}) \right.$$

$$+(a^+_{\underline{k}1-}a_{\underline{k}1-}a^+_{\underline{k}2+}a_{\underline{k}2+}+a^+_{\underline{k}1+}a_{\underline{k}1+}a^+_{\underline{k}+\underline{Q}2+}a_{\underline{k}+\underline{Q}2+}+a^+_{\underline{k}1-}a_{\underline{k}+\underline{Q}1-}$$
$$a^+_{\underline{k}2+}a_{\underline{k}+\underline{Q}2+})\Big] + \frac{K-J}{N}\Big[(a^+_{\underline{k}1+}a_{\underline{k}1+}a^+_{\underline{k}2+}a_{\underline{k}2+}+a^+_{\underline{k}1+}a_{\underline{k}1+}a^+_{\underline{k}+\underline{Q}2+}$$
$$a_{\underline{k}+\underline{Q}2+}+a^+_{\underline{k}1+}a_{\underline{k}+\underline{Q}1+}a^+_{\underline{k}2+}a_{\underline{k}2+})+(a^+_{\underline{k}1-}a_{\underline{k}1-}a^+_{\underline{k}2-}a_{\underline{k}2-}+a^+_{\underline{k}1-}$$
$$a_{\underline{k}1-}a^+_{\underline{k}+\underline{Q}2-}a_{\underline{k}+\underline{Q}2-}+a^+_{\underline{k}1-}a_{\underline{k}+\underline{Q}1-}a^+_{\underline{k}2-}a_{\underline{k}+\underline{Q}2-})\Big]\Big\}$$

We now Gorkov factorize each four operator product $a^+_1a_2a^+_3a_4$ into form:

$$(3.12)\quad a^+_1a_2a^+_3a_5 = \langle a^+_1a_2\rangle\, a^+_3a_4+\langle a^+_3a_4\rangle a^+_1a_2-\langle a^+_1a_4\rangle-\langle a^+_3a_2\rangle a^+_1a_4$$

and tabulate the resultant term subscripts. All such averages as $\langle a_4a_4\rangle$ and $\langle a^+_1a^+_3\rangle$ of two creation and two annihilation, which occur in superconductivity theory correlation operators, are ignored.

Table 4. Gorkov Factorized Terms in $V^{(2)}_{\text{Bloch}}$.

Sign	$\langle a^+$	$a\rangle$	a^+	a	Sign	$\langle a^+$	$a\rangle$	a^+	a
+	$\underline{k}1+$	$\underline{k}1+$	$\underline{k}2-$	$\underline{k}2-$	+	$\underline{k}2-$	$\underline{k}2-$	$\underline{k}1+$	$\underline{k}1+$
−	$\underline{k}1+$	$\underline{k}2-$	$\underline{k}2-$	$\underline{k}1+$	−	$\underline{k}2-$	$\underline{k}1+$	$\underline{k}1+$	$\underline{k}2-$
+	$\underline{k}1+$	$\underline{k}+\underline{Q}1+$	$\underline{k}2-$	$\underline{k}+\underline{Q}2-$	+	$\underline{k}2-$	$\underline{k}+\underline{Q}2-$	$\underline{k}1+$	$\underline{k}+\underline{Q}1+$
−	$\underline{k}1+$	$\underline{k}+\underline{Q}2-$	$\underline{k}2-$	$\underline{k}+\underline{Q}1+$	−	$\underline{k}2-$	$\underline{k}+\underline{Q}1+$	$\underline{k}1+$	$\underline{k}+\underline{Q}2-$
+	$\underline{k}1+$	$\underline{k}1+$	$\underline{k}+\underline{Q}2-$	$\underline{k}+\underline{Q}2-$	+	$\underline{k}2-$	$\underline{k}2-$	$\underline{k}+\underline{Q}1+$	$\underline{k}+\underline{Q}1+$
−	$\underline{k}1+$	$\underline{k}+\underline{Q}2-$	$\underline{k}+\underline{Q}2-$	$\underline{k}1+$	−	$\underline{k}+\underline{Q}2-$	$\underline{k}1+$	$\underline{k}1+$	$\underline{k}+\underline{Q}2-$
+	$\underline{k}1-$	$\underline{k}1-$	$\underline{k}2+$	$\underline{k}2+$	+	$\underline{k}2+$	$\underline{k}2+$	$\underline{k}1-$	$\underline{k}1-$
−	$\underline{k}1+$	$\underline{k}2+$	$\underline{k}2+$	$\underline{k}1-$	−	$\underline{k}2+$	$\underline{k}1-$	$\underline{k}1-$	$\underline{k}2+$
+	$\underline{k}1-$	$\underline{k}+\underline{Q}1-$	$\underline{k}+\underline{Q}2+$	$\underline{k}2+$	+	$\underline{k}+\underline{Q}2+$	$\underline{k}2+$	$\underline{k}1-$	$\underline{k}+\underline{Q}1-$
−	$\underline{k}1-$	$\underline{k}2+$	$\underline{k}+\underline{Q}2+$	$\underline{k}+\underline{Q}1-$	−	$\underline{k}2+$	$\underline{k}1-$	$\underline{k}+\underline{Q}1-$	$\underline{k}+\underline{Q}2+$

Table 4 (cont'd)

Sign	$<a^+$	a>	a^+	a	Sign	$<a^+$	a>	a^+	a
+	k1-	k1-	k+Q2+	k+Q2+	+	k+Q2+	k+Q2+	k1-	k1-
-	k1-	k+Q2+	k+Q2+	k1-	-	k+Q2+	k1-	k1-	k+Q2+
+	k1+	k1+	k1-	k1-	+	k1-	k1-	k1+	k1+
-	k1+	k1-	k1-	k1+	-	k1-	k1+	k1+	k1-
+	k1+	k+Q1+	k+Q1+	k1±	+	k+Q1-	k1-	k1+	k+Q1+
-	k1+	k1-	k+Q1-	k+Q1+	-	k+Q1-	k+Q1+	k1+	k1-
+	k1+	k1+	k+Q1-	k+Q1-	+	k+Q1-	k+Q1-	k1+	k1+
-	k1+	k+Q1-	k+Q1-	k1+	-	k+Q1-	k1+	k1+	k+Q1-
+	k2+	k2+	k2-	k2-	+	k2-	k2-	k2+	k2+
-	k2+	k2-	k2-	k2+	-	k2-	k2+	k2+	k2-
+	k2+	k+Q2+	k2-	k+Q2-	+	k2-	k+Q2-	k2+	k+Q2+
-	k2-	k+Q2+	k2+	k+Q2-	-	k2+	k+Q2-	k2-	k+Q2+
+	k2+	k2+	k+Q2-	k+Q2-	+	k+Q2-	k+Q2-	k2+	k2+
-	k2+	k+Q2-	k+Q2-	k2+	-	k+Q2-	k2+	k2+	k+Q2-
+	k2+	k2+	k1+	k1+	+	k1+	k1+	k2+	k2+
-	k2+	k1+	k1+	k2+	-	k1+	k2+	k2+	k1+
+	k2+	k+Q2+	k+Q1+	k1+	+	k+Q1+	k1+	k2+	k+Q2+
-	k2+	k1+	k+Q1+	k+Q2+	-	k1+	k2+	k+Q2+	k+Q1+
+	k1+	k1+	k+Q2+	k+Q2+	+	k2+	k2+	k+Q1+	k+Q1+
-	k1+	k+Q2+	k+Q2+	k1+	-	k+Q2+	k1+	k1+	k+Q2+
+	k1-	k1-	k2-	k2-	+	k2-	k2-	k1-	k1-
-	k1-	k2-	k2-	k1-	-	k2-	k1-	k1-	k2-
+	k1-	k+Q1-	k+Q2-	k2-	+	k+Q2-	k2-	k1-	k+Q1-
-	k1-	k2-	k+Q2-	k+Q1-	-	k2-	k1-	k+Q1-	k+Q2-
+	k1-	k1-	k+Q2-	k+Q2-	+	k+Q2-	k+Q2-	k1-	k1-
1	k1-	k+Q2-	k+Q2-	k1-	-	k+Q2-	k1-	k1-	k+Q2-

We exclude all correlations of form A_{mnk12} or A_{mnk21} as "orbital ordering". (These are terms on lines 2, 4, 6, 8, 10, 12, 26, 28,

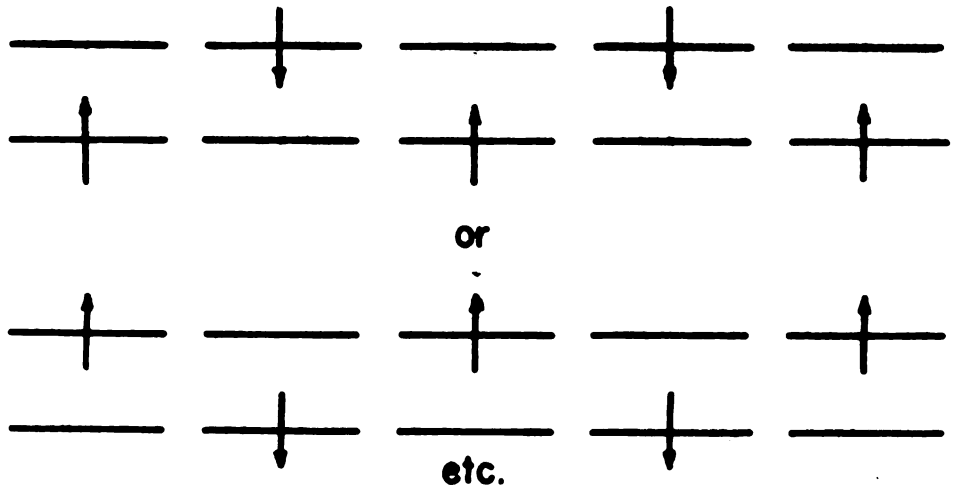
30,32,34,36), a spin arrangement in which the orbital that the spin is in is as important as what lattice site it is on and what its nearest neighbors are. We do this since no evidence for any such ordering exists in the transition metals.

We arrive at $V^{(2)}_{Bloch}$ in terms of four types of correlation functions. If we define our correlation functions as:

$$(3.13)\quad A = \sum_{\underline{k}}^{\text{Brillouin zone}} \langle a^{+}_{abc} a_{dec} \rangle$$

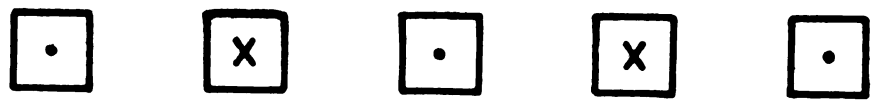
as type A(obecc) or type A($\underline{Q}$becc), where c is the orbital index, b and e are the spin indices. o (representing $\underline{k}$) and $\underline{Q}$ (representing $\underline{k}+\underline{Q}$) are the crystal momentum indices. This is unlike Penn's definitions (2.21) - (2.26) in that all are positive, and Co and N are not included in the definition. We prefer to carry them along in the calculation explicitly. Penn's Co will no longer be a simple s subband term, so we prefer to keep it visible throughout all steps we make. Type A(obecc) and A($\underline{Q}$becc) correspond to the pair (a,d) being ($\underline{k}$,$\underline{k}$), ($\underline{k}+\underline{Q}$, $\underline{k}+\underline{Q}$) or ($\underline{k}$, $\underline{k}+\underline{Q}$), ($\underline{k}+\underline{Q}$,$\underline{k}$) respectively.

We can rewrite $V^{(2)}_{Bloch}$ (equation 3.11) after the Gorkov factorization represented in Table 4 in terms of the nonzero correlation functions for a general magnetic state without "12" type "orbital" correlations. The specific relations between the correlation functions for the specific magnetic states are held in abeyance until later.



On each site we have one up spin or one down spin in either of two orbital states in the two-fold degenerate case (or in the five orbital states in the five-fold degenerate case).

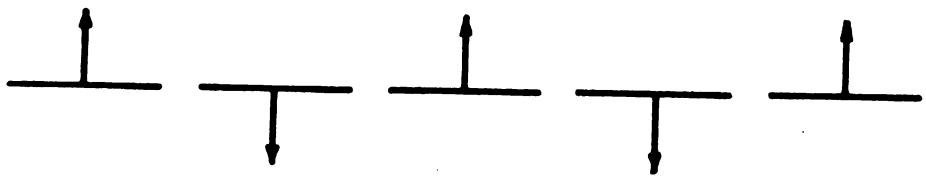
In a zero frequency probe, which measures $X(0) = M(0)/H(0)$, these would all appear the same as viewed from the top as:



where "." and "X" denote up or down spins on each site. Physically, this is because of the zero frequency probe H(0) (where H(0) is the applied magnetic field; M(0), the resulting macroscopic magnetization; and X(0) is the magnetic susceptibility relating the two) which does not excite orbital transitions, i.e. does not probe the orbital degeneracy. The definitions of our

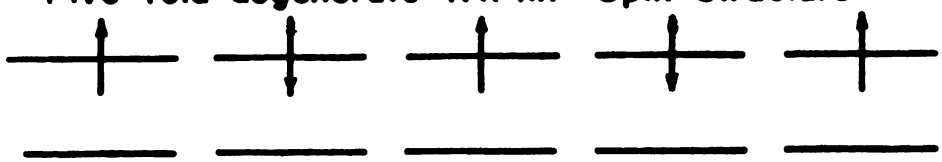
We must examine the physical reasons for this neglect of "12", cross-orbit correlations, $A(o^{++}_{+-}ij)$, where i and j here are two orbital indices. ij can be pairs 12, 21, in the two-fold degenerate case or 12, 13, 14, 15, 21, 23, 24, 25, 31, 32, 34, 35, 41, 32, 43, 45, 51, 52, 53, 54, in the five-fold degenerate case. Consider an AFM spin structure:

Nondegenerate |AFM> Spin Structure

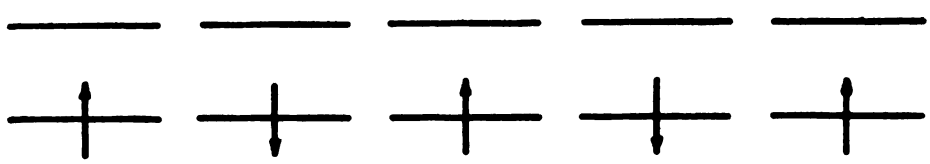


In the two-fold degenerate case (the same considerations hold in the five-fold degenerate case) this array could look like any of the following:

Five fold degenerate |AFM> Spin Structure



or



or

three magnetic states, AFM, PM, and FM, depend on macroscopic measurements which are probes of net spin on a particular lattice site, regardless of which degenerate orbital state that spin is in. Hence, orbital indices only play a physical role in putting new correlation terms into the total energy of a particular state, which adds more direct; and exchange terms with coefficient J. The interactions term in the Hamiltonian is also altered as seen by $V^{(2)}_{Bloch}$ being considerable enlarged. New correlations with K and J coefficients enter as we shall see in equation (3.14)

By mathematical reasoning, we can represent a sequence of correlation functions as a symmetric array[63]:

$$\begin{bmatrix} A(o^{++}_{\pm\mp}11) & A(o^{++}_{\pm\mp}21) \\ A(o^{++}_{\pm\mp}12) & A(o^{++}_{\pm\mp}22) \end{bmatrix}$$

Since $A(o^{++}_{\pm\mp}12) \equiv A(o^{++}_{\pm\mp}21)$, diagonalization by a similar transformation becomes, trivially:

$$\begin{bmatrix} A(o^{++}_{\pm\mp}11) & 0 \\ 0 & A(o^{++}_{\pm\mp}22) \end{bmatrix}$$

since these two correlations are assumed to be zero. Since we need only two independent one-electron wave functions, then:

$$\Psi^{(1)}_{\underline{k}}(\underline{R}) = B_1 \ell^{i\underline{k}_{1+}\cdot\underline{r}} + B_3 \ell^{i\underline{k}_{1+}\cdot\underline{r}} \ell^{i\underline{Q}\cdot\underline{r}} \quad \text{(contains } A(o^{++}_{\pm\mp}11)\text{)}$$

$$\Psi^{(2)}_{\underline{k}}(\underline{R}) = B_5 \ell^{i\underline{k}_{2+}\cdot\underline{r}} + B_7 \ell^{i\underline{k}_{2+}\cdot\underline{r}} \ell^{i\underline{Q}\cdot\underline{r}} \quad \text{(contains } A(o^{++}_{\pm\mp}22)\text{)}$$

$$\psi_{\underline{k}}^{(3)}(\underline{R}) = B_1 \ell_{1+}^{i\underline{k}\cdot\underline{r}} + B_5 \ell_{2+}^{i\underline{k}\cdot\underline{r}} \ell^{i\underline{Q}\cdot\underline{r}} \quad \text{(contains } A(o_{\pm\pm}^{++}12)\text{)}$$

$$\psi_{\underline{k}}^{(4)}(\underline{R}) = B_5 \ell_{2+}^{i\underline{k}\cdot\underline{r}} + B_1 \ell_{1+}^{i\underline{k}\cdot\underline{r}} \ell^{i\underline{Q}\cdot\underline{r}} \quad \text{(contains } A(o_{\pm\pm}^{++}21)\text{)}$$

Only two are independent. We assume the other two are zero by assume $A(o_{\pm\pm}^{++}12) \equiv A(o_{\pm\pm}^{++}21) = 0$. Electrons in different orbital states interact (as seen in the diagonalization where this is included) but are not correlated, i.e. our magnetic state one-electron wave functions are not constructed of mixed orbital electron states.

A physical justification for neglecting spin-orbit splitting is the large overlap of the d orbital subbands so that the total d electron band width is much greater than the spin-orbit splitting in transition metals.

In our neglect of cross-orbit correlations, we can further be assured that we are not probing the orbital structure so that the orbital angular momentum operator L_z is never used. It is usually quenched in transition metals in a cubic crystal field so that orbital angular momentum eigenvalues do not influence the magnetization definition of our magnetic states (2.108 - 2.125); they are electron spin-produced magnetization. S_z, the spin angular momentum operator, is used to operate on our electron wave functions; its eigenvalues are the important ones.

Table 5. $V^{(2)}_{\text{Bloch}}$ in Terms of $\underline{k}$ Space Correlation Functions.

We find:

$$
\begin{aligned}
(3.14)\quad V^{(2)}_{\text{Bloch}} = \Bigg[\sum_{\underline{k}} \frac{K}{N} \;& A(o{+}{+}11)\, a^{+}_{\underline{k}2-} a_{\underline{k}2-} + A(o{-}{-}22)\, a^{+}_{\underline{k}1+} a_{\underline{k}1+} \\
& + A(\underline{Q}{+}{+}11)\, a^{+}_{\underline{k}2-} a_{\underline{k}+\underline{Q}2-} + A(\underline{Q}{-}{-}22)\, a^{+}_{\underline{k}1+} a_{\underline{k}+\underline{Q}1+} \\
& + A(o{+}{+}11)\, a^{+}_{\underline{k}+\underline{Q}2-} a_{\underline{k}+\underline{Q}2+} + A(o{-}{-}22)\, a^{+}_{\underline{k}+\underline{Q}1+} a_{\underline{k}+\underline{Q}1-} \\
& + A(o{-}{-}11)\, a^{+}_{\underline{k}2+} a_{\underline{k}2+} + A(o{+}{+}22)\, a^{+}_{\underline{k}1-} a_{\underline{k}1-} \\
& + A(o{+}{+}11)\, a^{+}_{\underline{k}1-} a_{\underline{k}1-} + A(o{-}{-}22)\, a^{+}_{\underline{k}+\underline{Q}2+} a_{\underline{k}+\underline{Q}2+} \\
& + A(\underline{Q}{+}{+}11)\, a^{+}_{\underline{k}2-} a_{\underline{k}2-} + A(\underline{Q}{-}{-}22)\, a^{+}_{\underline{k}1+} a_{\underline{k}+\underline{Q}1+} \\
& + A(o{+}{+}11)\, a^{+}_{\underline{k}+\underline{Q}1-} a_{\underline{k}+\underline{Q}1-} + A(o{-}{-}22)\, a^{+}_{\underline{k}+\underline{Q}1+} a_{\underline{k}+\underline{Q}1+} \\
& + A(o{-}{-}11)\, a^{+}_{\underline{k}+\underline{Q}1+} a_{\underline{k}+\underline{Q}1+} + A(o{+}{+}22)\, a^{+}_{\underline{k}+\underline{Q}2-} a_{\underline{k}+\underline{Q}2-} \\
& + A(\underline{Q}{-}{-}11)\, a^{+}_{\underline{k}+\underline{Q}2+} a_{\underline{k}2+} + A(\underline{Q}{+}{+}22)\, a^{+}_{\underline{k}1-} a_{\underline{k}+\underline{Q}1-} \\
& + A(o{-}{-}11)\, a^{+}_{\underline{k}+\underline{Q}2+} a_{\underline{k}+\underline{Q}2+} + A(o{+}{+}22)\, a^{+}_{\underline{k}+\underline{Q}1-} a_{\underline{k}+\underline{Q}1-} \\
& + A(o{+}{+}11)\, a^{+}_{\underline{k}1-} a_{\underline{k}1-} + A(o{-}{-}11)\, a^{+}_{\underline{k}1+} a_{\underline{k}1+} \\
& - A(o{+}{-}11)\, a^{+}_{\underline{k}1-} a_{\underline{k}1+} - A(o{+}{-}11)\, a^{+}_{\underline{k}1+} a_{\underline{k}1-} \\
& + A(\underline{Q}{+}{+}11)\, a^{+}_{\underline{k}+\underline{Q}1-} a_{\underline{k}1-} + A(\underline{Q}{-}{-}11)\, a^{+}_{\underline{k}1+} a_{\underline{k}+\underline{Q}1+} \\
& - A(o{+}{-}11)\, a^{+}_{\underline{k}+\underline{Q}1-} a_{\underline{k}+\underline{Q}1+} - A(o{+}{-}11)\, a^{+}_{\underline{k}+\underline{Q}1+} a_{\underline{k}+\underline{Q}1-} \\
& - A(\underline{Q}{+}{-}11)\, a_{\underline{k}+\underline{Q}1-} a_{\underline{k}1+} - A(\underline{Q}{+}{-}11)\, a_{\underline{k}1+} a_{\underline{k}+\underline{Q}1-} \\
& + A(o{+}{+}22)\, a^{+}_{\underline{k}2-} a_{\underline{k}2-} + A(o{-}{-}22)\, a^{+}_{\underline{k}2+} a_{\underline{k}2+} \\
& - A(o{+}{-}22)\, a^{+}_{\underline{k}2-} a_{\underline{k}2+} - A(o{+}{-}22)\, a^{+}_{\underline{k}2+} a_{\underline{k}2-} \\
& + A(\underline{Q}{+}{+}22)\, a^{+}_{\underline{k}2-} a_{\underline{k}+\underline{Q}2-} + A(\underline{Q}{-}{-}22)\, a^{+}_{\underline{k}2+} a_{\underline{k}+\underline{Q}2+} \\
& - A(\underline{Q}{+}{-}22)\, a^{+}_{\underline{k}2+} a_{\underline{k}+\underline{Q}2-} - A(\underline{Q}{+}{-}22)\, a^{+}_{\underline{k}2-} a_{\underline{k}+\underline{Q}2+} \\
& - A(\underline{Q}{+}{-}22)\, a^{+}_{\underline{k}+\underline{Q}2-} a_{\underline{k}2+} - A(\underline{Q}{+}{-}22)\, a^{+}_{\underline{k}2+} a_{\underline{k}+\underline{Q}2-} \Bigg]
\end{aligned}
$$

Table 5 (cont'd)

$$+\sum_{\underline{k}}\frac{K-J}{N}\Big[A(o{+}{+}22)a^{+}_{\underline{k}1+}a_{\underline{k}1+}+A(o{+}{+}11)a^{+}_{\underline{k}2+}a_{\underline{k}2+}$$

$$+A(Q{+}{+}22)a^{+}_{\underline{k}+\underline{Q}1+}a_{\underline{k}1+}+A(Q{+}{+}11)a^{+}_{\underline{k}2+}a_{\underline{k}+\underline{Q}2+}$$

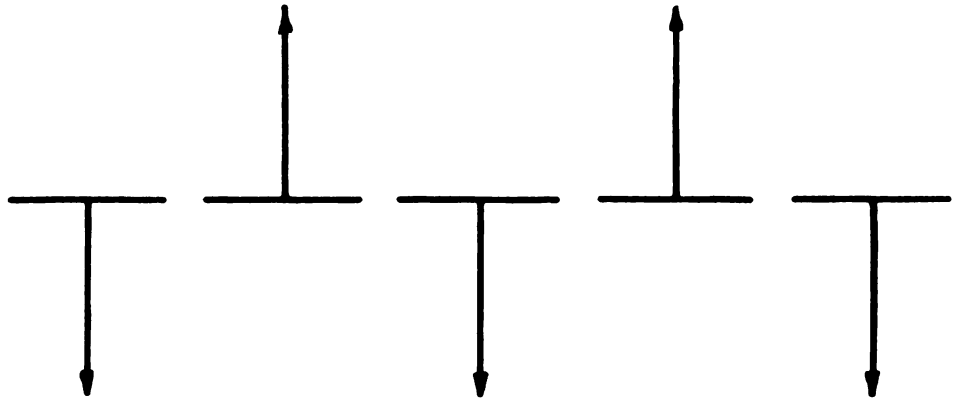
$$+A(o{+}{+}11)a^{+}_{\underline{k}+\underline{Q}2+}a_{\underline{k}+\underline{Q}2+}+A(o{+}{+}22)a^{+}_{\underline{k}+\underline{Q}1+}a_{\underline{k}+\underline{Q}1+}$$

$$+A(o{-}{-}11)a^{+}_{\underline{k}2-}a_{\underline{k}2-}+A(o{-}{-}22)a^{+}_{\underline{k}1-}a_{\underline{k}1-}$$

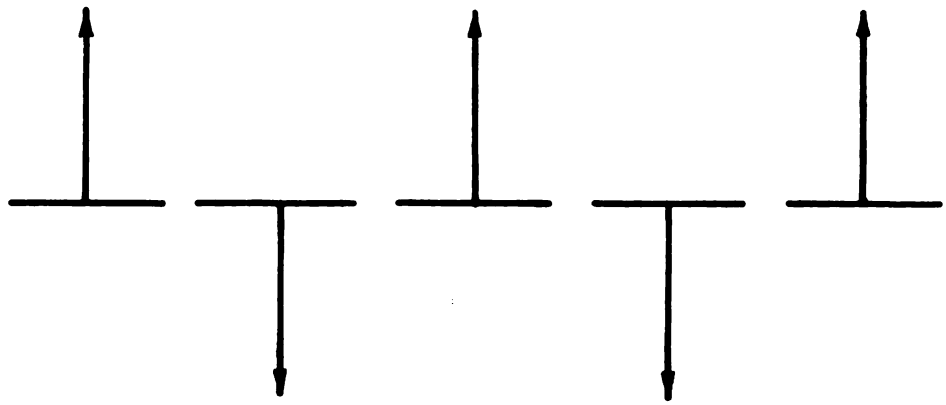
$$+A(Q{-}{-}11)a^{+}_{\underline{k}+\underline{Q}2-}a_{\underline{k}2-}+A(Q{-}{-}22)a^{+}_{\underline{k}1-}a_{\underline{k}+\underline{Q}1-}$$

$$+A(o{-}{-}11)a^{+}_{\underline{k}+\underline{Q}2-}a_{\underline{k}+\underline{Q}2-}+A(o{-}{-}22)a^{+}_{\underline{k}+\underline{Q}1-}a_{\underline{k}+\underline{Q}1-}\Big]$$

Lastly, degeneracies in the physical makeup of the spin structure of our states do not have to be all of an orbital filling nature as we have just indicated. The GM state has M_z with any magnitude from M_z^{MAX}, when all the spins are polarized along $\hat{z}$ to $M_z \approx 0$, and few spins are polarized along $\hat{z}$. Also $\hat{z}$ can have any direction in space. Therefore, there is a 2^N fold spatial rotation degeneracy in defining FM. The AFM state can be represented even in the single s-band calculation of Penn, as:



or as:



with a phase shift in its spatial spin structure of one lattice site. This will not matter macroscopically in a M_x or M_z definition.

In conclusion, we must look upon our magnetic states as being defined solely by their nonzero correlation functions, and not take intuitive spatial spin structures too seriously. This approach is a necessity in any practical calculation. Macroscopic M's and n's determine our magnetic states, and these depend solely upon the correlation functions as in (2.102) - (2.107).

We group the terms in (3.14). Noting that $a^+_{\underline{k}2+}\, a_{\underline{k}1+}$ is equivalent to $a^+_{\underline{k}1+} a_{\underline{k}2+}$ we can further group them in terms of a smallest set of independent two-operator product:

$$(3.15)\quad V^{(2)}_{Bloch} = \sum_{\underline{k}} \frac{1}{N}\{a^+_{\underline{k}2-} a_{\underline{k}2-}[KA(o++11)+KA(o++22)+KA(o--11)]$$

$$+a^{+}_{\underline{k}1+}a_{\underline{k}1+}[KA(o--11)+KA(o--22)+(K-J)A(o++22)]$$

$$+a^{+}_{\underline{k}2+}a_{\underline{k}2+}[KA(o--11)+KA(o--22)+(K-J)A(o++11)]$$

$$+a^{+}_{\underline{k}1-}a_{\underline{k}1-}[KA(o++11)+KA(o++22)+(K-J)A(o--22)]$$

$$+a^{+}_{\underline{k}2-}a_{\underline{k}+\underline{Q}2-}[KA(\underline{Q}++11)+KA(\underline{Q}++22)+(K-J)A(\underline{Q}--11)]$$

$$+a^{+}_{\underline{k}+\underline{Q}2+}a_{\underline{k}2+}[KA(\underline{Q}--11)+KA(\underline{Q}--22)+(K-J)A(\underline{Q}++11)]$$

$$+a^{+}_{\underline{k}1+}a_{\underline{k}+\underline{Q}1+}[KA(\underline{Q}--11)+KA(\underline{Q}--22)+(K-J)A(\underline{Q}++22)]$$

$$+a^{+}_{\underline{k}1-}a_{\underline{k}+\underline{Q}1-}[KA(\underline{Q}++11)+KA(\underline{Q}++22)+(K-J)A(\underline{Q}--22)]$$

$$+a^{+}_{\underline{k}1+}a_{\underline{k}+\underline{Q}1-}[-KA(\underline{Q}+-11)-KA(\underline{Q}+-11)]$$

$$+a^{+}_{\underline{k}+\underline{Q}1+}a_{\underline{k}+\underline{Q}1-}[-KA(o+-11)-KA(o+-11)]$$

$$+a^{+}_{\underline{k}2-}a_{\underline{k}+\underline{Q}2+}[-KA(\underline{Q}+-22)$$

$$+a^{+}_{\underline{k}2+}a_{\underline{k}+\underline{Q}2-}[-KA(\underline{Q}+-22)-KA(\underline{Q}+-22)-KA(\underline{Q}+-22)]$$

$$+a^{+}_{\underline{k}1+}a_{\underline{k}1-}[-KA(o+-11)-KA(o-+11)]$$

$$+a^{+}_{\underline{k}2+}a_{\underline{k}2-}[-KA(o-+22)-KA(o-+22)]\}$$

where the first $(\underline{k}\ \underline{k}+\underline{Q}\ 1\ 2\ +\ -)$ denotes the subscript of an a^{+} and the second denotes the subscript of an a. This is still the Gorkov factorized one-body, quasi-particle Hamiltonian.

We label the above terms in (3.5) in brackets as C, D, E, F, K, L, M, N, O, P, R, S, T, U, V, W, X, Y, Z, respectively.

We must now commute $[V^{(2)}_{Bloch}, \gamma^+_{\underline{k}}] = E_{\underline{k}}\gamma^+_{\underline{k}}$ to find the energy "eigenvalues", $E_{\underline{k}}$. The relevant commutators are such that for each term of $V^{(2)}_{Bloch}$, only two of the eight commutators with the operators making up $\gamma^+_{\underline{k}}$ are nonzero. The rest have delta functions, $\delta_{+,-}$ or $\delta_{1,2}$, which are automatically zero. In all of these terms, i is summed from one to eight to represent the eight terms in the linear combination of a"'s that is $\gamma^+_{\underline{k}}$. Each term has a "-" sign, since the commutator $[a^+_i, a^+_j a_{\underline{k}}]$ has been factored out as $(a^+_i a^+_j a_{\underline{k}} - a^+_j a_{\underline{k}} a^+_i) = a^+_j(a^+_i a_{\underline{k}} + a_{\underline{k}} a^+_i) = -a^+_j[a^+_i, a_{\underline{k}}]_+$. Note that here i and j have nothing to do with lattice site labels; this is just an unfortunate duplication of notation (also $\underline{k}$ above is just a dummy index, note a wave vector).

The actual anti-commutators are:

$$(3.16)\quad \sum_{i\underline{k}'} a^+_{\underline{k}'2-}[a^+_i, a_{\underline{k}'2-}]_+ = -B_6 a^+_{\underline{k}2+} - B_3 a^+_{\underline{k}+\underline{Q}2+}$$

$$(3.17)\quad \sum_{i\underline{k}'} a^+_{\underline{k}'+\underline{Q}1+}[a^+_i, a_{\underline{k}'1+}]_+ = -B_1 a^+_{\underline{k}1+} - B_3 a^+_{\underline{k}+\underline{Q}1+}$$

$$(3.18)\quad \sum_{i\underline{k}'} a^+_{\underline{k}'+\underline{Q}2+}[a^+_i, a_{\underline{k}'2+}]_+ = -B_5 a^+_{\underline{k}2+} - B_7 a^+_{\underline{k}+\underline{Q}2+}$$

$$(3.19)\quad \sum_{i\underline{k}'} a^+_{\underline{k}'+\underline{Q}1-}[a^+_i, a_{\underline{k}'1-}]_+ = -B_2 a^+_{\underline{k}1-} - B_4 a^+_{\underline{k}+\underline{Q}1-}$$

$$(3.20)\quad \sum_{i\underline{k}'} a^+_{\underline{k}'2-}[a^+_i, a_{\underline{k}'+\underline{Q}2-}]_+ = -B_8 a^+_{\underline{k}2-} - B_6 a^+_{\underline{k}+\underline{Q}2-}$$

$$(3.21)\quad \sum_{i\underline{k}'} a^+_{\underline{k}'+\underline{Q}2+}[a^+_i, a_{\underline{k}'2+}]_+ = -B_5 a^+_{\underline{k}+\underline{Q}2+} - B_7 a^+_{\underline{k}2+}$$

$$(3.22)\quad \sum_{i\underline{k}'} a^+_{\underline{k}'1+}[a^+_{\underline{k}}, a_{\underline{k}'+\underline{Q}1+}]_+ = -B_3 a^+_{\underline{k}1+} - B_1 a^+_{\underline{k}+\underline{Q}1+}$$

$$(3.23)\quad \sum_{i\underline{k}'} a^+_{\underline{k}'1-}[a^+_i, a_{\underline{k}'+\underline{Q}1-}]_+ = -B_2 a^+_{\underline{k}+\underline{Q}1-} - B_4 a^+_{\underline{k}1-}$$

$$(3.24)\quad \sum_{i\underline{k}'} a^{+}_{\underline{k}'1-}[a^{+}_{i}, a_{\underline{k}'+\underline{Q}1-}]_{+} = -B_2 a^{+}_{\underline{k}+\underline{Q}1-} - B_4 a^{+}_{\underline{k}1-}$$

$$(3.25)\quad \sum_{i\underline{k}'} a^{+}_{\underline{k}'1+}[a^{+}_{i}, a_{\underline{k}'+\underline{Q}1+}]_{+} = -B_2 a^{+}_{\underline{k}1+} - B_4 a^{+}_{\underline{k}+\underline{Q}1+}$$

$$(3.26)\quad \sum_{i\underline{k}'} a^{+}_{\underline{k}'2-}[a^{+}_{\underline{k}}, a_{\underline{k}'+\underline{Q}2+}]_{+} = -B_5 a^{+}_{\underline{k}+\underline{Q}2+} - B_7 a^{+}_{\underline{k}2-}$$

$$(3.27)\quad \sum_{i\underline{k}'} a^{+}_{\underline{k}'2+}[a^{+}_{i}, a_{\underline{k}'+\underline{Q}2-}]_{+} = -B_6 a^{+}_{\underline{k}+\underline{Q}2+} - B_8 a^{+}_{\underline{k}2+}$$

$$(3.28)\quad \sum_{i\underline{k}'} a^{+}_{\underline{k}'1+}[a^{+}_{i}, a_{\underline{k}'1-}]_{+} = -B_2 a^{+}_{\underline{k}1+} - B_4 a^{+}_{\underline{k}+\underline{Q}1-}$$

$$(3.29)\quad \sum_{i\underline{k}'} a^{+}_{\underline{k}'2+}[a^{+}_{i}, a_{\underline{k}'2-}]_{+} = -B_6 a^{+}_{\underline{k}2+} - B_8 a^{+}_{\underline{k}+\underline{Q}2+}$$

Gathering up all of these terms and the kinetic energy commutators calculated before, yields:

$$(3.30)\quad -a^{+}_{\underline{k}1+}(\epsilon_{\underline{k}} \pm E_{\underline{k}} + B_1 D + B_3 L + B_2 U + B_2 O + B_4 Z) = 0$$

$$(3.31)\quad -a^{+}_{\underline{k}1-}(\epsilon_{\underline{k}} - E_{\underline{k}} + B_2 F + B_4 N + B_4 Y + B_1 P \mp B_3 Z + B_1 P) = 0$$

$$(3.32)\quad -a^{+}_{\underline{k}+\underline{Q}1+}(\epsilon_{\underline{k}+\underline{Q}1+} - E_{\underline{k}} + B_3 D + B_1 L + B_4 U + B_2 Z + B_4 P) = 0$$

$$(3.33)\quad -a^{+}_{\underline{k}+\underline{Q}1-}(\epsilon_{\underline{k}+\underline{Q}1-} - E_{\underline{k}} + B_4 F + B_2 N + B_2 Y + B_1 Z + B_3 P + B_4 O + B_3 P) = 0$$

$$(3.34)\quad -a^{+}_{\underline{k}2+}(\epsilon_{\underline{k}2+} - E_{\underline{k}} + B_5 E + B_7 M + B_8 K + B_8 T + B_6 R) = 0$$

$$(3.35)\quad -a^{+}_{\underline{k}2-}(\epsilon_{\underline{k}2-} - E_{\underline{k}} + B_6 C + B_8 K \mp B_7 W + B_7 V + B_5 X) = 0$$

$$(3.36)\quad -a^{+}_{\underline{k}+\underline{Q}2+}(\epsilon_{\underline{k}+\underline{Q}2+} - E_{\underline{k}} + B_7 E + B_5 M + B_6 K + B_6 T + B_8 R) = 0$$

$$(3.37)\quad -a^{+}_{\underline{k}+\underline{Q}2-}(\epsilon_{\underline{k}+\underline{Q}2-} - E_{\underline{k}} + B_8 C + B_6 K + B_5 W + B_5 V + B_7 S) = 0$$

where

$$S = 0,\ P+Y = Z,\ N = L,\ T = K,\ K+T = W+V,\ P = Y = X$$

Thus by making the determinant of the coefficients equal to zero (the condition for the simultaneous solution of these eight homogeneous equations in eight unknowns, (3.30) - 3.37)) the following determinental secular equation for the "general magnetic state" with all the previously discussed correlations included is:

$$
\begin{array}{|c|c|c|c|}
\hline
\begin{array}{l} N(\epsilon_{\underline{k}}-E_{\underline{k}}) \\ +KA(o--11) \\ +KA(o--22) \\ +(K-J)A(o++22) \end{array} & -2KA(o-+11) & \begin{array}{l} KA(\underline{Q}-+11) \\ +KA(\underline{Q}--22) \\ +(K-J) \\ \quad A(\underline{Q}++22) \end{array} & -KA(\underline{Q}-+11) \\
\hline
-2KA(o-+11) & \begin{array}{l} N(\epsilon_{\underline{k}}-E_{\underline{k}}) \\ +KA(o++11) \\ +KA(o++22) \\ +(K-J) \\ \quad A(o--22) \end{array} & -KA(\underline{Q}-+11) & \begin{array}{l} KA(\underline{Q}++11) \\ +KA(\underline{Q}++22) \\ +(K-J) \\ \quad A(\underline{Q}--22) \end{array} \\
\hline
\begin{array}{l} KA(\underline{Q}--11) \\ +KA(\underline{Q}--22) \\ +(K-J) \\ \quad A(\underline{Q}++22) \end{array} & -KA(\underline{Q}-+11) & \begin{array}{l} N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}) \\ +KA(o--11) \\ +KA(o--22) \\ +(K-J) \\ \quad A(o++22) \end{array} & -2KA(o-+11) \\
\hline
 & \begin{array}{l} KA(\underline{Q}++11) \\ +KA(\underline{Q}++22) \\ +(K-J) \\ \quad A(\underline{Q}--22) \end{array} & & \begin{array}{l} N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}) \\ +KA(o++11) \\ +KA(o++22) \\ +(K-J)A(o--22) \end{array} \\
\hline
\end{array}
$$

(3.38)

$$
= 0
$$

$$
\begin{array}{|c|c|c|c|}
\hline
 & & \begin{array}{l} N(\epsilon_{\underline{k}}-E_{\underline{k}}) \\ +KA(o--11) \\ +KA(o--22) \\ +(K-J) \\ \quad A(o++11) \end{array} & -KA(o+-22) \\
\hline
 & & -KA(o+-22) & \begin{array}{l} N(\epsilon_{\underline{k}}-E_{\underline{k}}) \\ +KA(o++11) \\ +KA(o++22) \\ +(K-J)A(o--11) \end{array} \\
\hline
 & & \begin{array}{l} KA(\underline{Q}--11) \\ +KA(\underline{Q}--22) \\ +(K-J) \\ \quad A(\underline{Q}++11) \end{array} & -2KA(\underline{Q}-+22) \\
\hline
 & & -2KA(\underline{Q}-+22) & \begin{array}{l} KA(\underline{Q}++11) \\ +KA(\underline{Q}++22) \\ +(K-J) \\ \quad A(\underline{Q}--11) \end{array} \\
\hline
\end{array}
$$

$$
\begin{array}{|c|c|c|c|}
\hline
\begin{array}{l} N(\epsilon_{\underline{k}}-E_{\underline{k}}) \\ +KA(o--11) \\ +KA(o--22) \\ +(K-J) \\ \quad A(o++11) \end{array} & -KA(o+-22) & \begin{array}{l} KA(\underline{Q}--11) \\ +KA(\underline{Q}--22) \\ +(K-J) \\ \quad A(\underline{Q}++11) \end{array} & -2KA(\underline{Q}-+22) \\
\hline
-KA(o+-22) & \begin{array}{l} N(\epsilon_{\underline{k}}-E_{\underline{k}}) \\ +KA(o++11) \\ +KA(o++22) \\ +(K-J)A(o--11) \end{array} & -2KA(\underline{Q}-+22) & \begin{array}{l} KA(\underline{Q}++11) \\ +KA(\underline{Q}++22) \\ +(K-J) \\ \quad A(\underline{Q}--11) \end{array} \\
\hline
\begin{array}{l} KA(\underline{Q}--11) \\ +KA(\underline{Q}--22) \\ +(K-J) \\ \quad A(\underline{Q}++11) \end{array} & -2KA(\underline{Q}-+22) & \begin{array}{l} N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}) \\ +KA(o--11) \\ +KA(o--22) \\ +(K-J) \\ \quad A(o++11) \end{array} & -KA(o-+22) \\
\hline
-2KA(\underline{Q}-+22) & \begin{array}{l} KA(\underline{Q}++11) \\ +KA(\underline{Q}++22) \\ +(K-J) \\ \quad A(\underline{Q}--11) \end{array} & -KA(o-+22) & \begin{array}{l} N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}) \\ +KA(o++11) \\ +KA(o++22) \\ +(K-J) \\ \quad A(o--11) \end{array} \\
\hline
\end{array}
$$

In the two-fold degenerate AFM case we know the correlation functions relations:

(3.39) $A(o--22) = A(o--11) = A(o++11) = A(o++22) \equiv A(o--) \neq 0$

$A(\underline{Q}++11) = A(\underline{Q}++22) = A(\underline{Q}--11) = A(\underline{Q}--22) \equiv A(\underline{Q}--) \neq 0$

All other correlations are zero.

(3.40)

$\equiv 0$

$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+(3K-J)$ $A(o--)$ $\equiv 11$	0	12	0	33	0	12	0	33
0	$(3K-J)$ $A(\underline{Q}--)$ $\equiv 12$	0	$N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}})$ $+(3K-J)$ $A(o--)$ $\equiv 33$	0	12	0	33
0	11	0	12	0	11	0	12
0	12	0	33	0	12	0	33

Here we have only two independent matrix element correlations, A(o--) and A($\underline{Q}$--) as defined in (3.39). The 33 term is equivalent to the 11 term. For brevity we have labeled redundant matrix elements by their row-column indices in the matrix format presented here. These indices bear no relation to the physical indices "1" or "2" in the A's, which are subband labels in this two-subband degenerate model.

In the two-fold degenerate PM case, the correlation functions are related as:

(3.41) $A(o{+}{+}11) = A(o{-}{-}11) = A(o{+}{+}22) = A(o{-}{-}22) \neq 0$

All other A's are identically zero.

There is only <u>one</u> independent matrix element since the 33 and 11 terms are again equivalent.

(3.42)

$$\begin{vmatrix} N(\epsilon_{\underline{k}}-E_{\underline{k}}) & & & \\ +(3K-J) & 0 & 0 & 0 \\ A(o--) & & & \\ \equiv 11 & & & \\ 0 & 11 & 0 & 0 \\ & & N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}) & \\ 0 & 0 & +(3K-J) & 0 \\ & & A(o--) & \\ & & \equiv 33 & \\ 0 & 0 & 0 & 33 \end{vmatrix} \quad \begin{vmatrix} & & & \\ & 0 & & \\ & & & \end{vmatrix}$$

$$\begin{vmatrix} & & & \\ & 0 & & \\ & & & \end{vmatrix} \quad \begin{vmatrix} 11 & 0 & 0 & 0 \\ 0 & 11 & 0 & 0 \\ 0 & 0 & 33 & 0 \\ 0 & 0 & 0 & 33 \end{vmatrix} = 0$$

In the two-fold degenerate FM case we have the following correlation function relations:

(3.43) $A(o--11) = A(o--22) \equiv A(o--) \neq 0$, $A(o++11) = A(o++22) \equiv A(o++) \neq 0$

All other A's are identically zero. There are <u>two</u> independent matrix elements, $A(o--\_$ and $A(o++)$. Thus, the 11 and 33 matrix elements are <u>not</u> equivalent.

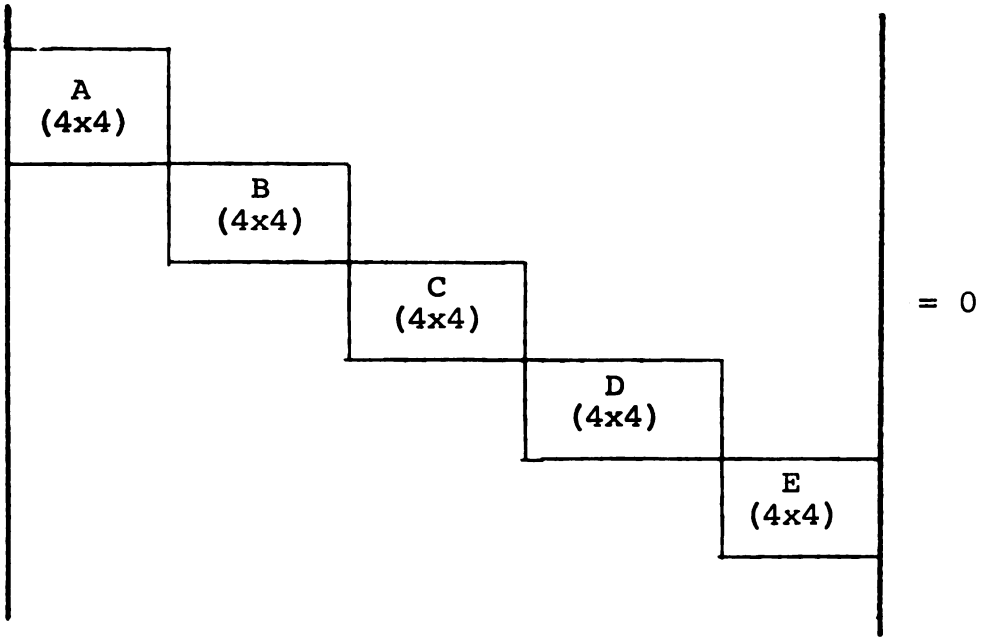
(3.44)

$$
\begin{vmatrix}
N(\epsilon_{\underline{k}}-E_{\underline{k}}) & & & \\
+2K\bar{A}(o--) & & & \\
+(K-J) & 0 & 0 & 0 \\
A(o++) & & & \\
\equiv 11 & & & \\
0 & 11 & 0 & 0 \\
0 & 0 & \begin{matrix} N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}}) \\ +2K\bar{A}(o++) \\ +(K-J) \\ A(o--) \\ \equiv 33 \end{matrix} & 0 \\
0 & 0 & 0 & 33
\end{vmatrix}
\begin{vmatrix}
 & & & \\
 & & & \\
 & & & \\
 & & & \\
 & & & \\
 & & & \\
 & & & \\
 & & & \\
 & & & \\
11 & 0 & 0 & 0 \\
0 & 11 & 0 & 0 \\
0 & 0 & 33 & 0 \\
0 & 0 & 0 & 33
\end{vmatrix}
= 0
$$

As it should be, we note that only the AFM state had $\underline{Q}$ dependent correlation functions in its secular equation.

We can easily generalize to the five-fold d-subband degeneracy problem by writing down the answer modeled after the two-fold results as shown in equation (3.44).

(We spread out the matrix subblocks on a few pages due to lack of room to include the 20 x 20 determinant.) There are five 4 x 4 subblocks. (Note that the symbols A, B, C, D, E, here are for the subblocks and just notational. They in no way should be mixed up with A's (correlation functions) or B's (linear combination coefficients) used before.) The subblocks of these subblocks have the correlation A; and, therefore, the coefficient B in them.



In the five-fold degenerate AFM case, the correlation functions are related as:

(3.45) $A(\underline{Q}++ii) = A(\underline{Q}--ii) \neq 0$, $A(o++ii) = A(o--ii) \neq 0$, $i = 1 \cdots 5$

There will be two independent A's, since 11 and 22 are equivalent. The 4 x 4 subblocks will be:

(3.46)

A =

$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+K\sum_{i=1}^{5} A(o--ii)$ $+(K-J)\sum_{i=2}^{5} A(o++ii)$ $\equiv 11$	0	$k\sum_{i=1}^{5} A(\underline{Q}--ii)$ $+(K-J)\sum_{i=2}^{5} A(\underline{Q}++ii)$ $\equiv 13$	0
0	$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+k\sum_{i=1}^{5} A(o++ii)$ $+(K-J)\sum_{i=2}^{5} A(o--ii)$ $\equiv 22$ $\equiv 11$	0	$K\sum_{i=1}^{5} A(Q++ii)$ $+(K-J)\sum_{i=2}^{5} A(\underline{Q}--ii)$ $\equiv 24$
13	0	11, but with $\epsilon_{\underline{k}+\underline{Q}}$ instead of $\epsilon_{\underline{k}}$	0
0	24	0	11, but with ϵ_{k+Q} instead of $\epsilon_{\underline{k}}$

(3.47)

$B =$

$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+K\sum_{i=1}^{5} a(o--ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 2}}^{5} A(o++ii)$ $=1,1'$	0	$K\sum_{i=1}^{5} A(Q--ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 2}}^{5} A(Q++ii)$ $\equiv 1,3'$	0
0	$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+K\sum_{i=1}^{5} A(o++ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 2}}^{5} A(o--ii)$ $=2,2'$	0	$K\sum_{i=1}^{5} A(Q++ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 2}}^{5} A(Q--ii)$ $=2,4'$
$1,3'$	0	$1,1'$ with $\epsilon_{\underline{k}+Q}$ in place of $\epsilon_{\underline{k}}$	0
0	$2,4'$	0	$2,2'$ but with $\epsilon_{\underline{k}+Q}$ in place of $\epsilon_{\underline{k}}$

(3.48)

$C =$

$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+K\sum_{i=1}^{5} A(o--ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 3}}^{5} A(o++ii)$ $\equiv 1,1"$	0	$K\sum_{i=1}^{5} A(\underline{Q}--ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 3}}^{5} A(Q++ii)$ $=1,3"$	0
0	$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+K\sum_{i=1}^{5} A(o++ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 3}}^{5} A(o--ii)$ $=2,2"$	0	$K\sum_{i=1}^{5} A(\underline{Q}++ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 3}}^{5} A(\underline{Q}--ii)$ $=2,4"$
$1,3"$	0	$1,1"$ but with $\epsilon_{\underline{k}+\underline{Q}}$ replacing $\epsilon_{\underline{k}}$	0
0	$2,4"$	0	$2,2"$ but with $\epsilon_{\underline{k}+\underline{Q}}$ replacing $\epsilon_{\underline{k}}$

(3.49)

$D =$

$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+K\sum_{i=1}^{5} A(o++ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 4}}^{5} A(o++ii)$ $=1,1'''$	0	$K\sum_{i=1}^{5} A(\underline{Q}--ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 4}}^{5} A(Q++ii)$ $=1,3'''$	0
0	$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+K\sum_{i=1}^{5} A(o++ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 4}}^{5} A(o--ii)$ $=2,2'''$	0	$K\sum_{i=1}^{5} A(Q++ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 4}}^{5} A(\underline{Q}--ii)$ $=2,4'''$
$1,3'''$	0	$1,1'''$ but with $\epsilon_{\underline{k}+\underline{Q}}$ replacing $\epsilon_{\underline{k}}$	0
0	$2,4'''$	0	$2,2'''$ but with $\epsilon_{\underline{k}+\underline{Q}}$ replacing $\epsilon_{\underline{k}}$

(3.50)

$E=$

$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+K\sum_{i=1}^{5} A(o--ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 5}}^{5} A(o++ii)$ $\equiv 1,1''''$	0	$K\sum_{i=1}^{5} A(\underline{Q}--ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 5}}^{5} A(\underline{Q}++ii)$ $=1,3''''$	0
0	$N(\epsilon_{\underline{k}}-E_{\underline{k}})$ $+K\sum_{i=1}^{5} A(o++ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 5}}^{5} A(o--ii)$ $=2,2''''$	0	$K\sum_{i=1}^{5} A(\underline{Q}++ii)$ $+(K-J)\sum_{\substack{i=1\\ i\neq 5}}^{5} A(\underline{Q}--ii)$ $=2,4''''$
$1,3''''$	0	$1,1''''$ but with $\epsilon_{\underline{k}+\underline{Q}}$ replacing $\epsilon_{\underline{k}}$	0
0	$2,4''$	0	$2,2''''$ but with $\epsilon_{\underline{k}+\underline{Q}}$ replacing $\epsilon_{\underline{k}}$

For the FM state in the five-fold d-subband degeneracy problem, the correlation functions are related:

$$(3.51)\quad A(o--) \equiv A(o--ii) \neq 0,\ A(o++) \equiv A(o++ii) \neq 0$$

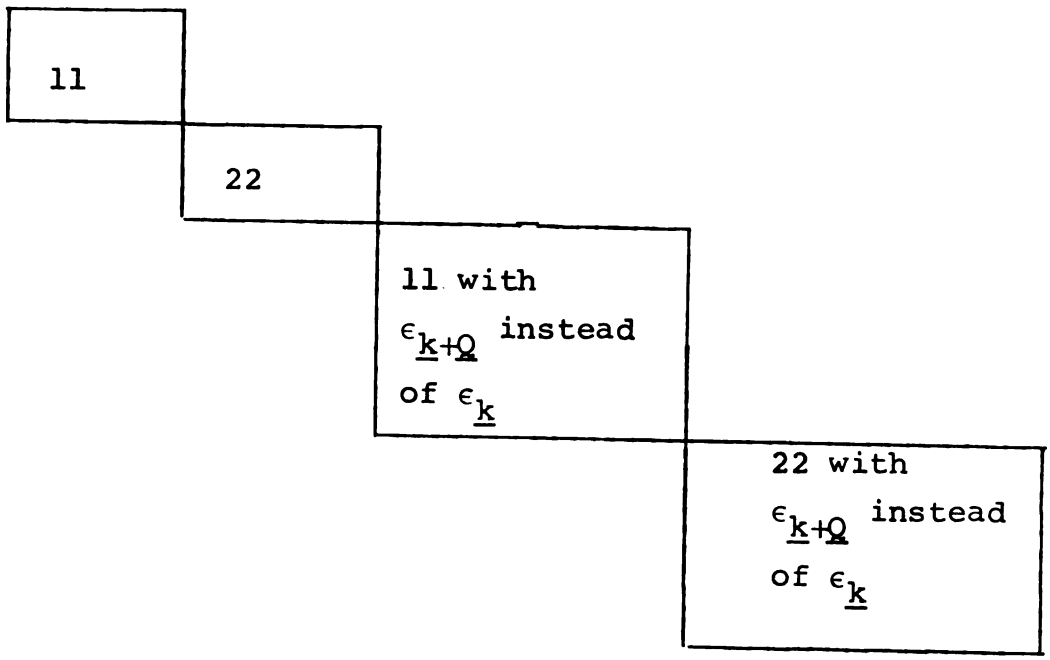
All other A's are identically zero. There are two independent correlations as in the two orbit case, A(o--) and A(o++ , but there are three more of each since 11 and 22 terms are not equivalent. We find a diagonal 20 x 20 secular determinant with five subblocks.

(3.52)

$$A = \begin{array}{|l|l|l|l|}
\hline
N(\epsilon_{\underline{k}}-E_{\underline{k}}) & & & \\
+(9K-4J) & & & \\
A(o++) & & & \\
\equiv 11 & & & \\
\hline
 & N(\epsilon_{\underline{k}}-E_{\underline{k}}) & & \\
 & +5KA(o++) & & \\
 & +4(K-J)A(o--) & & \\
 & \equiv 22 & & \\
\hline
 & & 11 \text{ with } \epsilon_{\underline{k}+\underline{Q}} \text{ replacing } \epsilon_{\underline{k}} & \\
\hline
 & & & 11 \text{ with } \epsilon_{\underline{k}+\underline{Q}} \text{ replacing } \epsilon_{\underline{k}} \\
\hline
\end{array}$$

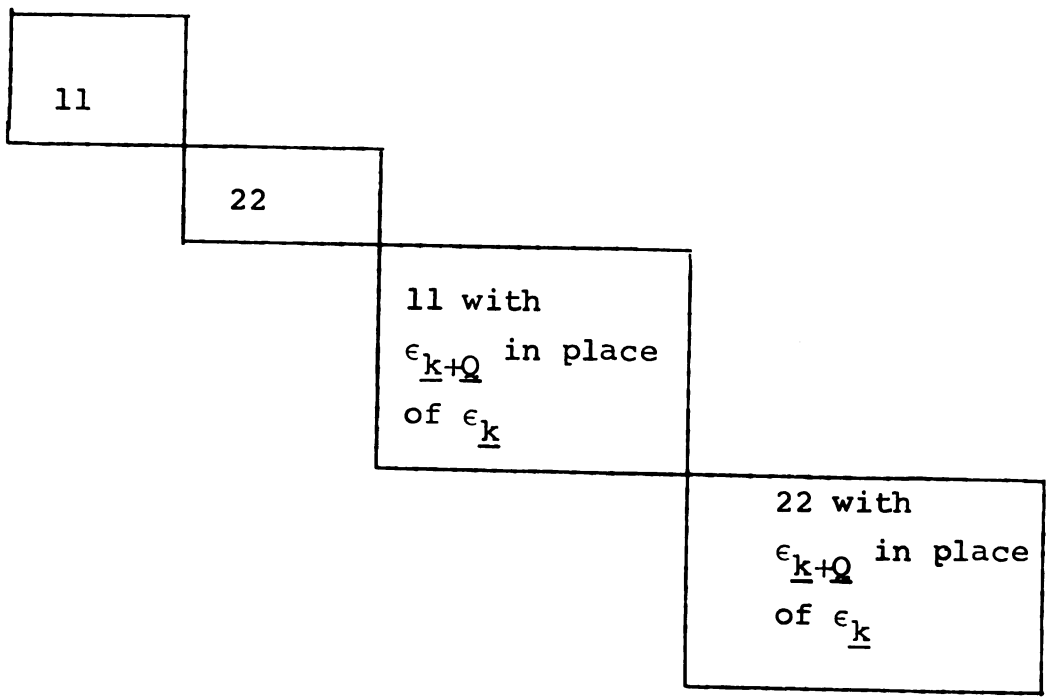
(3.53)

$B =$


11
22
11 with
$\epsilon_{\underline{k}+\underline{Q}}$ instead
of $\epsilon_{\underline{k}}$
22 with
$\epsilon_{\underline{k}+\underline{Q}}$ instead
of $\epsilon_{\underline{k}}$

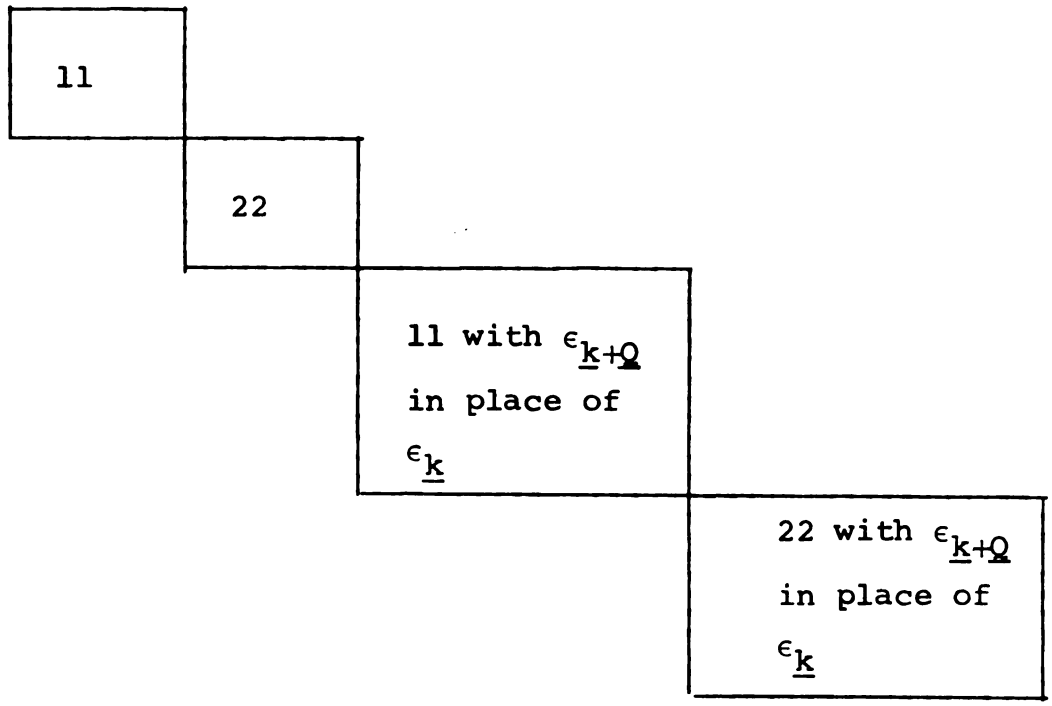
(3.54)

$C =$

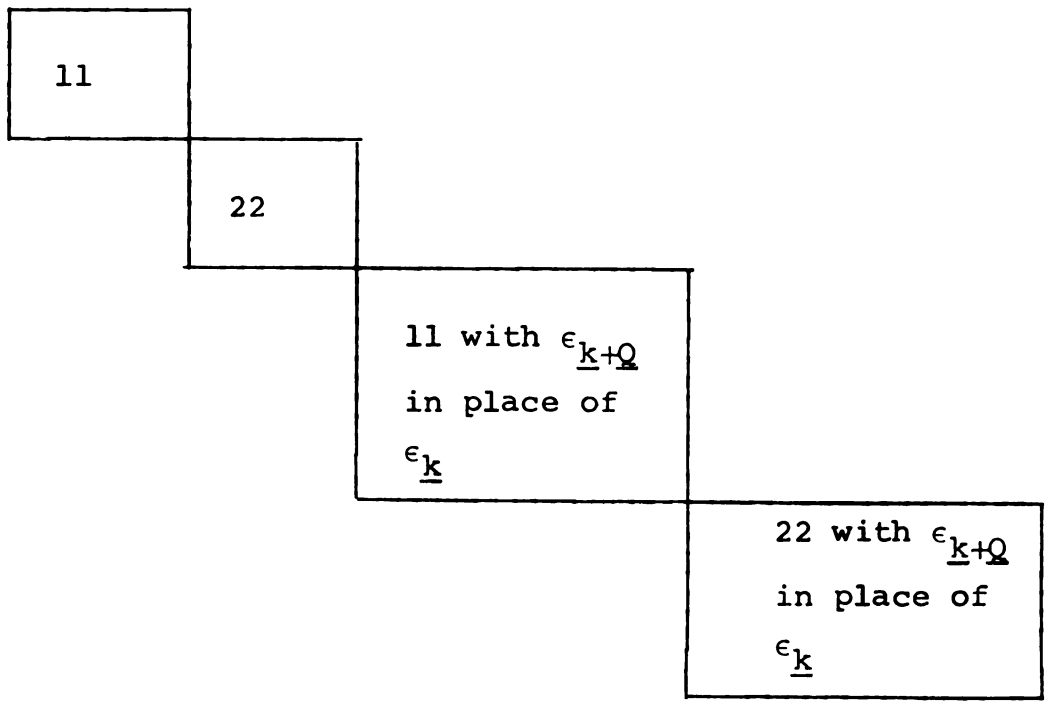

11
22
11 with
$\epsilon_{\underline{k}+\underline{Q}}$ in place
of $\epsilon_{\underline{k}}$
22 with
$\epsilon_{\underline{k}+\underline{Q}}$ in place
of $\epsilon_{\underline{k}}$

(3.55)

D =



E =



Subblocks A through E are all the same here.

For the PM state in the five-fold d-subband degeneracy problem, the correlation functions are related:

$$(3.57)\quad A(o{+}{+}ii) = A(o{-}{-}ii) \equiv A(o{+}{+}) \neq 0$$

All other A's are identically zero. There is one independent correlation function, A(o++), but there are four more of them. We find a diagonal 20 x 20 secular determinant with five exactly identical subblocks:

(3.58)

$$A = \begin{vmatrix} N(\epsilon_{\underline{k}} - E_{\underline{k}}) + (9K-4J)A(o{+}{+}) = 11 & & & \\ & 11 & & \\ & & 11 \text{ with } \epsilon_{\underline{k}+\underline{Q}} \text{ replacing } \epsilon_{\underline{k}} & \\ & & & 11 \text{ with } \epsilon_{\underline{k}+\underline{Q}} \text{ replacing } \epsilon_{\underline{k}} \end{vmatrix}$$

The following subblocks are identical.

(3.59) $B = A$

(3.60) $C = A$

(3.61) $D = A$

(3.62) $E = A$

We can transform the AFM 20 x 20 secular determinant for the five-fold degenerate subband case into block form as follows: Each of the five 4 x 4 subblocks of the 20 x 20 determinant can be changed from:

(3.63)
$$\begin{vmatrix} A & O & B & O \\ O & C & O & D \\ E & O & F & O \\ O & G & O & H \end{vmatrix}$$

into:

(3.64)
$$\begin{vmatrix} A & O & B & O \\ E & O & F & O \\ O & C & O & D \\ O & G & O & H \end{vmatrix}$$

and then into:

(3.65)
$$\begin{vmatrix} A & B & O & O \\ E & F & O & O \\ O & O & C & D \\ O & O & G & H \end{vmatrix}$$

by permuting the rows and columns. The resulting minus signs have no meaning since the secular equation is homogeneous, and the minus signs factor out of the whole 20 x 20 secular determinant. (Note that A, B, C, D, E, F, G, H here are just notations for the elements of a 4 x 4 subblock. They are in no way related to the same symbols that were used before for correlations and for terms in our development of a shorthand expression for $V^{(2)}_{Bloch}$ in (3.15) before we did the commutations in (3.16) - (3.29).)

We thus get, putting $A(o{+}{+}ii) = A(o{-}{-}ii) \equiv A(o{+}{+}) \neq 0$ and $A(\underline{Q}{+}{+}ii) = A(\underline{Q}{-}{-}ii) = A(\underline{Q}{+}{+}) \neq 0$, five identical 4 x 4 subblocks for the 20 x 20 AFM five-fold d-subband degeneracy case:

(3.66)

$$A = \begin{array}{|c|c|} \hline N(\epsilon_k - E_k) + (9K-4J)A(o{+}{+}) \equiv 11 & (9K-4J)A(\underline{Q}{+}{+}) \equiv 12 \\ \hline 12 & N(\epsilon_{\underline{k}+\underline{Q}} - E_{\underline{k}}) + (9K-4J)A(o{+}{+}) \equiv 22 \\ \hline \end{array}$$

(3.67) $B = A$

(3.68) $C = A$

(3.69) $D = A$

(3.70) $E = A$

We now proceed to find the eigenvalues and total energies by expanding out our six determinental secular equations. Three are for the AFM, PM and FM two-fold degeneracy case. Three are for the AFM, PM and FM five-fold degeneracy case. We will then solve the resulting equations for the eight or twenty roots as the case may be (two or five-fold degeneracy respectively), and sum those roots to get the total energy for an electron in state $\underline{k}$, $E_{\underline{k}}$.

Before we do this, we note that the five-fold degeneracy case for the AFM, PM, and FM states has a seemingly complex 20 x 20 secular determinant. However, this determinant is already diagonal in the PM and FM cases with only a few independent elements. It is easily diagonalizable in the AFM case when the 4 x 4 subblocks are all transformed to diagonal block form. We will not attempt Penn's SSDW or FIM states in the two- or five-fold degenerate case since the 20 x 20 secular matrix would be difficult to diagonalize. Also, the existence of these two states in real transition metals is in some doubt (except for Overhauser's work in chromium). The AFM, PM and FM are the most common transition metal magnetic states.

The secular equation for the five-fold degenerate PM state reduces to:

$$(3.71)\quad [N(\epsilon_{\underline{k}}-E_{\underline{k}})+(9K-4J)A(o++)]^{10}\cdot[N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}})+(9K-4J)A(o++)]^{10} = 0$$

There are ten roots of form:

$$(3.72)\quad \epsilon_{\underline{k}} + \frac{(9K-4J)}{N} A(o{+}{+}) = E_{\underline{k}}^{(1-10)}$$

and ten roots of form:

$$(3.73)\quad \epsilon_{\underline{k}+\underline{Q}} + \frac{(9K-4J)}{N} A(o{+}{+}) = E_{\underline{k}}^{(11-20)}$$

which are the same.

The secular equation for the five-fold degenerate FM state reduces to:

$$(3.74)\quad [N(\epsilon_{\underline{k}}-E_{\underline{k}})+5K(Ao{-}{-})+4(K-J)A(o{+}{+})]^5\cdot[N(\epsilon_{\underline{k}}-E_{\underline{k}})+5KA(o{+}{+})$$
$$+4(K-J)A(o{-}{-})]^5\cdot[N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}})+5KA(o{-}{-})+4(K-J)A(o{+}{+})]^5\cdot$$
$$[N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}})+5KA(o{+}{+})+4(K-J)A(o{-}{-})]^5 = 0$$

There are five roots of form:

$$(3.75)\quad E_{\underline{k}}^{(1-5)} = \epsilon_{\underline{k}} + \frac{5K}{N} A(o{-}{-}) + \frac{4(K-J)}{N} A(o{+}{+})$$

five roots of form:

$$(3.76)\quad E_{\underline{k}}^{(6-10)} = \epsilon_{\underline{k}} + \frac{5K}{N} A(o{+}{+}) + \frac{4(K-J)}{N} A(o{-}{-})$$

five roots to form:

$$(3.77)\quad E_{\underline{k}}^{(11-15)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{5K}{N} A(o{-}{-}) + \frac{4(K-J)}{N} A(o{+}{+})$$

and five roots of form:

$$(3.78)\quad E_{\underline{k}}^{(16-20)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{5K}{N} A(o{+}{+}) + \frac{4(K-J)}{N} A(o{-}{-})$$

The secular equation in the five-fold degenerate FM state is:

$$(3.79)\quad [(11)(22) - (12)^2]^{10} = 0$$

which becomes:

$$(3.80)\quad \{[N(\epsilon_{\underline{k}}-E_{\underline{k}})+(9K-4J)A(o++)]\cdot[N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}})+(9K-4J)A(o++)]-[(9K-4J)A(\underline{Q}++)]^2\}^{10} = 0$$

The solution expanding this out yields:

$$(3.81)\quad E_{\underline{k}}{}^2N^2+E_{\underline{k}}[-N^2\epsilon_{\underline{k}}-N^2\epsilon_{\underline{k}+\underline{Q}}-2N(9K-4J)A(o++)]+[-(9K-4J)(N\epsilon_{\underline{k}}+N\epsilon_{\underline{k}+\underline{Q}})Ao++)+(9K-4J)^2][A^2(o++)+N^2\epsilon_{\underline{k}}\epsilon_{\underline{k}+\underline{Q}}+(9K-4J)^2][A^2(\underline{Q}++)] = 0$$

Thus, the two groups of ten roots apiece are of form:

$$(3.82)\quad E_{\underline{k}}^{(i)} = N^2\epsilon_{\underline{k}}+N^2\epsilon_{\underline{k}+\underline{Q}}+2N(9K-4J)A(o++)$$

$$\pm\frac{1}{2N^2}\sqrt{[-N^2\epsilon_{\underline{k}}-N^2\epsilon_{\underline{k}+\underline{Q}}-2N(9K-4J)A(o++)]^2-4N^2[-(9K-4J)(N\epsilon_{\underline{k}}+N\epsilon_{\underline{k}+\underline{Q}})A(o++)+N^2\epsilon_{\underline{k}}\epsilon_{\underline{k}+\underline{Q}}+(9K-4J)^2][A^2(o++)+A^2(\underline{Q}++)]}$$

$$= \frac{\epsilon_{\underline{k}}}{2} + \frac{\epsilon_{\underline{k}+\underline{Q}}}{2} + \frac{(9K-4J)}{N}A(o++) \pm \frac{1}{2N^2}\sqrt{\text{square root above}}$$

There are ten roots $E_{\underline{k}}^{(i)}$ with the minus sign and then roots $E_{\underline{k}}^{(i)}$ with the plus sign.

Since the band is split in the AFM case, for the less-than or just half-filled band case, $(1/2\ n/2N \leq 1/2)$, we take all twenty roots with the minus sign.

The secular equation for the two-fold degenerate PM state is:

$$(3.83)\quad [N(\epsilon_{\underline{k}}-E_{\underline{k}})+(3K-J)A(o{+}{+})]^2\cdot[N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}})+(3K-J)A(o{+}{+})]^2\mp 0$$

There are four roots of form:

$$(3.84)\quad E_{\underline{k}}^{(1-4)} = \epsilon_{\underline{k}} + \frac{(3K-J)}{N} A(o{+}{+})$$

and four roots of form:

$$(3.85)\quad E_{\underline{k}}^{(5-8)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{(3K-J)}{N} A(o{+}{+})$$

The secular equation for the two-fold degenerate FM state is:

$$\begin{aligned}(3.86)\quad & [N(\epsilon_{\underline{k}}-E_{\underline{k}})+2KA(o{-}{-})+(K-J)A(o{+}{+})]^2\cdot[N(\epsilon_{\underline{k}}-E_{\underline{k}})+2KA(o{+}{+}) \\ & +(K-J)A(o{+}{+})]^2\cdot[N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}})+2KA(o{-}{-})+(K-J)A(o{+}{+})]^2\cdot \\ & [N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}})+2KA(o{+}{+})+(K-J)A(o{-}{-})]^2 = 0\end{aligned}$$

There are two roots of form:

$$(3.87)\quad E_{\underline{k}}^{(1,2)} = \epsilon_{\underline{k}} + \frac{2K}{N} A(o{-}{-}) + \frac{(K-J)}{N} A(o{+}{+})$$

two of form:

$$(3.88)\quad E_{\underline{k}}^{(3,4)} = \epsilon_{\underline{k}} + \frac{2K}{N} A(o{+}{+}) + \frac{(K-J)}{N} A(o{-}{-})$$

two of form:

$$(3.89)\quad E_{\underline{k}}^{(5,6)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{2K}{N} A(o{-}{-}) + \frac{(K-J)}{N} A(o{+}{+})$$

and two of form:

$$(3.90)\quad E_{\underline{k}}^{(7,8)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{2K}{N} A(o{+}{+}) + \frac{(K-J)}{N} A(o{-}{-})$$

The secular equation for the two-fold degenerate AFM state is:

$$(3.91)\quad [(11)(22)-(12)^2]^4 = 0$$

This becomes:

$$(3.92)\quad \{[N(\epsilon_{\underline{k}}-E_{\underline{k}})-(3K-J)A(o{+}{+})]\cdot[N(\epsilon_{\underline{k}+\underline{Q}}-E_{\underline{k}})+(3K-J)A(o{+}{+})] -[(3K-J)^2[A(\underline{Q}{+}{+})]^2]^2\}^4 = 0$$

There are four roots of form:

$$(3.93)\quad E_{\underline{k}}^{(1-4)} = \frac{\epsilon_{\underline{k}}}{2} + \frac{\epsilon_{\underline{k}+\underline{Q}}}{2} + \frac{(3K-J)}{2N}A(o{+}{+}) + \frac{1}{2\cdot 2N^2}\cdot \sqrt{\begin{array}{l}[N\epsilon_{\underline{k}}+N\epsilon_{\underline{k}+\underline{Q}}+2N(3K-J)A(o{+}{+})]^2-4N^2[N^2\epsilon_{\underline{k}}\epsilon_{\underline{k}+\underline{Q}}+(3K-J)^2 \\ [A^2(o{+}{+})+A^2(\underline{Q}{+}{+})]-(3K-J)(N\epsilon_{\underline{k}}+N\epsilon_{\underline{k}}+N\epsilon_{\underline{k}+\underline{Q}})A(o{+}{+})\end{array}}$$

and four of form:

$$(3.94)\quad E_{\underline{k}}^{(5-8)} = \frac{\epsilon_{\underline{k}}}{2} + \frac{\epsilon_{\underline{k}+\underline{Q}}}{2} + \frac{(3K-J)}{2N}A(o{+}{+}) - \frac{1}{2\cdot 2N^2}\cdot \sqrt{\text{square root above}}$$

In this chapter, the two-fold degenerate problem is worked out and the answers are included for completeness. It is the five-fold degenerate case which is of actual physical interest. We have patterned our five-fold degenerate case's 20 x 20 secular equation after the two-fold degenerate case's 8 x 8 secular equation. We then worked out all the corresponding expressions in the two- and five-fold cases separately and independently, as a check on one another since they should always be of similar form with proportional coefficients.

Before continuing, it is important to illustrate the physical meaning of the expressions for the total energy of state $\underline{k}$ which

will be seen in equations (3.137), (3.138), (3.139), (3.140), (3.141), and (3.142). They are all sums over the roots of the secular equations, taking into account each root and summing it over the two- or five- orbital states that an electron could be in. Each expression $E_{\underline{k}}$ total is the total energy of an electron in state $\underline{k}$. These would add up to give the total energy (minus some corrections for double counting derived later on) of a magnetic state as follows. Each spin on a particular site is composed of a sum of the electron spins on each site. Each electron is labeled by a wave vector $\underline{k}$, implying which state it is in. For example, a totally FM array might look like (with 100% spin polarization):

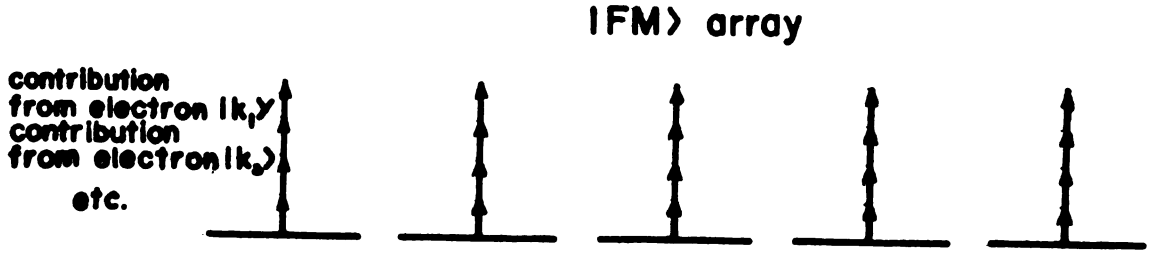


Figure 6. Itinerant Electron Contributions to FM Array.

A PM array might look like:

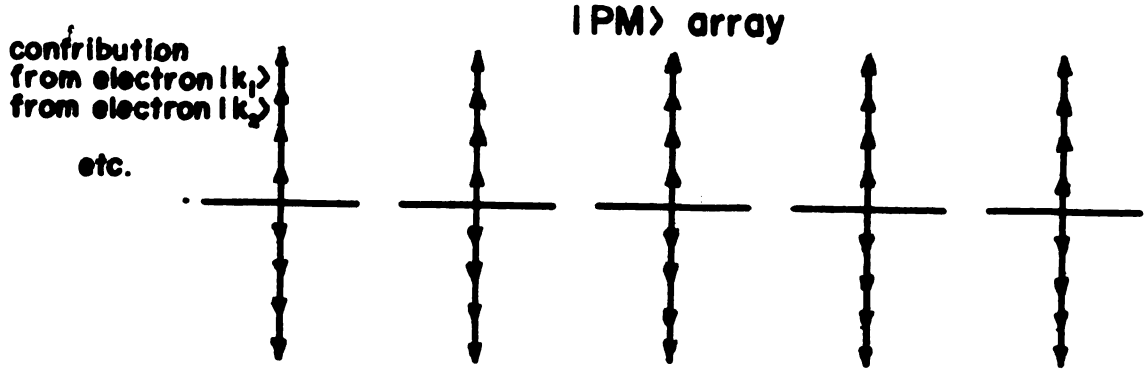


Figure 7. Itinerant Electron Contributions to PM Array.

and an AFM array might look like:

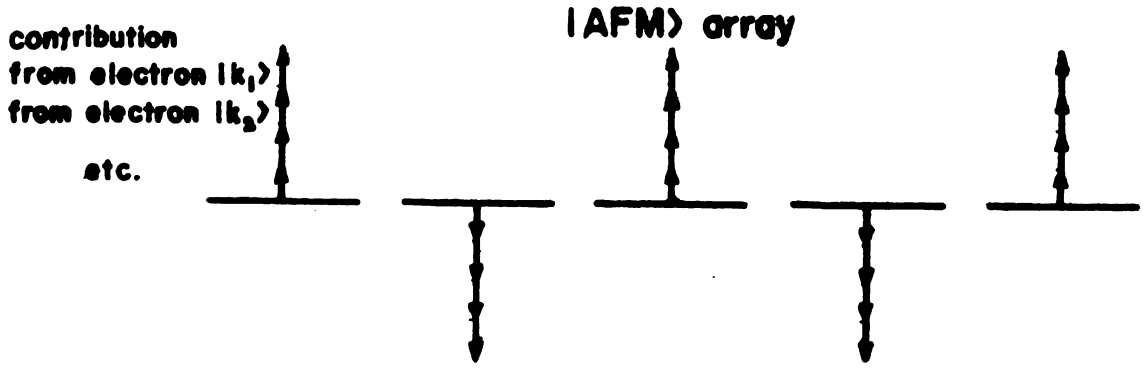


Figure 8. Itinerant Electron Contributions to AFM Array.

As we have stated before, in the AFM state, $\underline{Q}$ occurs. Therefore, it also appears in the AFM correlation function. $A(\underline{Q}...)$ will be seen for AFM only. This means that the AFM wave function has an $e^{i\underline{Q}\cdot\underline{r}} = e^{i\underline{\pi}\cdot\underline{r}}$ term in our simple cubic lattice, so the spin contribution is flipped in sign on alternating sites as $e^{i\underline{\pi}\cdot\underline{r}}$ oscillates between ± 1. This yields the AFM array seen in Fig. 8. In this regard, Penn took exactly the same approach.

We must now generalize Penn's original definitions of the correlation functions, A, in terms of the linear combinations, B, to our two- and five-fold degenerate cases where the B's could be functions of $\underline{k}$ in general. The two-orbit general state have a wave function as a linear combination of eight terms; hence, eight B's. The five-orbit general state had a wave function as a linear combination of twenty terms; hence, twenty B's.

For the two-fold degenerate case, we generalize equations (2.91) - (2.96) to:

$$(3.95)\quad A(o+-) = \sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (B_1B_2+B_3B_4+B_5B_6+B_7B_8)$$

$$(3.96)\quad A(o++) = \sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (B_2^2+B_4^2+B_6^2+B_8^2)$$

$$(3.97)\quad A(o--) = \sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (B_1^2+B_3^2+B_5^2+B_7^2)$$

$$(3.98)\quad A(Q+-) = \sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (B_1B_4+ B_2B_3 + B_5B_8+B_6B_7)$$

$$(3.99)\quad A(Q++) = \sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (B_2B_4+B_6B_8)$$

$$(3.100)\quad A(Q--) = \sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (B_1B_3+B_5B_7)$$

We do not include the 11, 12, 21, or 22 combinations for the orbital indices since each A is either for orbit 1 or orbit 2. Therefore, 11 = 22 and 12 and 21 orbital correlations have been purposely neglected, as mentioned previously. Also, the 1/N and "-" factors are excluded, contrary to Penn's work, so that we may carry them along explicitly. Similarly, the interaction coupling coefficients, K (Penn's Co), and J are not included in Penn's work.

For the five-fold degenerate case, we generalize equations (2.91) - (2.96) to:

$$(3.101)\quad A(o+-) = \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}\,(B_1B_2+B_3B_4+B_5B_6+B_7B_8+B_9B_{10}+B_{11}B_{12}$$

$$+B_{12}B_{13}+B_{13}B_{14}+B_{15}B_{16}+B_{17}B_{18}+B_{19}B_{20})$$

$$(3.102)\quad A(o++) = \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2+B_6^2+B_8^2+B_{10}^2+B_{12}^2+B_{14}^2$$

$$+B_{16}^2+B_{18}^2+B_{20}^2)$$

$$(3.103)\quad A(o--) = \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1^2+B_3^2+B_5^2+B_7^2+B_9^2+B_{11}^2+B_{13}^2$$

$$+B_{15}^2+B_{17}^2+B_{19}^2)$$

$$(3.104)\quad A(Q+-) = \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_4+B_2B_3+B_5B_8+B_6B_7+B_9B_{12}+B_{10}B_{11}$$

$$+B_{13}B_{16}+B_{14}B_{15}+B_{17}B_{20}+B_{18}B_{19})$$

$$(3.105)\quad A(Q++) = \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2B_4+B_6B_8+B_{10}B_{12}+B_{14}B_{16}+B_{18}B_{20})$$

$$(3.106)\quad A(Q--) = \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_3+B_5B_7+B_9B_{11}+B_{13}B_{15}+B_{17}B_{19})$$

We can rewrite these as:

$$(3.101)\quad A(o+-) = \sum_{i=1\ \text{odd}}^{19} \sum_{\underline{k}} F_{\underline{k}}/N\ (B_iB_{i+1})$$

$$(3.102)\quad A(o++) = \sum_{i=1\ \text{even}}^{20} \Sigma F_{\underline{k}}/N\ B_i^2$$

$$(3.103)\quad A(o--) = \sum_{i=1\ \text{odd}}^{20} \sum_{\underline{k}} F_{\underline{k}}/N\ B_i^2$$

$$(3.104)\quad A(Q+-) = \sum_{i=1\ \text{odd}}^{20} \sum_{\underline{k}} F_{\underline{k}}/N(B_iB_{i+3}+B_{i+2}B_{i+1})$$

$$(3.105)\quad A(Q++) = \sum_{i=1\ \text{even}}^{20} \sum_{\underline{k}} F_{\underline{k}}/N(B_iB_{i+2})$$

$$(3.106)\quad A(Q--) = \sum_{i=1\ \text{odd}}^{19} \sum_{\underline{k}} F_{\underline{k}}/N\ (B_iB_{i+2})$$

where these i's have no relation to the lattice coordinate i's used before. They are just dummy indices to be summer over.

There are certain simple relations between the B's which come out when we put in the relations between the correlation functions, A, using (3.95) - (3.106).

In the two-fold degenerate PM case we have:

$$(3.107)\quad A(o--) = A(o++) \text{ leads to } \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1^2+B_3^2+B_5^2+B_7^2)$$
$$= \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2+B_6^2+B_8^2)$$

$$(3.108)\quad A(o+-) = 0 \text{ leads to } \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_2+B_3B_4+B_5B_6+B_7B_8)=0$$

$$(3.109)\quad A(\underline{Q}+-) = 0 \text{ leads to } \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_4+B_2B_3+B_5B_8+B_6B_7)=0$$

$$(3.110)\quad A(\underline{Q}++) = 0 \text{ leads to } \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2B_4+B_6B_8) = 0$$

$$(3.111)\quad A(\underline{Q}--) = 0 \text{ leads to } \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_3+B_5B_7) = 0$$

In the two-fold degenerate FM case we have:

$$(3.112)\quad A(o+-) = 0 \text{ leads to } \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_2+B_3B_4+B_5B_6+B_7B_8)=0$$

$$(3.113)\quad A(\underline{Q}+-) = 0 \text{ leads to } \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_4+B_2B_3+B_5B_8+B_6B_7)=0$$

$$(3.114)\quad A(\underline{Q}++) = 0 \text{ leads to } \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2B_4+B_6B_8) = 0$$

$$(3.115)\quad A(\underline{Q}--) = 0 \text{ leads to } \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_3+B_5B_7) = 0$$

In the two-fold degenerate AFM case we have:

(3.116) $A(o+-) = 0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_2+B_3B_4+B_5B_6+B_7B_8)=0$

(3.117) $A(\underline{Q}+-) = 0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_4+B_2B_3+B_5B_8+B_6B_7)=0$

(3.118) $A(\underline{Q}++) = A(\underline{Q}--)$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2B_4+B_6B_8) =$

$\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_3+B_5B_7)$

In the five-fold degenerate PM case we have:

(3.119) $A(o--)=A(o++)$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1^2+B_3^2+B_5^2+B_7^2+B_9^2$

$+B_{11}^2+B_{13}^2+B_{15}^2+B_{17}^2+B_{19}^2)= \frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2^2+B_4^2+B_6^2+B_8^2$

$+B_{10}^2+B_{12}^2+B_{14}^2+B_{16}^2+B_{18}^2+B_{20}^2)$

(3.120) $A(o+-)=0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_2+B_3B_4+B_5B_6+B_7B_8+B_9B_{10}$

$+B_{11}B_{12}+B_{13}B_{14}+B_{15}B_{16}+B_{17}B_{18}+B_{19}B_{20})=0$

(3.121) $A(\underline{Q}+-)=0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_4+B_2B_3+B_5B_8+B_6B_7+B_9B_{12}$

$+B_{13}B_{16}+B_{14}B_{15}+B_{17}B_{20}+B_{18}B_{19})=0$

(3.122) $A(\underline{Q}++)=0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2B_4+B_6B_8+B_{10}B_{12}+B_{14}B_{16}$

$+B_{18}B_{20})=0$

(3.123) $A(\underline{Q}--)=0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_3+B_5B_7+B_9B_{11}+B_{13}B_{15}$

$+B_{17}B_{19})=0$

In the five-fold degenerate FM case we have:

(3.124) $A(o+-)=0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_2+B_3B_4+B_5B_6+B_7B_8+B_9B_{10}$

$+B_{11}B_{12}+B_{13}B_{14}+B_{15}B_{16}+B_{17}B_{18}+B_{19}B_{20})=0$

(3.125) $A(\underline{Q}+-)=0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_2+B_2B_3+B_5B_8+B_6B_7+$

$B_9B_{12}+B_{10}B_{11}+B_{13}B_{16}+B_{14}B_{15}+B_{17}B_{20}+B_{18}B_{19})=0$

(3.126) $A(\underline{Q}++)=0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2B_4+B_6B_8+B_{10}B_{12}+B_{14}B_{16}$

$+B_{18}B_{20})=0$

(3.127) $A(\underline{Q}--)=0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_3+B_5B_7+B_9B_{11}+B_{13}B_{15}$

$+B_{17}B_{19})=0$

In the five-fold degenerate AFM case we have:

(3.128) $A(o+-)=0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_2+B_3B_4+B_5B_6+B_7B_8$

$+B_9B_{10}+B_{11}B_{12}+B_{13}B_{14}+B_{15}B_{16}+B_{17}B_{18}+B_{19}B_{20})=0$

(3.129) $A(\underline{Q}+-)=0$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_4+B_2B_3+B_5B_8+B_6B_7+B_9B_{12}$

$+B_{10}B_{11}+B_{13}B_{16}+B_{14}B_{15}+B_{17}B_{20}+B_{18}B_{19})=0$

(3.130) $A(\underline{Q}++)=A(\underline{Q}--)$ leads to $\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_2B_4+B_6B_8+B_{10}B_{12}+B_{14}B_{16}$

$+B_{18}B_{20})=\frac{1}{N}\sum_{\underline{k}} F_{\underline{k}}(B_1B_3+B_5B_7+B_9B_{11}+B_{13}B_{15}+B_{17}B_{19})$

In the five-fold case, we note that relations (3.120), (3.124), and (3.129) all stem from $A(o+-)=0$. (3.121), (3.125), and

(3.129) stem from $A(\underline{Q}+-)=0$, and so on. The same correlation function relations in different magnetic states lead to the same relations among the B's. This is also true of the two-fold state.

We now express our roots, $E_{\underline{k}}^{(i)}$ in terms of these B coefficients. In the two-fold degenerate PM case we have:

$$(3.131)\quad E_{\underline{k}}^{(1-4)} = \epsilon_{\underline{k}} + \frac{(3K-J)}{N} \sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2+B_6^2+B_8^2) \text{ and}$$

$$E_{\underline{k}}^{(5-8)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{(3K-J)}{N} \sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2+B_6^2+B_8^2)$$

In the two-fold degenerate FM case we have:

$$(3.132)\quad E_{\underline{k}}^{(1,2)} = \epsilon_{\underline{k}} + \frac{2K}{N} \sum_{\underline{k}} F_{\underline{k}} (B_1^2+B_3^2+B_5^2+B_7^2) + \frac{(K-J)}{N} \sum_{\underline{k}} F_{\underline{k}}$$

$$(B_2^2+B_4^2+B_6^2+B_8^2)$$

$$E_{\underline{k}}^{(3,4)} = \epsilon_{\underline{k}} + \frac{2K}{N} \sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2+B_6^2+B_8^2) + \frac{(K-J)}{N} \sum_{\underline{k}} F_{\underline{k}}$$

$$(B_1^2+B_3^2+B_5^2+B_7^2)$$

$$E_{\underline{k}}^{(5,6)} = \epsilon_{\underline{k}} + \frac{2K}{N} \sum_{\underline{k}} F_{\underline{k}} (B_1^2+B_3^2+B_5^2+B_7^2) + \frac{(K-J)}{N} \sum_{\underline{k}} F_{\underline{k}}$$

$$(B_2^2+b_4^2+B_6^2+B_8^2)$$

$$E_{\underline{k}}^{(7,8)} = \epsilon_{\underline{k}} + \frac{2K}{N} \sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2+B_6^2+B_8^2) + \frac{(K-J)}{N} \sum_{\underline{k}} F_{\underline{k}}$$

$$(B_1^2+B_3^2+B_5^2+B_7^2)$$

In the two-fold degenerate AFM case we have:

$$(3.133)\quad E_{\underline{k}}^{(1-4)}_{(5-8)} = \frac{\epsilon_{\underline{k}}}{2} + \frac{\epsilon_{\underline{k}+\underline{Q}}}{2} + \frac{(3K-J)}{N} - \sum_{\underline{k}} F_{\underline{k}} (B_2^2+B_4^2+B_6^2+B_8^2)$$

$$\pm \frac{1}{2N^2} \sqrt{\begin{array}{l} [N^2\epsilon_{\underline{k}}+n^2\epsilon_{\underline{k}+\underline{Q}}+2N(3K-J)\Sigma F_{\underline{k}}(B_2^2+B_4^2+B_6^2+B_8^2)]^2 \\ -4N^2[N^2\epsilon_{\underline{k}}\epsilon_{\underline{k}+\underline{Q}}+(3K-J)^2[\{\Sigma\frac{F_{\underline{k}}}{N}(B_2^2+B_4^2+B_6^2+B_8^2)\}^2+\Sigma\frac{F_{\underline{k}}}{N} \\ (B_2B_4B_6B_8)\}^2]-(3K-J)(N\epsilon_{\underline{k}}+N\epsilon_{\underline{k}+\underline{Q}})\Sigma\frac{F_{\underline{k}}}{N}(B_2^2+b_4^2+B_6^2+B_8^2)] \end{array}}$$

We will use the compressed summation notation of (3.101) - (3.106) for the correlation functions in terms of the coefficients, B, in the five-fold degenerate case. In the five-fold degenerate PM case we have:

$$(3.134)\quad E_{\underline{k}}^{(1-10)} = \epsilon_{\underline{k}} + \frac{(9K-4J)}{N}\Sigma F_{\underline{k}}\left(\sum_{i=1\ \text{even}}^{20} B_i^2\right)$$

$$E_{\underline{k}}^{(11-20)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{(9K-4J)}{N}\Sigma F_{\underline{k}}\left(\sum_{i=1\ \text{even}}^{20} B_i^2\right)$$

In the five-fold degenerate FM case we have:

$$(3.135)\quad E_{\underline{k}}^{(1-5)} = \epsilon_{\underline{k}} + \frac{5K}{N}\Sigma F_{\underline{k}}\left(\sum_{i=1\ \text{odd}}^{20} B_i^2\right) + \frac{4(K-J)}{N}\Sigma F_{\underline{k}}\left(\sum_{i=1\ \text{even}}^{20} B_i^2\right)$$

$$E_{\underline{k}}^{(6-10)} = \epsilon_{\underline{k}} + \frac{5K}{N}\Sigma F_{\underline{k}}\left(\sum_{i=1\ \text{even}}^{20} B_i^2\right) + \frac{4(K-J)}{N}\Sigma F_{\underline{k}}\left(\sum_{i=1\ \text{odd}}^{20} B_i^2\right)$$

$$E_{\underline{k}}^{(11-15)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{5K}{N}\Sigma F_{\underline{k}}\left(\sum_{i=1\ \text{odd}}^{20} B_i^2\right) + \frac{4(K-J)}{N}\Sigma F_{\underline{k}}\left(\sum_{i=1\ \text{even}}^{20} B_i^2\right)$$

$$E_{\underline{k}}^{(16-20)} = \epsilon_{\underline{k}+\underline{Q}} + \frac{5K}{N}\Sigma F_{\underline{k}}\left(\sum_{i=1\ \text{even}}^{20} B_i^2\right) + \frac{4(K-J)}{N}\Sigma F_{\underline{k}}\left(\sum_{i=1\ \text{odd}}^{20} B_i^2\right)$$

In the five-fold degenerate AFM case we have:

$$(3.136)\quad E_{\underline{k}}^{\substack{(1-10)\\(11-20)}} = \frac{\epsilon_{\underline{k}}}{2} + \frac{\epsilon_{\underline{k}+Q}}{2} + \frac{(9K-4J)}{N} \sum_{\substack{i=1\\ \text{even}}}^{20} (\Sigma F_{\underline{k}} B_i)^2$$

$$\pm\frac{1}{2N^2} \cdot \sqrt{\begin{array}{l} [N^2\epsilon_{\underline{k}} + N_2\epsilon_{\underline{k}+Q} - 2N(9K-4J)\sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (\sum_{\substack{i=1\\ \text{even}}}^{20} B_i^2)]^2 + N^2\epsilon_{\underline{k}}\epsilon_{\underline{k}+Q} \\ -4N^2[-(9K-4J)(N\epsilon_{\underline{k}} + N\epsilon_{\underline{k}+Q}) \sum_{\substack{i=1\\ \text{even}}}^{20} (\sum_{\underline{k}} \frac{F_{\underline{k}}}{N} B_i^2) + (9K-4J)^2 \\ [\sum_{\substack{i=1\\ \text{even}}}^{20} (\sum_{\underline{k}} \frac{F_{\underline{k}}}{N} B_i^2) + \sum_{\substack{i=1\\ \text{even}}}^{20} (\sum_{\underline{k}} \frac{F_{\underline{k}}}{N} B_i B_{i+2})]] \end{array}}$$

We note that factors (9K-4J) in the five-fold case and (3K-J0 in the two-fold case have emerged. They will do so next in the total energy. This is very significant as will be shown later.

Finally, we get the total energies of the three states in both the two- and five-orbit case in terms of the coefficients B.

For the two-orbit case (where the factor of 2 is again inserted in the correlation terms denominators to prevent double counting):

$$(3.137)\quad E_{TOT}^{2\ \text{orbit-PM}} = 2 \sum_{\underline{k}}^{B.Z.} \frac{F_{\underline{k}}}{N} E_{\underline{k}} = 2 \sum_{\underline{k}}^{B.Z.} \frac{F_{\underline{k}}}{N} \epsilon_{\underline{k}} + 2 \sum_{\underline{k}}^{B.Z.} \frac{F_{\underline{k}}}{N}$$
$$[(3K-J) \sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (B_2^2 + B_4^2 + B_6^2 + B_8^2)]$$

$$(3.138)\quad E_{TOT}^{2\ \text{orbit-FM}} = 2 \sum_{\underline{k}}^{B.Z.} \frac{F_{\underline{k}}}{N} \epsilon_{\underline{k}} + 2 \sum_{\underline{k}}^{B.Z.} \frac{F_{\underline{k}}}{N} [(3K-J)\{\sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (B_2^2 +$$
$$B_4^2 + B_6^2 + B_8^2) + \sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (B_1^2 + B_3^2 + B_5^2 + B_7^2)\}]$$

$$(3.139)\quad E_{TOT}^{2\ orbit\text{-}AFM}=2\sum_{\underline{k}}^{B.Z.}\frac{F_{\underline{k}}}{N}\epsilon_{\underline{k}}+2\sum_{\underline{k}}^{B.Z.}\frac{F_{\underline{k}}}{N}[(3K-J)\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2^2+B_4^2+B_6^2+B_8^2)$$

$$\epsilon_{\underline{k}}+\epsilon_{\underline{k}+\underline{Q}}\pm\sqrt{\begin{array}{l}[N^2\epsilon_{\underline{k}}+N^2\epsilon_{\underline{k}+\underline{Q}}+2N^2(3K-J)\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2^2+B_4^2+B_6^2+B_8^2)]^2\\ -4N^2\{N^3\epsilon_{\underline{k}}\epsilon_{\underline{k}+\underline{Q}}-(3K-J)[N\epsilon_{\underline{k}}+N\epsilon_{\underline{k}+\underline{Q}}]\\ (\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2^2+B_4^2+B_6^2+B_8^2)+(3K-J)^2\{[\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2^2\\ +B_4^2+B_6^2+B_8^2)]^2+[\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2B_4+B_6B_8)]^2\}\}\end{array}}\Bigg]_{-}^{2\epsilon_{\underline{k}}}$$

where the kinetic energy term in (3.139) should more explicitly be written as:

$$\sum_{\substack{\text{half}\\ \text{Brillouin}\\ \text{zone}}}^{\underline{k}}\frac{F_{\underline{k}}}{N}\epsilon_{\underline{k}}+\sum_{\substack{\text{half}\\ \text{Brillouin}\\ \text{zone}}}^{\underline{k}+\underline{Q}}\frac{F_{\underline{k}+\underline{Q}}}{N}\epsilon_{\underline{k}+\underline{Q}}$$

For the five-orbit case:

$$(3.140)\quad E_{TOT}^{5\ orbit\text{-}PM}=5\sum_{\underline{k}}^{B.Z.}\frac{F_{\underline{k}}}{N}\epsilon_{\underline{k}}+5\sum_{\underline{k}}^{B.Z.}\frac{F_{\underline{k}}}{N}(9K-4J)[\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}$$
$$(B_2^2+B_4^2+B_6^2+B_8^2+B_{10}^2+B_{12}^2+B_{14}^2+B_{16}^2+B_{18}^2+B_{20}^2)]$$

$$(3.141)\quad E_{TOT}^{5\ orbit\text{-}FM}=5\sum_{\underline{k}}^{B.Z.}\frac{F_{\underline{k}}}{N}\epsilon_{\underline{k}}+5\sum_{\underline{k}}^{B.Z.}\frac{F_{\underline{k}}}{N}(9K-J)[\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}$$
$$(B_2^2+B_4^2+B_6^2+B_8^2+B_{10}^2+B_{12}^2+B_{14}^2+B_{16}^2+B_{18}^2+B_{20}^2)+\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}$$
$$(B_1^2+B_3^2+B_5^2+B_7^2+B_9^2+B_{11}^2+B_{13}^2+B_{15}^2+B_{17}^2+B_{19}^2)]$$

$$(3.142)\quad E_{TOT}^{5\ \text{orbit-AFM}} = 5\sum_{\underline{k}}^{B.Z.}\frac{F_{\underline{k}}}{N}\epsilon_{\underline{k}} + 5\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(9K-J)\Big[\sum_{\underline{k}}^{B.Z.}\frac{F_{\underline{k}}}{N}\Big(\sum_{\substack{i=1\\ \text{even}}}^{20} B_i^2\Big)$$

$$+\frac{5}{2.2}\sum_{\underline{k}}^{B.Z.}\frac{F_{\underline{k}}}{N}\Bigg[\epsilon_{\underline{k}}+\epsilon_{\underline{k}+\underline{Q}} \pm \Big[N^2\epsilon_{\underline{k}}+N^2\epsilon_{\underline{k}+\underline{Q}}+2N^2(9K-4J)\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2^2+B_4^2+B_6^2+B_8^2+B_{10}^2+B_{12}^2+B_{14}^2+B_{16}^2+B_{18}^2+B_{20}^2)\Big]^2 - 4N^2\{N^2\epsilon_{\underline{k}}\epsilon_{\underline{k}+\underline{Q}} - (9K-4J)[N\epsilon_{\underline{k}}+N\epsilon_{\underline{k}+\underline{Q}}]\Big(\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2^2+B_4^2+B_6^2+B_8^2+B_{10}^2+B_{12}^2+B_{14}^2+B_{16}^2+B_{18}^2+B_{20}^2)\Big) + (9K-4J)^2\Big\{\Big[\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2^2+B_4^2+B_6^2+B_8^2+B_{10}^2+B_{12}^2+B_{14}^2+B_{16}^2+B_{18}^2+B_{20}^2)\Big]^2 + \Big[\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2B_4+B_6B_8+B_{10}B_{12}+B_{14}B_{16}+B_{18}B_{20})\Big]^2\Big\}\Big]^{1/2} - 2\epsilon_{\underline{k}}\Bigg]$$

where the kinetic energy term in (3.142) could be more explicitly written as:

$$\frac{5}{2}\sum_{\substack{\underline{k}\\ \text{half Brillouin zone}}}\frac{F_{\underline{k}}}{N}\epsilon_{\underline{k}} + \frac{5}{2}\sum_{\substack{\underline{k}\\ \text{half Brillouin zone}}}\frac{F_{\underline{k}+\underline{Q}}}{N}\epsilon_{\underline{k}+\underline{Q}}$$

We note here that the restriction to one $\underline{Q}$, $\underline{Q}=\underline{G}/2a$ has nowhere been used explicitly in the antiferromagnetic state. This choice of $\underline{Q}$ would correspond to an antiferromagnetic order with wave length a in real space. One might think that in general one could write any term containing $\underline{Q}$ in terms of a generalized $\underline{Q}_j = \underline{G}/2n_j a$, with $n_1=1$, $n_j>1$ = an interger ≥ 2. (For example $\underline{Q}_2 = \underline{G}/4a$ would correspond to an antiferromagnetic order with wave

length 2a in real space.) Thus, for example, any correlation, $A(\underline{Q}++)$, occurring in an energy eigenvalue or total energy, would become $\sum_j A(\underline{Q}_j++)$.

The fallacy in this argument, which seems to imply that our off-diagonal terms in the 8 x 8 or 20 x 20 secular matrix would just become sums of the form indicated is seen when one considers the mapping between $\underline{k}$ and $\underline{k} + \underline{Q}$ in the Brillouin zone. For example, in two dimensions, the $\underline{k}$ and $\underline{k} + \underline{Q}$ pairing in the Brillouin zone in $\underline{k}$ space:

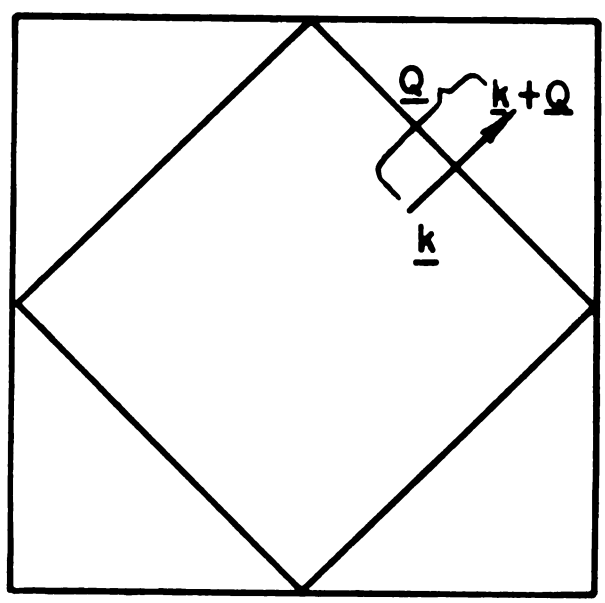


Figure 9. One to One Mapping of $\underline{k}$ and $\underline{k}+\underline{Q}$ in Two-Dimensional Brillouin Zone Projection.

corresponds to:

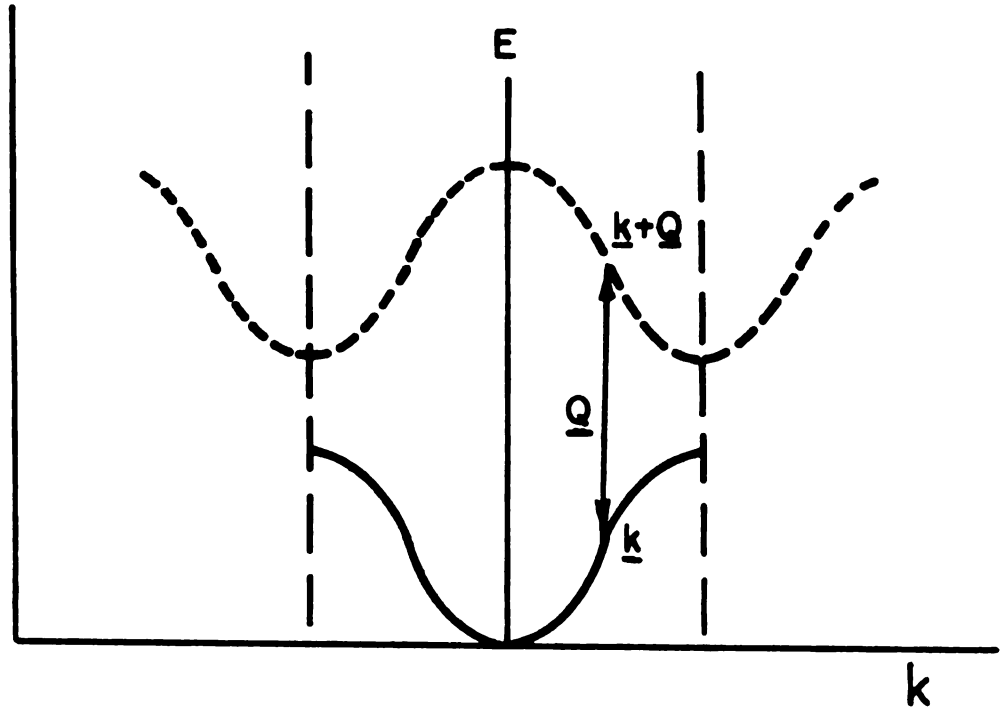


Figure 10. One to One Mapping of $\underline{k}$ and $\underline{k} + \underline{Q}$ in Dispersion Relation.

in one $\underline{k}$ direction in the dispersion relation. For $\underline{Q} = \underline{G}/2a$, there is a unique 1:1 pairing of states $\underline{k}$ and $\underline{k} + \underline{Q}$, both in the Brillouin zone and the dispersion relation. However, for $\underline{Q}_j = \underline{G}/2n_j a$, a 1:1 pairing breaks down giving a many to one pairing, which one does.

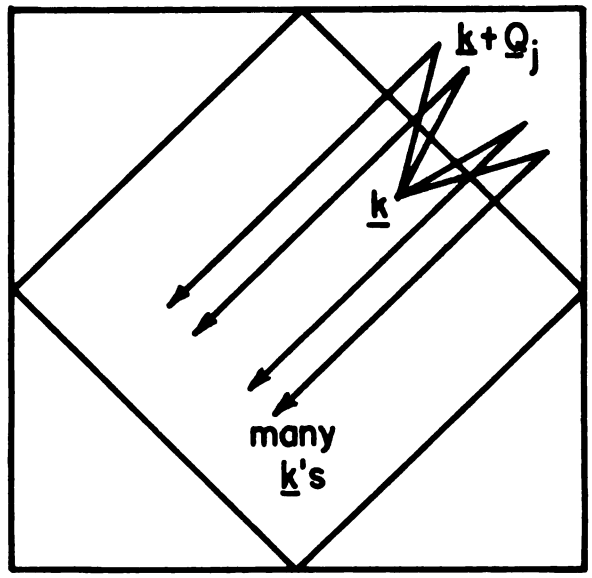


Figure 11. Many to One Mapping of $\underline{k}$ and $\underline{k} + \underline{Q}$ in Two-Dimensional Brillouin Zone Projection.

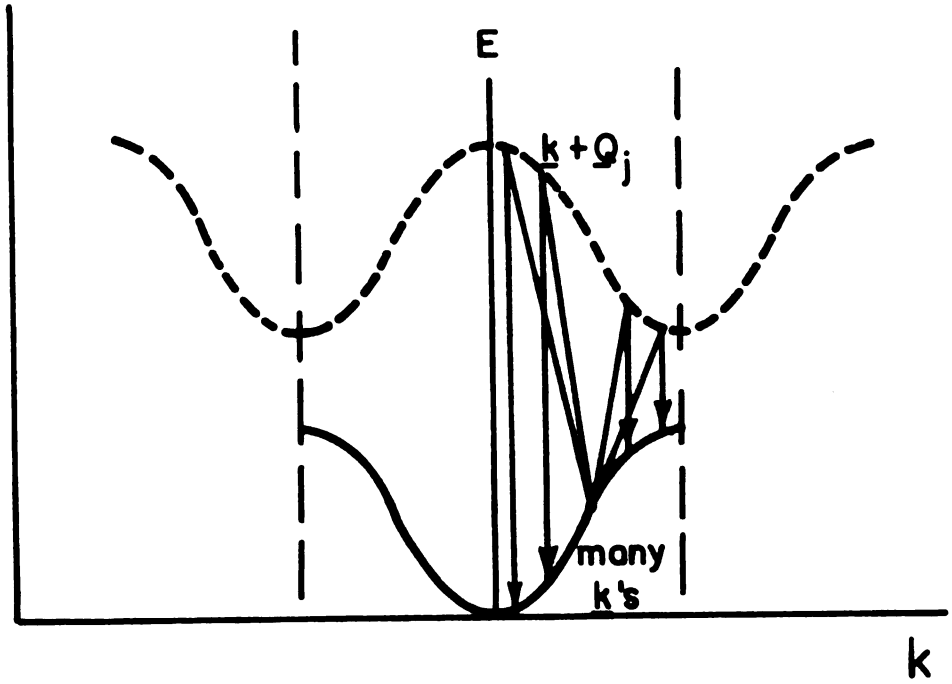


Figure 12. Many to One Mapping of $\underline{k}$ and $\underline{k} + \underline{Q}$ in Dispersion Relation.

Thus, an attempt to amend the antiferromagnetic secular determinant to include arbitrary $\underline{Q}_j$ is clearly doomed to failure because of this breakdown of 1:1 mapping of $\underline{k}$ and $\underline{k}+\underline{Q}$. One would need to make each off diagonal term equal to $K\sum_{i=1}^{5} A(\underline{Q}_j \overline{--}\overline{++}ii)+K\sum_{i\mp 2}^{5} A(\underline{Q}_j \overline{++}\overline{--}ii)$. Then, being four in each subblock, each term would become 2 x 2 larger for each $\underline{Q}$ added. The diagonal term would change from $\epsilon_{\underline{k}+\underline{Q}}$ to $\epsilon_{\underline{k}+\underline{Q}_j}$ or $\sum_j \epsilon_{\underline{k}+\underline{Q}_j}$, making two new diagonal terms for each new $\underline{Q}_j$.

This consideration will not be important for the general paramagnetic and ferromagnetic states we consider since these two states have diagonal secular matrices and no $A(\underline{Q})$'s appear; thus, the gap parameter, $\Delta\equiv 0$. There is no exchange splitting of the bands, and the question never arises.

We now calculate the self-consistent conditions for the energy in order to decide for which values of n/2N, J, K, and T, the E_{TOT} is minimized, and thus the F_{TOT} is minimized. The minima, not necessarily coinciding, tell us which of the three states, paramagnetic, ferromagnetic, or antiferromagnetic, has the lowest free energy and is thus stable.

A direct comparison of all three simultaneously is complicated, so we try to compare $F_{TOT}^{AFM}(J,K,n/2N,T)$ with $F_{TOT}^{PM}(J,K,n/2N,T)$ first, and then $F_{TOT}^{FM}(J,K,n/2N,T)$ with $F_{TOT}^{PM}(J,K,n/2N,T)$ second.

Matsubara and Yokota[64] and Kemeny and Caron[65] have derived the equation for the energy gap, Δ, used in the first comparison. We reproduce Kemeny and Caron's derivation.

We note at the outset that Kemeny and Caron's J becomes our K, the direct coulomb coupling constant. Our J is the exchange coulomb coupling constant, absent in their work. Also, Matsubara has an $(I_0 - zI_1)$ coupling constant, where I_0 is an intra-atomic "exchange integral" and I_1 is an inter-atomic "exchange integral". Since we are working in the Hubbard Model, we have no inter-atomic term in our potential part of the Hubbard Hamiltonian. Therefore, I_1 is absent in our work. Also, it is not clear whether Matsubara's I_0 is really an "exchange term". Our total coulomb coupling coefficient in our energy eigenvalues and total energies is (9K-4J) for the five-orbit degenerate case.

To derive the energy gap equation, the cornerstone for our first comparison involving a self-consistent calculation for the AFM state, we define a single particle symmetry breaking potential

$$(3.143) \quad \sum_{i\sigma}\sum \Delta^{H.F.}_{i\sigma} n_{i\sigma}$$

where $\Delta_{i\sigma}$ is a self-consistently defined Hartree-Fock potential seen by an electron in one of the 5-d subbands. We generalize Kemeny and Caron's expression for Δ (their J becomes K in our notation):

$$(3.144)\quad (\Delta_{i\sigma}^{H.F.})_{\alpha} = K n_{i,-\sigma,\alpha}$$

putting in an α as a subband index since they were considering one s-band. Summing over the 5-d subbands we find:

$$(3.145)\quad \Delta_{i\sigma}^{H.F.} = \sum_{\alpha=1}^{5} (\Delta_{i\sigma}^{H.F.})_{\alpha} = K \sum_{\alpha=1}^{5} n_{i,-\sigma,\alpha} + (K-J) \sum_{\beta(\neq\alpha)=1}^{5}$$

$$n_{i,-\sigma,\alpha} = (9K-4J) n_{i,-\sigma}$$

a generalized total Δ for all the five subbands (although we may still talk of five Δ_{α}'s, one for each d-subband, and consider their gaps separately).

Note that since we have introduced exchange by adding d-subband degeneracy on each site, our Δ in a true Hartree-Fock gap parameter. In single s-band calculations, Δ is actually only a Hartree gap parameter, since exchange was not included.

The Hubbard Hamiltonian in the Matsubara approximation becomes:

$$(3.146)\quad H_M = \sum_{i,j} \sum_{\sigma} T_{ij} C_{i\sigma}^{+} C_{j\sigma} + \sum_{i} \sum_{\sigma} \Delta_{i\sigma}^{H.F.} n_{i\sigma}$$

in Wannier space. The potential term is in effective one-body form, equivalent to our Gorkov factorization result previously, if $\Delta_{i\sigma}^{H.F.}$ is taken as a parameter.

In $\underline{k}$ space, this becomes:

$$(3.147)\quad H_M = \sum\sum_{\underline{k}\sigma} [\epsilon(\underline{k}) + \frac{(9K-4J)}{2}] n_{\underline{k}\sigma} + \sum\sum_{\underline{k}\sigma} \frac{\Delta_{\sigma}^{H.F.}}{2} [C_{\underline{k}\sigma}^{+} C_{\underline{k}+\underline{\pi},\sigma}$$

$$+ C_{\underline{k}+\pi,\sigma}^{+} C_{\underline{k}\sigma}]$$

where $\underline{\pi} = \underline{Q} = \underline{G}/2$ (as in Penn's paper) and where

$$(3.148) \qquad \Delta_\sigma = \begin{cases} \Delta_{o+} - \dfrac{(9K-4J)}{2} = +\Delta \text{ for up spins} \\ \Delta_{o-} - \dfrac{(9K-4J)}{2} = -\Delta \text{ for down spins} \end{cases}$$

is related to our $B_1(\underline{k})$, $B_3(\underline{k})$ coefficients in the magnetic phase wave function:

$$(3.149) \qquad \Psi_+^{AFM} = B_1(\underline{k})\ \Psi_{\underline{k}1+} + B_3(\underline{k})\ \Psi_{\underline{k}+\underline{Q}1+}$$

by:

$$(3.150) \qquad B_1(\underline{k}) = \sqrt{\frac{1}{2}\left(1 - \frac{\epsilon_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}\right)}$$

$$(3.151) \qquad B_3(\underline{k}) = \sqrt{\frac{1}{2}\left(1 + \frac{\epsilon_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}\right)}$$

where we must remember that B_1 is equivalent to B_2, B_5, B_6, B_9, B_{10},B_{13},B_{14},B_{17},B_{18} since any of the pairs (B_1,B_3), (B_5,B_7), B_9,B_{11}), (B_{13},B_{15}), (B_{17},B_{18}) yield a Ψ_+^{AFM} while any of the pairs (B_2,B_4), (B_6,B_8), (B_{10},B_{12}), (B_{14},B_{16}), (B_{18},B_{20}) yields a Ψ_-^{AFM}. Any of these combinations will allow description of a pairing of a state $\underline{k}$ with state $\underline{k} + \underline{Q}$, the antiferromagnetic correlation.

Continuing our analogy with Kemeny and Caron's work, the eigenfunctions and eigenvalues are, for each d-subband, α (and for Bloch wave electron states):

$$(3.152)\quad \begin{cases} \psi^{AFM\alpha}_{1,\underline{k},\pm}(\underline{R}) = \dfrac{1}{\sqrt{N}}\, e^{i\underline{k}\cdot\underline{R}}\left[B_1(\underline{k}) \mp B_3(\underline{k})\, e^{i\underline{\pi}\cdot\underline{R}}\right] \\ E_1^{\alpha}(\underline{k}) = -\sqrt{\Delta^2+\epsilon_{\underline{k}}^{\,2}} + \dfrac{(9K-4J)}{2} \end{cases}$$

$$(3.153)\quad \begin{cases} \psi^{AFM\alpha}_{2,\underline{k},\pm}(R) = \dfrac{1}{\sqrt{N}}\, e^{i\underline{k}\cdot\underline{R}}\left[B_3(\underline{k}) \pm B_1(\underline{k})\, e^{i\underline{\pi}\cdot\underline{R}}\right] \\ E_2^{\alpha}(\underline{k}) = +\sqrt{\Delta^2+\epsilon_{\underline{k}}^{\,2}} + \dfrac{(9K-4J)}{2} \end{cases}$$

which can be written as above since if $A(o{+}{+}) = A(o{-}{-})$ in the state and $A(\underline{Q}{+}{+}) = A(\underline{Q}{-}{-})$, then:

$$(3.144)\quad \sum_{\underline{k}} F_{\underline{k}} B_1 = \sum_{\underline{k}} F_{\underline{k}} B_2 = \sum_{\underline{k}} F_{\underline{k}} B_3 = \sum_{\underline{k}} F_{\underline{k}} B_4 \text{ is a solution since:}$$

$$(3.145)\quad \sum_{\underline{k}} F_{\underline{k}} (B_1^{\,2}+B_3^{\,2}) = \sum_{\underline{k}} F_{\underline{k}} (B_2^{\,2}+B_4^{\,2}) \text{ i.e. } |\psi_+^{AFM}|^2 = |\psi_-^{AFM}|^2$$

the number of up spins being equal to the number of down spins.

A self-consistency condition is written by Kemeny and Caron[66] as:

$$(3.154)\quad \pm\Delta + \frac{K}{2} = \frac{K}{N} \sum_{\underline{k}<\underline{k}_F} |\psi_{1,\underline{k},\mp}(0)|^2$$

equivalent to: $\dfrac{K}{2} + \sum\limits_{\underline{k}<\underline{k}_F} \langle\psi|\, U_{(+)}(\underline{R}) - U_{(-)}(\underline{R})\,|\,\psi\rangle$

in Matsubara's notation for Δ (his equation (3)). Note that Δ can be $\gtrless 0$ depending on whether $U_+(\underline{R}) = U_-(\underline{R})$.

This condition says that in the AFM state a gap of width Δ opens up between the lower band (composed of overlapping d-subbands) and the higher band (also composed of overlapping d-subbands). The gap is caused by a magnetic Brillouin zone boundary occurring at II, halfway between the origin and the lattice Brillouin zone boundary corner. This is illustrated in Matsubara's and Penn's papers.

From the self-consistency condition, Kemeny and Caron derive a more explicit self-consistency condition:

$$(3.155)\quad \frac{K}{N}\sum_{\underline{k}<\underline{k}_F}\frac{F_{\underline{k}}(T,E_{\underline{k}}^{(i)})}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}} = 1$$

which we now reproduce:

$$(3.156)\quad n_{i,-\sigma} = \sum_{\underline{k}}[\Psi_1^2(\underline{k}) - \Psi_2^2(\underline{k})]$$

$$(3.157)\quad \text{where}\begin{cases}\Psi_1^2(\underline{k}) = B_1^2(\underline{k})+B_3^2(\underline{k})+2B_1(\underline{k})B_3(\underline{k})\\ \Psi_2^2(\underline{k}) = B_1^2(\underline{k})+B_3^2(\underline{k})\mp 2B_1(\underline{k})B_3(\underline{k})\end{cases}$$

subtracting these to get $n_{i,-\sigma}$.

$$(3.158)\quad n_{i,-\sigma} = \pm\sum_{\underline{k}} 4B_1(\underline{k})B_3(\underline{k})$$

$$(3.159)\quad \text{Now:}\quad B_1(\underline{k}) = \sqrt{\frac{1}{2}\left(1-\frac{\epsilon_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}\right)}$$

$$\text{and:}\quad B_3(\underline{k}) = \sqrt{\frac{1}{2}\left(1+\frac{\epsilon_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}\right)}$$

Thus:

$$(3.160)\quad \frac{K}{N}\sum_{\underline{k}}\sqrt{\frac{1}{2}\left(1-\frac{\epsilon_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}\right)\cdot\frac{1}{2}\cdot\left(1+\frac{\epsilon_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}\right)} \equiv \Delta$$

by the definition of Δ, or:

$$(3.161)\quad \frac{K}{N}\sum_{\underline{k}}\sqrt{1-\frac{\epsilon_{\underline{k}}}{\Delta^2+\epsilon_{\underline{k}}^2}} \equiv \Delta$$

Taking the least common denominator in the square root:

$$(3.162)\quad \frac{K}{N}\sum_{\underline{k}}\sqrt{\frac{\Delta^2+\cancel{\epsilon_{\underline{k}}^2}-\cancel{\epsilon_{\underline{k}}^2}}{\Delta^2+\epsilon_{\underline{k}}^2}} \equiv \Delta$$

or:

$$(3.163)\quad \frac{\cancel{\Delta}K}{N}\sum_{\underline{k}}\frac{1}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}} = \cancel{\Delta}$$

or:

$$(3.164)\quad \frac{K}{N}\sum_{\underline{k}}\frac{1}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}} = 1$$

Without putting it in explicitly, $F_{\underline{k}}(T,E_{\underline{k}}^{(i)})$ should be put in the sum over $\underline{k}$ on the left hand side to include filling of the states, or restrict the sum to $\underline{k}$ values $<\underline{k}_F$.

We must now generalize this equation:

$$(3.165)\quad \pm\Delta+\frac{K}{2}=\frac{K}{N}\sum_{k<k_F}\left|\Psi_{1,k,\mp}(0)\right|^2$$

and the equation we derived from it:

$$(3.166)\quad \frac{K}{N}\sum_{\underline{k}}\frac{1}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}} = 1$$

to our five-fold degenerate d-subband system for T = 0°K. The above derivation of the gap parameter equation from the relation between gap parameter and wave function is analogous for many such wave function terms. Thus a five-fold generalization of the wave-function-gap parameter relation is:

$$(3.167)\quad \pm\Delta + \frac{K}{2} = K\sum_{j=1}^{9}\Big[\sum_{\underline{k}=0}^{\underline{k}B1}\left|\Psi_{1,\underline{k},\pm}(0)\right|^2 - \sum_{\underline{k}=\underline{k}B2}^{k_F}\left|\Psi_{2,\underline{k},\pm}(0)\right|^2\Big]_j$$

$$-J\sum_{j=1}^{4}\Big[\sum_{\underline{k}=0}^{\underline{k}B1}\left|\Psi_{1,\underline{k},\pm}(0)\right|^2 - \sum_{\underline{k}=\underline{k}B2}^{k_F}\left|\Psi_{2,\underline{k},\pm}(0)\right|^2\Big]_j$$

where $\underline{k}B1$ is the upper band edge of the lower band and $\underline{k}B2$ is the lower band edge of the upper band.

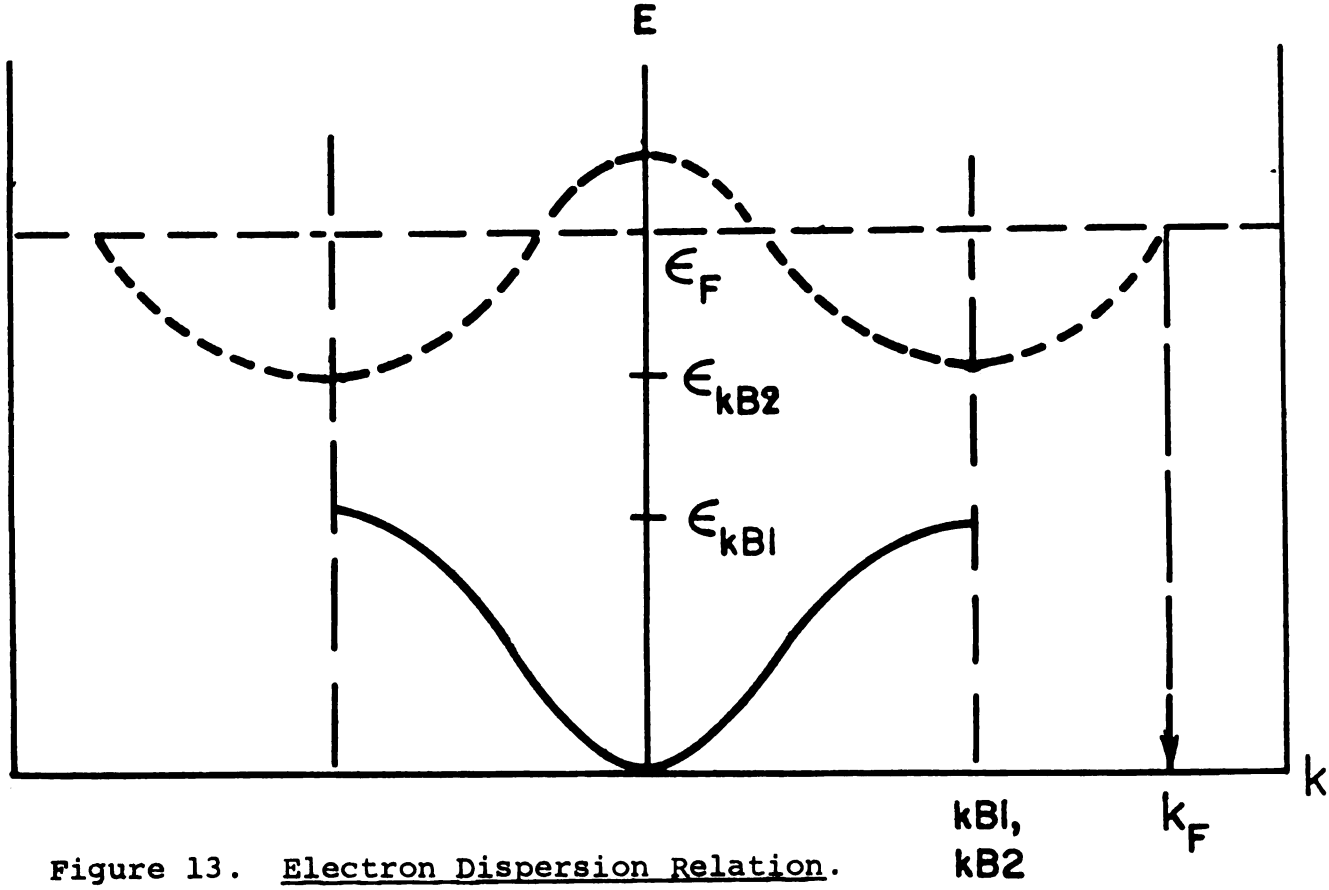


Figure 13. Electron Dispersion Relation.

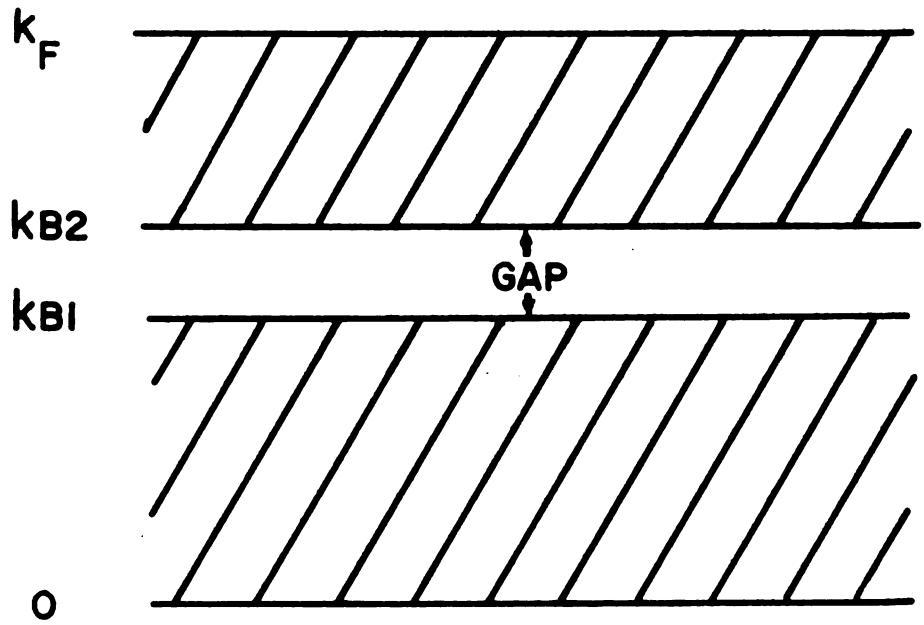


Figure 14. Allowed Wave Vectors in $\underline{k}$ Space.

where we sum over up and down spins separately for each $\underline{k}$.

The result of the transformation in the five-orbit case is (by analogy with Kemeny and Caron's derivation):

$$(3.168)\quad 1 = \left[\frac{K}{N}\sum_{j=1}^{9}\left\{\sum_{\underline{k}=0}^{\underline{k}_{B1}}\frac{F_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}} - \sum_{\underline{k}=\underline{k}_{B2}}^{\underline{k}_F}\frac{F_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}\right\}_j - \frac{J}{N}\sum_{j=1}^{4}\left\{\sum_{\underline{k}=0}^{\underline{k}_{B1}}\frac{F_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}} - \sum_{k=k_{B2}}^{\underline{k}_F}\frac{F_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}\right\}_j\right]$$

with the $F_{\underline{k}}$ Fermi factors put in:

$$(3.169)\quad F_{\underline{k}} = [1+\exp((E_{\underline{k}}^{(i)}-U)/\underline{k}_B T)]^{-1}$$

where the $E_{\underline{k}}^{(i)}$ depends on the Bi's, J, K, and the $\epsilon_{\underline{k}}$'s. We can improve upon the above expression by putting in Fermi factors:

$$(3.170)\quad 1 = [\frac{K}{N}\sum_{j=1}^{9}\sum_{\underline{k}=0}^{B\cdot Z\ bdry}\frac{F_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}} - \frac{J}{N}\sum_{j=1}^{4}\sum_{k=0}^{B.Z.\ bdry}\frac{F_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}]$$

the subtractive effects of the upper band filling being implied.

since $F_{\underline{k}}$ in the AFM case looks like, at T = 0 and at T > 0, when the gap shrinks.

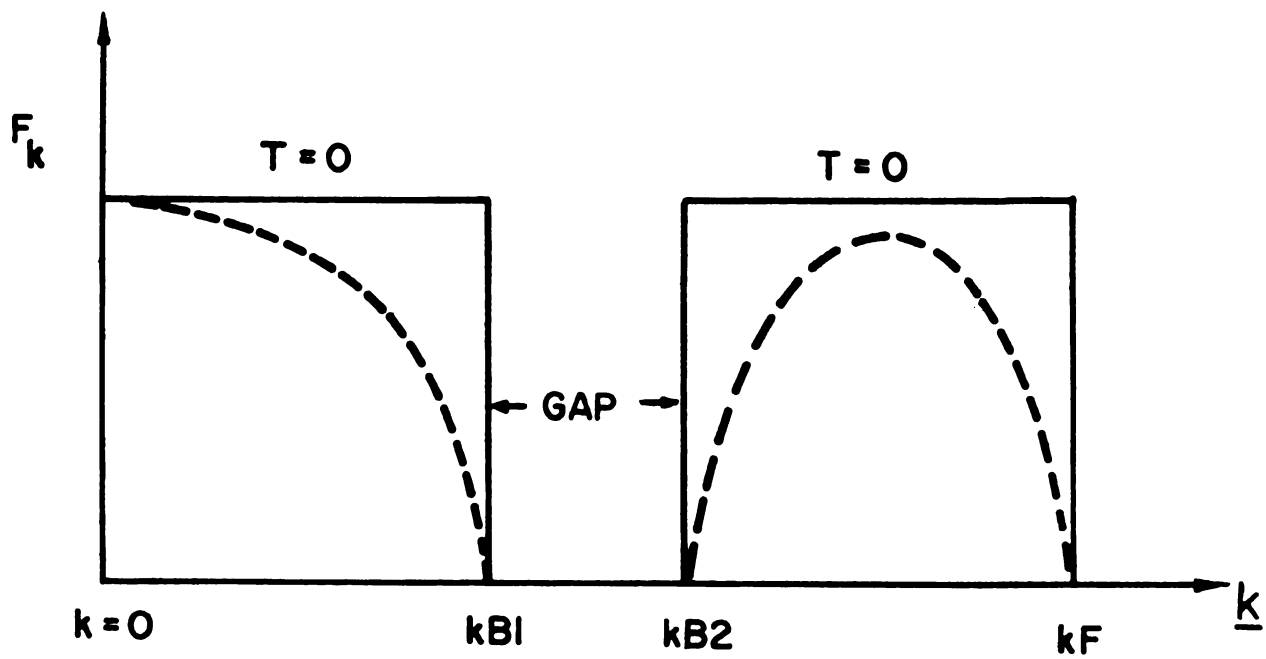
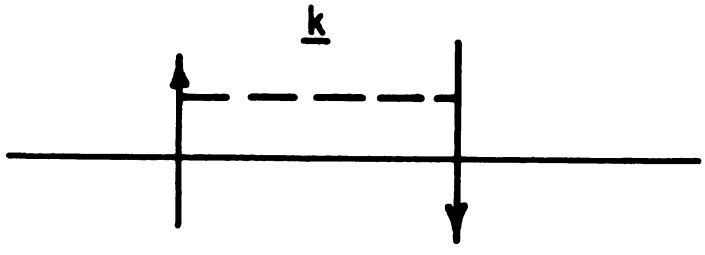


Figure 15. Fermi Factor Dependence on $\underline{k}$, Including AFM Gap.

We note the physical ideas embodied in this equation. The first term, with a coefficient, K, favors the AFM state while the second term, with a J coefficient, favors the AFM state by tending to increase the gap parameter magnitude and, therefore, the gap width, 2Δ. Thus, as more and more exchange between degenerate d-subband electrons takes place on any site, the tendency toward the AFM state is increased. J = 0, from an s-band



configuration on each site, gives the least tendency to the AFM order. As J increases from zero, new terms are added on each site. This is illustrated with the following progression:

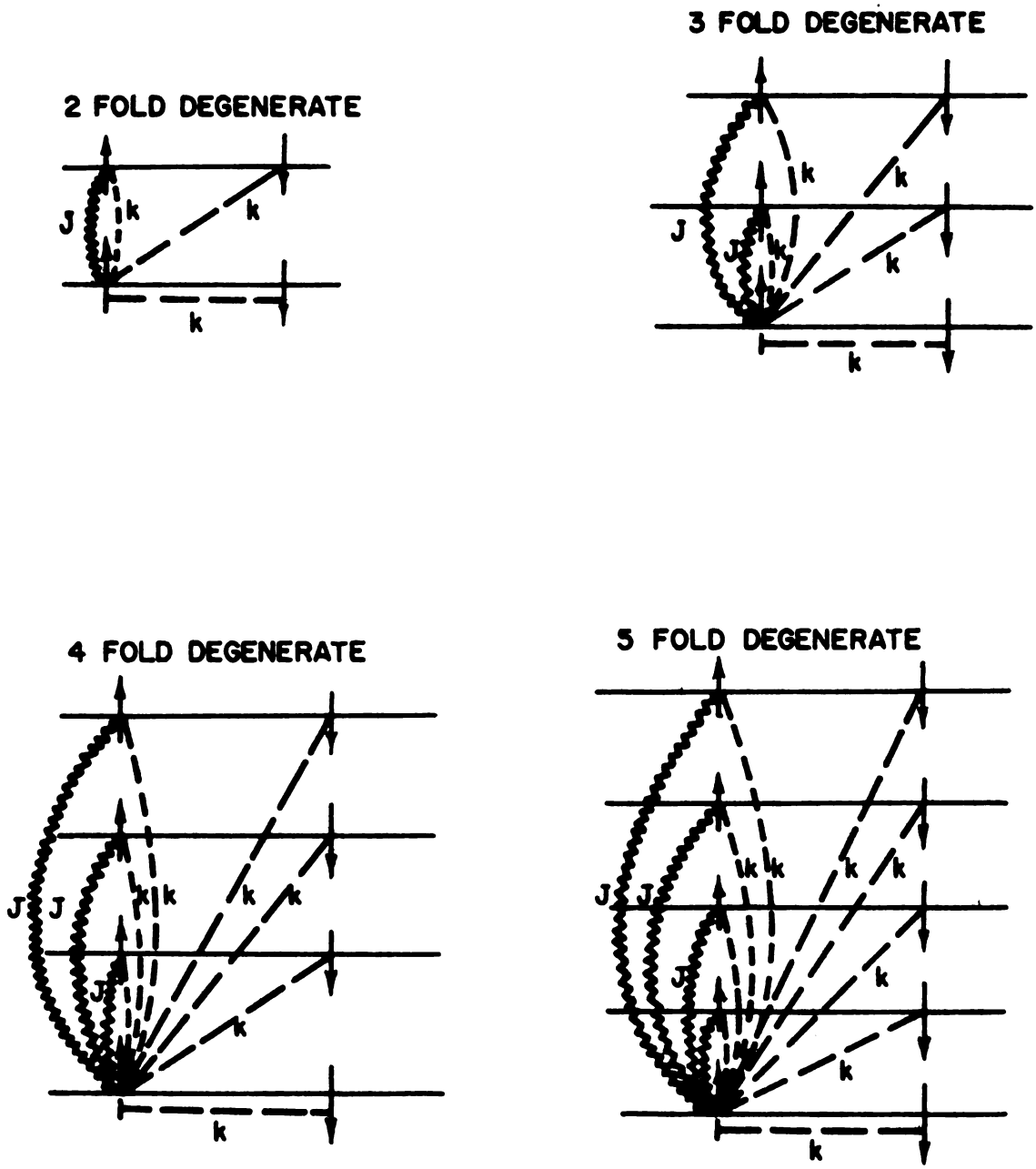


Figure 16. Direct and Exchange Couplings in 2-, 3-, 4-, and 5-Fold Degenerate Cases.

Of course, the extent to which this happens is governed by the n/2N filling of the whole d-electron band. Not all subband states will be occupied by electrons if the filling is not perfect.

Actually, for each J term added, a direct coulomb K term is added so that this effect would cancel out if $J \equiv K$, in which case 9K - 4J would become 5K, the direct coulomb interaction of five electrons in the five d-subbands with no exchange coupling constant. But $J \neq K$ in general, although there will be a $J = K$ plane in the three-dimensional (n/2N, K, J) parameter phase diagram we will plot. In this $J \equiv K$ plane, introducing five d-electron exchange as we have done, the tendency toward the AFM state would not be changed. It would raise the direct coulomb energy from Penn's Co to 5K, a five-fold increase in the coulomb interaction energy evaluation from the Hubbard-Hamiltonian since presumably for an s-band, Penn's Co $\equiv$ our K.

We will also alter this tendency for the AFM state in the band filling, n/2N, manifested by the subtractive effect in the brackets { } in our master self-consistent equation for Δ for filling above the half-filled d-band. For $n/2N < 1/2$, the tendency toward the AFM state rises as n/2N. But, after $n/2N = 1/2$, at which the tendency is a maximum, it falls off symmetrically as $n/2N(>1/2)$ goes to 1, the completely filled d-band. When

$n/2N \equiv 1$, the gap equation degenerates and the PM state should dominate. These ideas match those of Penn, and are mirrored in his three state phase diagram of Co/E" versus n/2N.

We note two further details to be used in the calculation. Firstly, to find $F_{tot} = E_{tot} - TS$, we need S. We can use the equation for the entropy of a Fermi gas:

$$(3.171)\quad S = -\underline{k}_B \cdot 10 \cdot \sum_{\underline{k}} \{[1+e^{(E_{\underline{k}}-U)/\underline{k}_B T}]^{-1} \ln\{[1+e^{(E_{\underline{k}}-U/\underline{k}_B T}]^{-1}\}$$

$$+(1-[1+e^{(E_{\underline{k}}-U)/\underline{k}_B T}]^{-1} \ln\{1-[1+e^{(E_k-U)/\underline{k}_B T}]^{-1}\}\}$$

where degeneracy in S is accounted for in the self-consistent u and $E_{\underline{k}}$ calculation.

It is now a clothed Fermi gas, rather than a free one, since in an energy band, m_e gets renormalized to an effective electron mass m_e^*. We, however, cannot use the usual formulas for the chemical potential of a free Fermi gas which are only valid when n/2N is very small or very large, but not near the middle of the n/2N axis, i.e., the half-filled band.

Secondly, our expressions for $E_{\underline{k}} = \sum_i E_{\underline{k}}^{(i)}$ must be amended as Penn does since in just summing up the eigenvalues, we are over-counting the interaction. In general:

$$(3.172)\quad E_{TOT} = \sum_{\underline{k}} F_{\underline{k}} E_{\underline{k}} - N(A_{o++}A_{o--} + A_{\underline{Q}++}A_{\underline{Q}--} - A_{o+-}^2 - A_{\underline{Q}+-}$$

where: $E_{\underline{k}} = \sum_i E_{\underline{k}}^{(i)}$

In our work: $A_{o+-} = A_{\underline{Q}+-} = 0$

for every state we consider, so that:

$$(3.173)\quad E_{TOT} = \sum_{\underline{k}} F_{\underline{k}} E_{\underline{k}} - N(A_{o++}A_{o--} + A_{\underline{Q}++}A_{\underline{Q}--})$$

For our three magnetic states this becomes:

$$(3.174)\quad E_{TOT}^{5\text{ fold-}\underline{PM}} = \sum_{\underline{k}} F_{\underline{k}} E_{\underline{k}}^{PM} - NA_{o++}^2 \text{ since } A_{o++}=A_{o--} \text{ and } A_{\underline{Q}ij}=0$$

$$(3.175)\quad E_{TOT}^{5\text{ fold-}\underline{FM}} = \sum_{k} F_k E_k^{FM} - NA_{o++}A_{o--} \text{ since } A_{o++}\neq A_{o--} \text{ and } A_{\underline{Q}ij}=0$$

$$(3.176)\quad E_{TOT}^{5\text{ fold-A}\underline{FM}} = \sum_{\underline{k}} F_{\underline{k}} E_{\underline{k}}^{AFM} - NA_{o++}^2 - NA_{\underline{Q}++}^2 \text{ since } A_{o++}=A_{o--}$$

and $A_{\underline{Q}++}=A_{\underline{Q}--}$

The general energy expression can be written in terms of the B's as:

$$(3.177)\quad E_{TOT}^{5\text{ fold}} = \sum_{\underline{k}} F_{\underline{k}} E_{\underline{k}} - N\{[\sum_{\underline{k}} \frac{F_{\underline{k}}}{N} (B_2^2+B_4^2+B_6^2+B_8^2+B_{10}^2+B_{12}^2+$$

$$B_{14}^2+B_{16}^2+B_{18}^2+B_{20}^2]\cdot\sum_{\underline{k}} \frac{F_{\underline{k}}}{N}(B_1^2+B_3^2+B_5^2+B_{11}^2+B_{13}^2+$$

$$B_{15}^2+B_{17}^2+B_{19}^2)]\cdot[\sum_{\underline{k}} \frac{F_{\underline{k}}}{N}(B_1B_3+B_5B_7+B_9B_{11}+B_{13}B_{15}+$$

$$B_{17}B_{19})]\}$$

We have not put Co=(9K-4J) in the denominator of these subtractive expressions since we did not include any coupling constants in

our definition of the A's, whereas Penn did. Thus, he needed to divide by Co to make E_{TOT} dimensionally correct; we do not.

Our three final total energies are now:

$$(3.178)\quad E_{TOT}^{5\ fold-PM}=\sum_{\underline{k}}F_{\underline{k}}E_{\underline{k}}^{PM}-N\Big[\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}\,(B_2^2+B_4^2+B_6^2+B_8^2+B_{10}^2+B_{12}^2+B_{14}^2+B_{16}^2+B_{18}^2B_{20}^2)\Big]$$

$$(3.179)\quad E_{TOT}^{5\ fold-FM}=\sum_{\underline{k}}F_{\underline{k}}E_{\underline{k}}^{FM}-N\Big[\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_1^2+B_3^2+B_5^2+B_7^2+B_9^2+B_{11}^2+B_{13}^2+B_{15}^2+B_{17}^2+B_{19}^2)\Big]\cdot\Big[\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2^2+B_4^2+B_6^2+B_8^2+B_{10}^2+B_{12}^2+B_{14}^2+B_{16}^2+B_{18}^2+B_{20}^2)\Big]$$

$$(3.180)\quad E_{TOT}^{5\ fold-AFM}=\sum_{\underline{k}}F_{\underline{k}}E_{\underline{k}}^{AFM}-N\Big[\Big\{\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2^2+B_4^2+B_6^2+B_8^2+B_{10}^2+B_{12}^2+B_{14}^2+B_{16}^2+B_{18}^2+B_{20}^2)\Big\}^2-\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_1B_3B_5B_7B_9B_{11}B_{13}B_{15}B_{17}B_{19})\cdot\sum_{\underline{k}}\frac{F_{\underline{k}}}{N}(B_2B_4B_6B_8B_{10}B_{12}B_{14}B_{16}B_{18}B_{20})\Big]$$

We now derive our general subtractive expression:

$$(3.181)\quad E_{TOT}=\sum_{\underline{k}}F_{\underline{k}}E_{\underline{k}}-N(A_{o++}A_{o--}+A_{\underline{Q}++}A_{\underline{Q}--}-A_{o+-}^2-A_{\underline{Q}+-}^2)$$

from Penn's:

$$(3.182)\quad E_{TOT}=\sum_{\underline{k}\sigma}\epsilon_{\underline{k}}\langle a_{\underline{k}\sigma}^{+}a_{\underline{k}\sigma}\rangle+1/2Co\sum_{\ell\sigma}[\langle c_{\ell\sigma}^{+}c_{\ell\sigma}\rangle\langle c_{\ell\bar{\sigma}}^{+}c_{\ell\bar{\sigma}}\rangle-\langle c_{\ell\sigma}^{+}c_{\ell\bar{\sigma}}\rangle\langle c_{\ell\bar{\sigma}}^{+}c_{\ell\sigma}\rangle]$$

for completeness, simply by noting that $E_{TOT}=\sum_{\underline{k}}F_{\underline{k}}E_{\underline{k}}$ would double

count the effect of the various correlations on E_{TOT}. Thus, the true E_{TOT} must have them subtracted off.

We now outline the self-consistent decision procedure to decide whether at a particular point (n/2N,K,J,T) we shall find $F_{TOT}^{PM} \gtrless F_{TOT}^{FM}$. The minimum free energy will be the criterion for phase stability.

First we solve our master gap equation (3.168):

$$(3.168)\quad 1 = \left[\frac{K}{N}\sum_{j=1}^{9}\left\{\sum_{\underline{k}=0}^{kB1}\frac{F_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}} - \sum_{\underline{k}=\underline{k}B2}^{k_F}\frac{F_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}\right\}_j\right.$$

$$\left.-\frac{J}{N}\sum_{j=1}^{4}\left\{\sum_{\underline{k}=0}^{kB1}\frac{F_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}} - \sum_{k-kB1}^{k_F}\frac{F_{\underline{k}}}{\sqrt{\Delta^2+\epsilon_{\underline{k}}^2}}\right\}_j\right]$$

for Δ by guessing a value of $\Delta(=\Delta^{(i)})$:

We know: (a) $E_{\underline{k}}^{(i)}$ as a function of the bi's, $\epsilon_{\underline{k}}, \epsilon_{\underline{k}+\underline{Q}}, F_{\underline{k}}$

(b) $F_{\underline{k}}$ as a function of T, U, $E_{\underline{k}}^{(i)}$

(c) B_1 as a function of $\epsilon_{\underline{k}}$, Δ

(d) B_2 as a function of $\epsilon_{\underline{k}}$, Δ

(e) $\epsilon_k/4T = -1/2\sum_{i=1}^{3}\cos\varphi_i$, $\varphi = \underline{k}\cdot\underline{a}$

Now (a) and (b) together form a self-consistent calculation since we need $F_{\underline{k}}(\Delta)$ and $E_{\underline{k}}^{(i)}(\Delta)$ to solve the master gap equation above.

Second, we see if Δ is satisfactorily computed from our master gap equation, $(=\Delta^{(2)})$, by comparing with $\Delta^{(1)}$:

$$\Delta^{(2)}-\Delta^{(1)} \leq \text{an error factor}$$

If so, we have found the correct Δ and can proceed to calculate E_{TOT}^{AFM} as a function of Δ, $Bi(\Delta)$. If not so, we either increase or decrease our Δ and find a $\Delta^{(3)}$ from the master gap equation. We then test $\Delta^{(3)}$ as we tested $\Delta^{(2)}$, etc. This is conveniently summarized in the flow-charts (Figures 18 and 19).

The testing of F_{TOT}^{PM} versus F_{TOT}^{FM} to determine whether PM or FM has a minimum for a given parameter set (n/2N,K,J,T) is different from the AFM-PM calculation since a gap equation cannot be used.

Here, we must write an E+ for up spins and an E- for down spins, sum them to get an E_{TOT}, and then minimize E_{TOT} with respect to $\delta = n_+ - n_-$, the difference between up spin and down spin electron densities. A $\delta=0$ determination means the PM state is stable for a particular parameter choice (n/2N,K,J,T). A $\delta>0$ implies a FM state, with varying degrees of net spin polarization from $n_+ \approx n_-$ so that $\delta>0$, but just barely, to $n_+ = n_{total}$ so that δ reaches a maximum, the completely polarized FM state. (The PM-FM flow chart is given in Figure 17).

Figure 17. FM-PM Flow Chart.

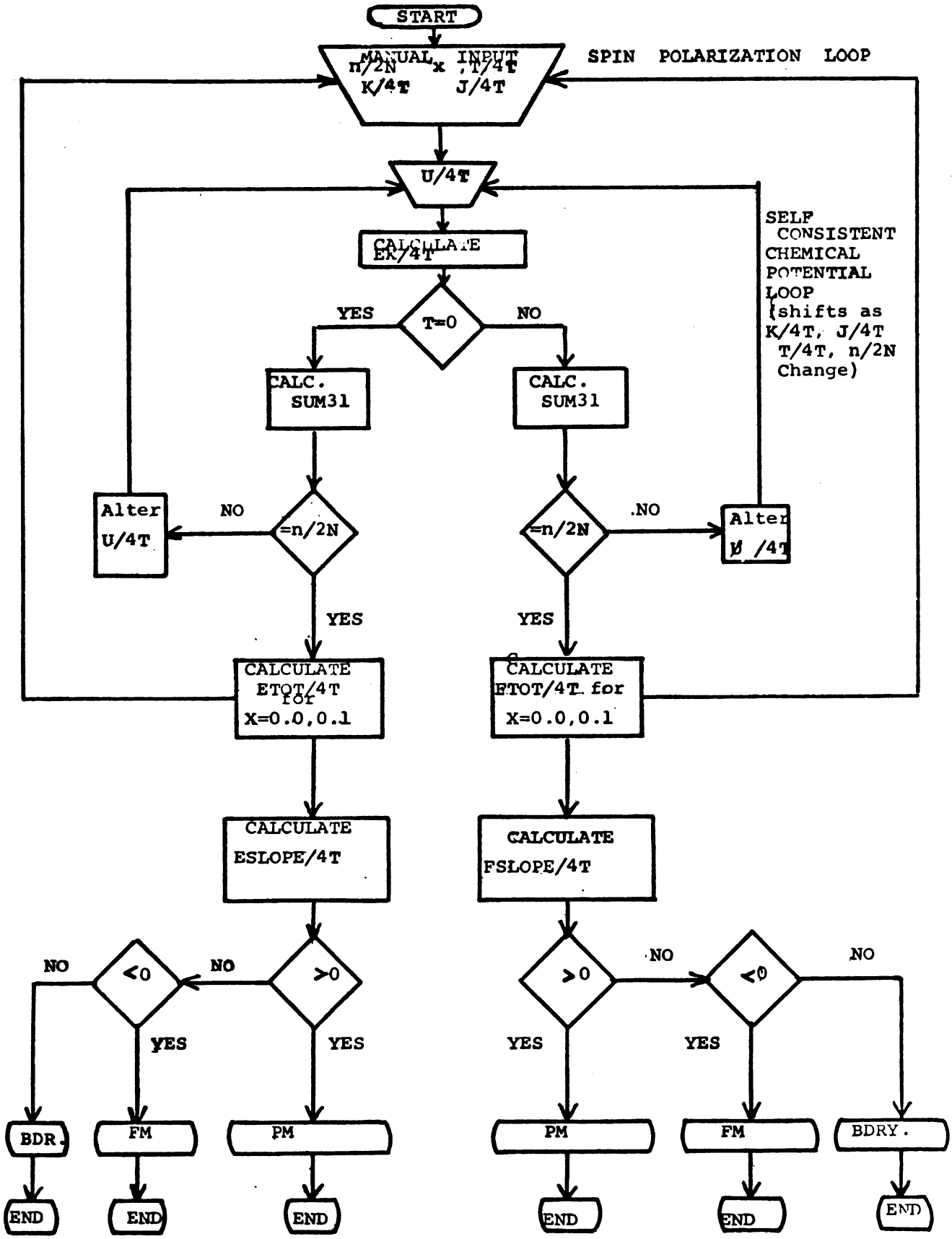

START
MANUAL INPUT
n/2N x ,T/4T
K/4T J/4T
SPIN POLARIZATION LOOP
U/4T
CALCULATE ER/4T
SELF CONSISTENT CHEMICAL POTENTIAL LOOP (shifts as K/4T, J/4T T/4T, n/2N Change)
T=0
YES
NO
CALC. SUM31
CALC. SUM31
Alter U/4T
NO
=n/2N
=n/2N
.NO
Alter
YES
YES
CALCULATE ETOT/4T for X=0.0,0.1
CALCULATE ETOT/4T for X=0.0,0.1
CALCULATE ESLOPE/4T
CALCULATE FSLOPE/4T
NO
<0
NO
>0
>0
NO
<0
NO
YES
YES
YES
YES
BDR.
FM
PM
PM
FM
BDRY.
END
END
END
END
END
END

Figure 18. AFM-PM Flow Chart (Any T, $K/4T < 3.5$).

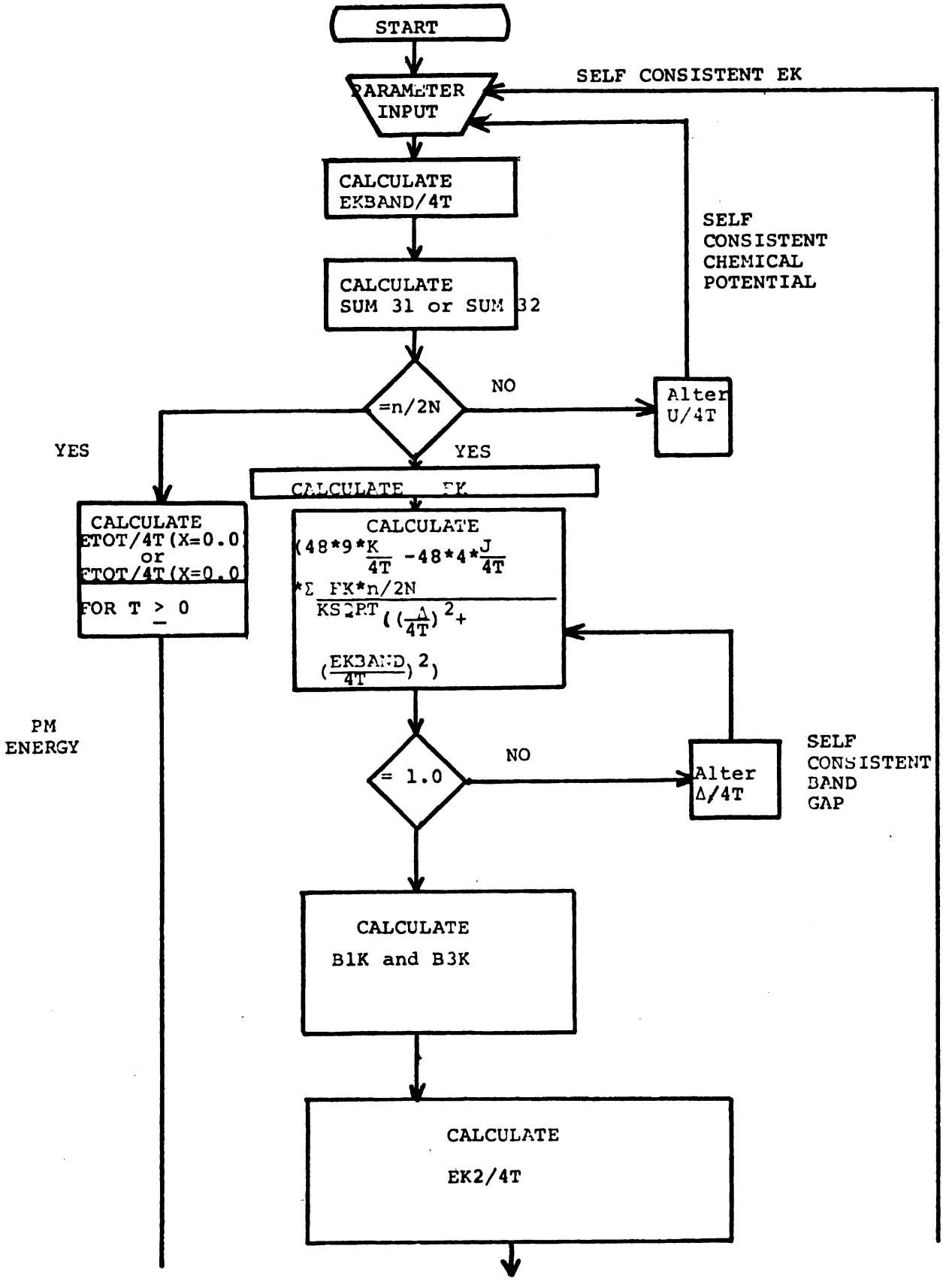

START
PARAMETER INPUT
SELF CONSISTENT EK
CALCULATE EKBAND/4T
CALCULATE SUM 31 or SUM 32
SELF CONSISTENT CHEMICAL POTENTIAL
=n/2N
NO
Alter U/4T
YES
YES
CALCULATE EK
CALCULATE ETOT/4T (X=0.0 or ETOT/4T (X=0.0
FOR T ≥ 0
CALCULATE
(48*9*K/4T -48*4*J/4T
*Σ FK*n/2N / KSQRT((Δ/4T)^2+
(EKBAND/4T)^2)
PM ENERGY
= 1.0
NO
Alter Δ/4T
SELF CONSISTENT BAND GAP
CALCULATE
B1K and B3K
CALCULATE
EK2/4T

Figure 18 (cont'd.)

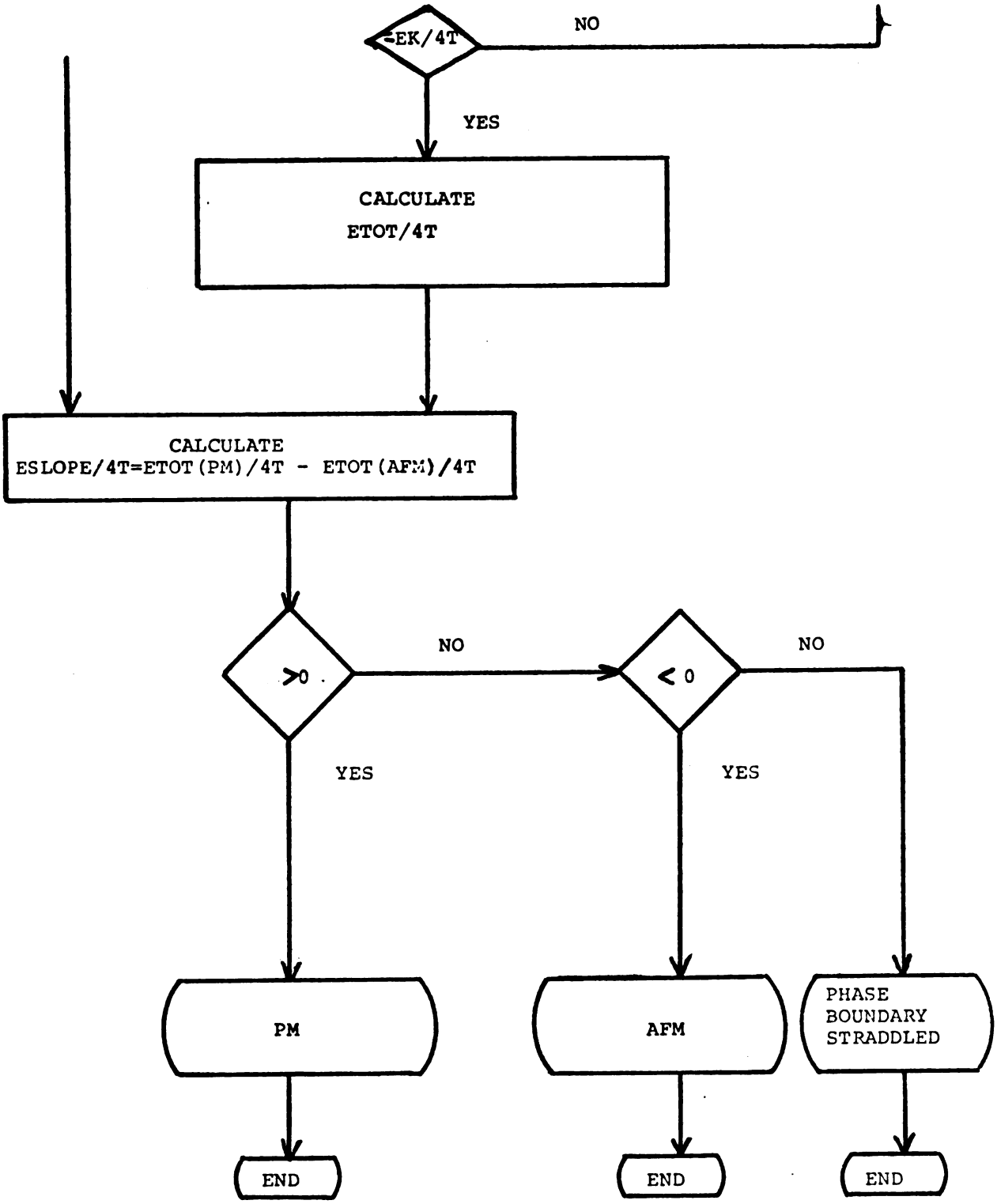

=EK/4T
NO
YES
CALCULATE
ETOT/4T
CALCULATE
ESLOPE/4T=ETOT(PM)/4T - ETOT(AFM)/4T
>0
NO
< 0
NO
YES
YES
PM
AFM
PHASE
BOUNDARY
STRADDLED
END
END
END

Figure 19. AFM-FM Flow Chart (Any T) $K/4T \geq 3.5$).

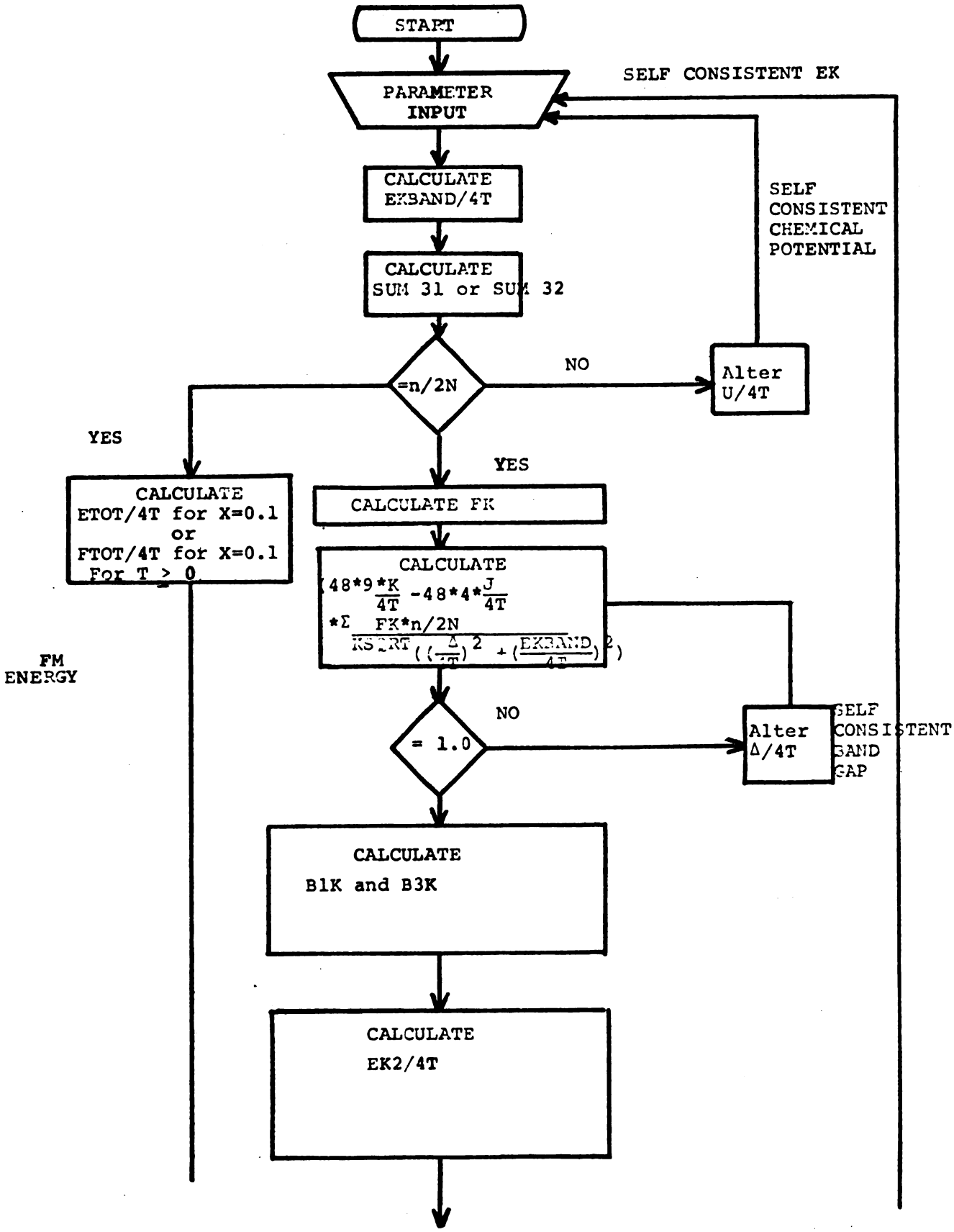
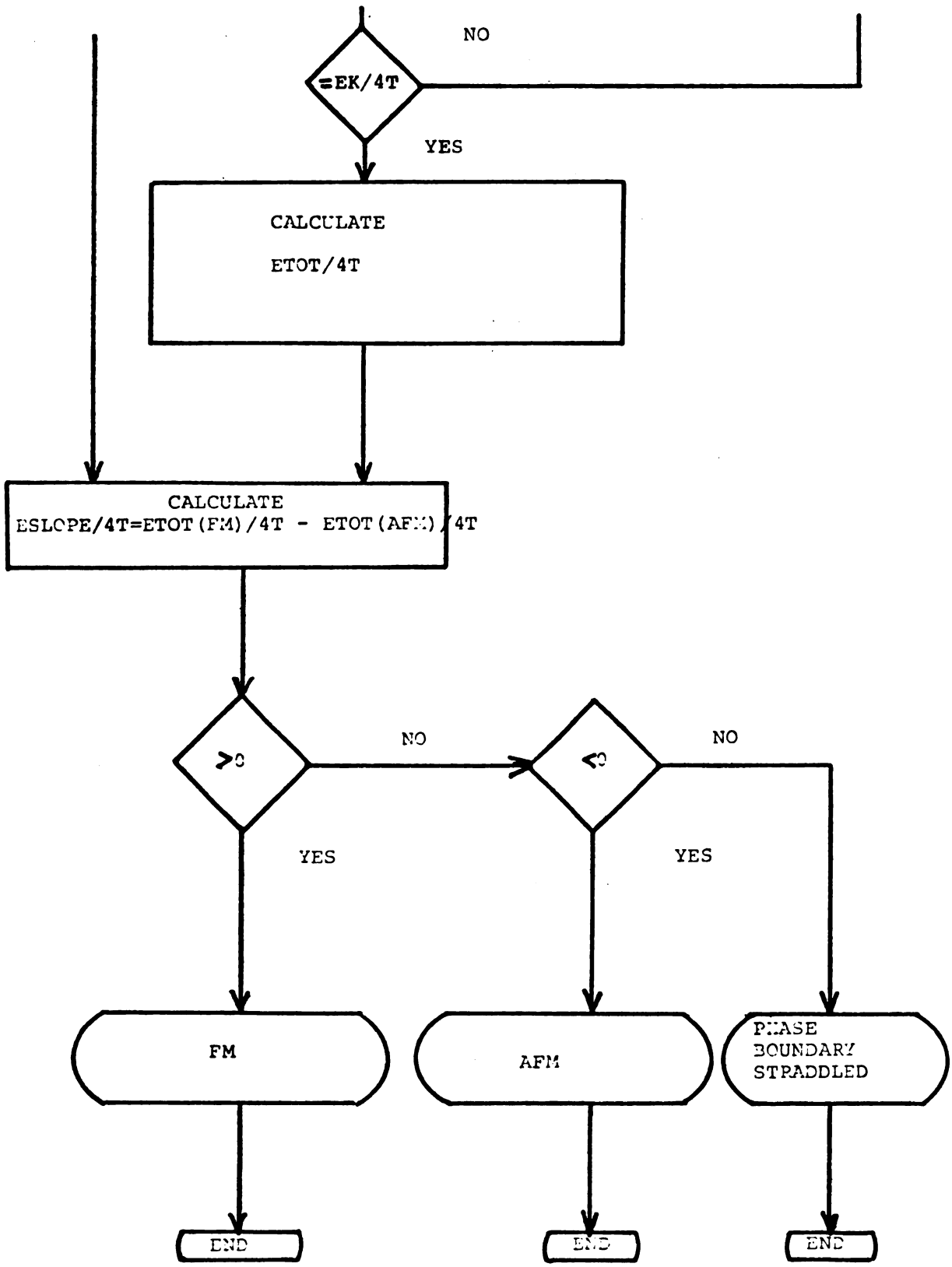

START
PARAMETER INPUT
SELF CONSISTENT EK
CALCULATE EKBAND/4T
SELF CONSISTENT CHEMICAL POTENTIAL
CALCULATE SUM 31 or SUM 32
=n/2N
NO
Alter U/4T
YES
YES
CALCULATE ETOT/4T for X=0.1 or FTOT/4T for X=0.1 For T > 0
CALCULATE FK
CALCULATE
48*9*K/4T -48*4*J/4T
*Σ FK*n/2N
RSQRT((Δ/4T)^2 + (EKBAND/4T)^2)
FM ENERGY
NO
= 1.0
Alter Δ/4T
SELF CONSISTENT BAND GAP
CALCULATE B1K and B3K
CALCULATE EK2/4T

Figure 19 (cont'd.)


NO
=EK/4T
YES
CALCULATE
ETOT/4T
CALCULATE
ESLOPE/4T=ETOT(FM)/4T - ETOT(AFM)/4T
>0
NO
<0
NO
YES
YES
FM
AFM
PHASE
BOUNDARY
STRADDLED
END
END
END

We programmed an interactive summation over 1540 points in 1/48 of the Brillouin zone, allowing for a 540 point overcount by weighing points on the [111] axis by 1/6 and points on the 1/4 zone planes by 1/2. Therefore, we effectively count 1,000 points per 1/48 of the Brillouin zone. The renormalized energies, EK1, Ek2, were calculated as functions of J/4T, K/4T, n/2N, X, U and $\underline{k}_B T$ and used in the appropriate total energy (at small $k_B T$). In the FM-PM comparison program, U was iteratively calculated as a sum of Fermi factors and compared with its initial value until a self-consistent U was achieved. In the AFM-PM comparison, this was done for Δ as well as U. The Δ and U iterative loops are concentric so that one self-consistency depended upon the other. In the FM-PM comparison we calculated F_{TOT} (X=0.0) and F_{TOT}(X=0.1), X being the net spin polarization for constant $k_B T$, n/2N, J/4T, K/4T and $U_{S.C.F.}$. The sign of the slope of the difference, $[F_{TOT}(X=0.0)-F_{TOT}(X=0.1)]$/increment n/2N yielded a measure of whether at any point in the K/4T, J/4T, n/2N three dimensional space, the FM state had lower or higher energy than the PM state. If a small slope was found, n/2N was increased by 0.01 until a large slope appeared, indicating a FM-PM second order phase transition line had been crossed. Then a smaller K/4T value was chosen and the same process redone. Finally, J/4T was manually changed and we then had derived the FM-PM phase diagram for a given kT. Indicating electron and hole symmetry in the problem, the n/2N axis only when up to

$n/2N = 0.5$ since Penn's phase diagram is symmetric about $n/2N = 0.5$. As we expected our FM region to be larger at low k_BT, we limited $n/2N$ to 0.2, Penn's lowest FM phase boundary intercept of a horizontal line. Our FM phase boundary line should be outside his; hence, intercept some horizontal line (some K/4T value not necessarily his) at a lower $n/2N$ value.

The flow charts for both programs are given with the running FM-PM program. High k_BT and low k_BT cases were run on the same program with appropriate instructions for skipping the entropy calculation for low k_BT (≈ 0.0001) and summing Fermi factors = 1 or 0, rather than doing out the actual exponential summation of Fermi factors as was done at higher k_BT.

In this program, we sum $\underline{k}$ over 1,000 points in 1/48 of the cubic lattice Brillouin zone so that, since the number of states equals the number of atoms in the solid, N = 48,000. For every Σ we have a 1/N to normalize $\Sigma F_{\underline{k}}/N$ to a number less than 1. N is meaningless when we compare total free energies of the various states; it cancels out.

We can utilize the symmetry of d-electrons and d-holes in reducing the number of values of 1/2 n/N, the band filling, we must calculate with Penn's phase diagram, since for s-electrons (Fig. 5) is symmetric about 1/2 n/N = 1/2, the half-filled band

Table 6. Running FM-PM Program.

```
            PROGRAM FERRO (OUTPUT=200)
C-------------COMMENT--MUST ALWAYS HAVE DIRECT .GE. EXCHANGE-----------------CAUTION
C---------------- -----------COMMENT-------STRADDLE STORAGE-------------------------
C---------------- -----------COMMENT-------STRADDLE STORAGE-------------------------
 3          REAL NDIV2N
 4          REAL KB
C------COMMENT-----------WEIGHING STORAGE-----------------------------------------
C------COMMENT-----------WEIGHING STORAGE-----------------------------------------
           DIMENSION FTOT(2),FTOT(2),E1(2000),E2(2000),EK1(2000),EK2(2000),
          1  R(2000),G(10),H(10)
           DATA (FTOT=10004*0.)
           DATA (H(I),I=1,8)/3.3,3.5,4.4,5.7,7.0,7.5,8.0,8.5/
           DATA (G(I),I=1,8)/.08,.12,.16,.20,.24,.28,.32,.36/
           DO 8888 MI=1,8
           NDIV2N=G(MI)
           SUM32=0.
           SUM31=0.
           NUMLOOP=0
           ILOOPY=0
           ILOOPZ=0
           ETOTI=0.0
           FTOTI=0.0
           ETOT(1)=0.0
           ETOT(2)=0.0
           FTOT(1)=0.0
           FTOT(2)=0.0
           ESLOPE=0.0
           ETOT1=0.0
           ETOT2=0.0
           FSLOPE=0.0
           FTOT1=0.0
           FTOT2=0.0
```

Table 6 (cont'd.)

```
10          KB=.00008613960
9800        FORMAT(* *95X,15)
9998        FORMAT(* *315,2F10.5)
            TT=0.0001
C-------COMMENT-TT IS A MANUAL VARIABLE-------------------------MANUAL TT------------
30          T=TT/.00008613960
50          EXCHANGE=0.0
C-------COMMENT-EXCHANG IS A MANUAL VARIABLE----------------------MANUAL EXCHA
60 DIRECT=3.2
C-------- ---------------- -- ---------- ----------MANUAL K/4T IN 60    ---------------
C-------- ---------------- -- ---------- ----------MANUAL N/2N IN 70-------------------
80 DO 505 lX=1,2
            IC=0
            NUMLOOP=0
            ILOOPY=0
            ILOOPZ=0
81          XX=IX-1
82          X=XX/10.0
83          GO TO 90
85          PRINT 86
86          FORMAT(* U HAS EXCEEDED -1.5*)
87          GO TO 9999
90          U=H(MI)
C---------COMMENT-THE INITIAL U VALUE IS A MANUAL VARIABLE  ---MANUAL U INPUT
C-------  ----------COMMENT------BEGINNING OF LOW TEMP CALC OF Y --------------------
            PI=3.14159
94          DO 130 I=1,20
95          DO 131 L=1,I
96          DO 132 N=1,L
            IC=IC+1
97          A = I
98          B = L
99          C = N
```

Table 6 (cont'd.)

```
101         FIX=PI*(A-.5)/20.0
102         FIY=PI*(B-.5)/20.0
103         FIZ=PI*(C-.5)/20.0
C--         WEIGHING SCHEME TO BE USED IN FTOT AND ETOT CALCS ONLY   ----WEIGHING------
            IF(A.EQ.B)  GO TO 105
            IF(A.EQ.C)  GO TO 124
            IF(B.EQ.C)  GO TO 124
            GO TO 121
105         IF(B.EQ.C)  GO TO 122
            GO TO 124
121         R(IC)=1.
C------- ------------COMMENT---------A .NE~ B .NE. C CASE
            GO TO 125
122         R(IC)=1./6.
C----------------COMMENT---------A = B = C CASE
            GO TO 125
124         R(IC)=0.5
C------------COMMENT-----------A = B .NE. C  OR  B = C .NE. A CASES
C-----END OF WEIGHING SCHEME        ----------------------------------WEIGHING
125         EK1(IC)=-.5*(COS(FIX)+COS(FIY)+COS(FIZ))+4.*(DIRECT-EXCHANG)*
            1 NDIV2N*(1.+X)+5.*DIRECT*NDIV2N*(1.-X)
            EK2(IC)=-.5*(COS(FIX)+COS(FIY)+COS(FIZ))+4.*(DIRECT-EXCHANG)*
            1 NDIV2N*(1.-X)+5.*DIRECT*NDIV2N*(1.+X)
132         CONTINUE
131         CONTINUE
130         CONTINUE
            NARR=IC
91          IF (U .LT. -1.5) GO TO 85
92          IF (NUMLOOP .GT. 50) GO TO 9700
            PRINT 93, IX, NUMLOOP, ILOOPY, ILOOPZ
93          FORMAT(1H ,*IX=*,13, * NUMLOP =*,13, *  ILOY =*,13, * ILOZ = *,
            1  I3, )
146         IF (TT .GT. ).0001) GO TO 205
```

Table 6 (cont'd.)

```
            SUM3=0.0
            SUM31=0.0
            Y=0.0
            DO 165 IC=1,NARR
148         IF(EK2(IC).LE.U) GO TO 150
149         FK2=0.0
            GO TO 151
150         FK2=1.0
151         IF(EK1(IC).LE.U)  GO TO 154
153         FK1=0.0
            GO TO 160
154         FK1=1.0
160         SUM3=0.5 * (FK1+FK2)/1540.0
161         SUM31=SUM31+SUM3
162         Y=SUM31-NDIV2N
165         CONTINUE
            GO TO 240
C--------------- --------------COMMENT-----------END OF LOW TEMP CALCULATION OF Y ----
C--------------- --------------COMMENT----------BEGINNING OF HIGH TEMP CALC OF Z------
205         SUM32=0.0
            Z=0.0
            THREE=0.0
            DO 135 IC=1,NARR
            E1 (IC)=(FK1(IC)-/)/TT
            E2UIC)=(EK2(IC)-U)/TT
            IF (E1(IC).GE.0.0.AND.E2(IC).GE.0.0)  GO TO 227
            IF UE1 (IC).LT.0.0.AND.E2(IC).LT.0.0)  GO TO 216
            IF (E1 (IC).LT.0.0.AND.E2(IC).GE.0.0)  GO TO 212
            IPOS=1
20          VV=1.0/EXP(-1.0*E2(IC))
209         PITHREE=1.0/(1.0+EXP(E1(IC)))
210         P2THREE=(1.0+VV)**(-1)
211         GO TO 221
```

Table 6 (cont'd.)

```
212         V=1.0/EXP(-1.)*E1(IC))
            IPOS=4
213         PITHREE=(1.0+V)**(-1)
214         P2THREE=1.0/(1.0+EXP(E2(IC)))
215         GO TO 221
216         V=1.0/EXP(-1.0*E1(IC))
217         VV=1.0/EXP(-1.0*E2(IC))
            IPOS=2
219         PITHREE=1.0/(1.0+V)
220         P2THREE=1.0/(1.0+VV)
221         THREE=(0.5/1540.0)*(PITHREE+P2THREE)
222         GO TO 228
227         THREE=1.0/(1.0+EXP(E1(IC)))+ 1.0/(1.0+EXP(E2(IC)))
            THREE=THREE*0.5/1540.0
            IPOS=3
228         SUM 32 = SUM 32 + THREE
229         Z=SUM 32 - NDIV2N
230         PRINT 231, IPOS, E1(IC),E2(IC)
231         FORMAT(* *25X,14,5X,2E20.13)
135         CONTINUE
240         PRINT 245
245         FORMAT(* SUM31*,10X,* SUM32*,10X,* NDIV2N*,10X,* U*,10X,* X*,10X,
            1* EXCHANG*,10X,* DIRECT*,10X,* T*,10X,* Y*,10X,* Z*)
            PRINT 250,SUM31,SUM32,NDIV2N,U,X,EXCHANG,DIRECT,T,Y,Z
250         FORMAT(1H , 10(F9.4,4X))
            IF(TT.LE.0.0001) GO TO 265
C------- ---------COMMENT--------END OF HIGH TEMP CALC OF Z-------------------------
C------- -----------COMMENT--------BEGINNING OF Z DECISION AREA---------------------
244         IF (ABS(Z) .LF. 0.5) GO TO 248
            IF (Z .LT. 0.0) GO TO 247
246         U=U+0.5
            NUMLOOP=NUMLOOP+1
            ILOOPZ=1
```

Table 6 (cont'd.)

```
          GO TO 91
247       U=U-0.5
          NUMLOOP=NUMLOOP+1
          ILOOPZ=1
          GO TO 91
248       IF (ABS(Z) .LE. 0.4) GO TO 252
249       IF (Z .LT. 0.0) GO TO 251
          U=U+0.2
          NUMLOOP=NUMLOOP+1
          ILOOPZ=2
          GO TO 91
251       U=U-0.2
          NUMLOOP=NUMLOOP+1
          ILOOPZ=2
          GO TO 91
252       IF (ABS(Z) .LE. 0.3) GO TO 256
253       IF (Z .LT. 0.0) GO TO 255
254       U=U+0.075
          NUMLOOP=NUMLOOP+1
          ILOOPZ=3
          GO TO 91
255       U=U-0.075
          NUMLOOP=NUMLOOP+1
          ILOOPZ=3
          GO TO 91
256       IF (ABS(Z) .LE. 0.1) GO TO 260
257       IF (Z .LT. 0.0) GO TO 259
258       U=U+0.03
          NUMLOOP=NUMLOOP+1
          ILOOPZ=4
          GO TO 91
259       U=U-0.03
          NUMLOOP=NUMLOOP+1
```

Table 6 (cont'd.)

```
            ILOOPZ=4
            GO TO 91
260         IF (ABS(Z) .LF. 0.01) GO TO 264
261         IF (Z .LT. 0.0) GO TO 263
262         U=U+0.01
            NUMLOOP=NUMLOOP+1
            ILOOPZ=5
            GO TO 91
263         U=U-0.01
            NUMLOOP=NUMLOOP+1
            ILOOPZ=5
            GO TO 91
264         GO TO 278
C---- COMMENT-END OF Z COMPARISON WITH NDIV2N TO GET RIGHT U AT HIGH TEMP----------
C--------------COMMENT--------BEGINNING OF Y DECISION AREA-------------------------
265         IF (ABS(Y) .LE. 0.5) GO TO 267
            IF (Y .LT. 0.0) GO TO 266
            U=U-0.5
            NUMLOOP=NUMLOOP+1
            ILOOPY=1
            GO TO 91
266         U=U+0.5
            NUMLOOP=NUMLOOP+1
            ILOOPY=1
            GO TO 91
267         IF (ABS(Y) .LE. 0.4) GO TO 269
            IF (Y .LT. 0.0) GO TO 268
            U=U-0.2
            NUMLOOP=NUMLOOP+1
            ILOOPY=2
            GO TO 91
268         U=U+0.2
            NUMLOOP=NUMLOOP+1
            ILOOPY=2
```

Table 6 (cont'd.)

```
          GO TO 91
269       IF (ABS(Y) .LT. 0.3) GO TO 271
          IF (Y .LT. 0.0) GO TO 270
          U=U-0.15
          NUMLOOP=NUMLOOP+1
          ILOOPY=3
          GO TO 91
270       U=U+0.15
          NUMLOOP=NUMLOOP+1
          ILOOPY=3
          GO TO 91
271       IF (ABS(Y) .LT~ 0.1) GO TO 273
          IF (Y .LT. 0.0) GO TO 272
          U=U-0.06
          NUMLOOP=NUMLOOP+1
          ILOOPY=4
          GO TO 91
272       U=U+0.06
          NUMLOOP=NUMLOOP+1
          ILOOPY=4
          GO TO 91
273       IF (ABS(Y) .LE. 0.01) GO TO 275
          IF (Y .LT. 0.0) GO TO 274
          U=U-0.02
          NUMLOOP=NUMLOOP+1
          ILOOPY=5
          GO TO 91
274       U=U+0.02
          NUMLOOP=NUMLOOP+1
          ILOOPY=-5
          GO TO 91
275       CONTINUE
278       PRINT 279, Y,Z,U
```

Table 6 (cont'd.)

```
279         FORMAT(1HO,  3E12.6)
C-------COMMENT-END OF Y COMPARISON WITH NDIV2N TO GET RIGHT U AT LOW TEMP----------
C------BEGINNING OF ETOT OR FTOT DECISION DEPENDING ON TEMP-------------------------
            IF (TT .GT. 0.0001) GO TO 400
C---------END OF ETOT OR FTOT DECISION DEPENDING ON TEMP---------------------------
C-------BEGINNING OF ETOT COMPUTATION-----------------------------------------------
317         DO 330 IC=1,NARR
            ETOTI=0.0
            IF (EK2(IC).LE.U) GO TO 318
            ZAMM=0.0
            GO TO 319
318         ZAMM=1.0
319         IF (EK1(IC).LE.U) GO TO 321
            ZIM=0.0
            GO TO 322
321         ZIM=1.0
322         CONTINUE
            E1(IC)=(EK1(IC)-U)/TT
            E2(IC)=(EK2(IC)-U)/TT
326         ETOTI=(5.*48./48000.)*(E1(IC)*ZIM+E2(IC)*ZAMM)-
            1 (240./48000.)*(NDIV2N*(1.+X)*NDIV2N*(1.-X) )
            ETOTI=ETOTI*R(IC)
328         ETOT(IX)=ETOT(IX)+ETOTI
C-------------COMMENT-------------------------WEIGHING
330         CONTINUE
360         PRINT 370,ETOT,DIRECT,EXCHANG,U,X,NDIV2N,T
370         FORMAT(1H1, 7(F10.4,5X))
C-----------END OF ETOT COMPUTATION-----------------------------------------------
            IF (IX.GT.1) GO TO 372
371         GO TO 505
C----------BEGINNING OF ETOT STRADDLE ROUTINE-------------------------------------
372         ETOT2=ETOT(1)
C-----------COMMENT--------ETOT2 IS ETOT(X=0.0)
373         ETOT1=ETOT(2)
C-------------COMMENT----------ETOT1 IS ETOT(X=0.01)
```

Table 6 (cont'd.)

```
375         ESLOPE=(ETOT2-ETOT1)/0.1
376         IF (ESLOPE .GT. 0.0) GO TO 382
377         IF (ESLOPE .LT. 0.0) GO TO 387
380         PRINT 381
381         FORMAT (1H1, 10X, *ETOT HAS ZERO SLOPE FOR THIS NDIV2N BAND FILLING
            1 VALUE* )
            GO TO 9999
382         PRINT 383
383         FORMAT (1HO, *PARAMAGNETIC*,9X,*K*,9X, *N/2N*,9X,*J*,9X, *T*,9X,
            1 9X, *SUM31*,9X, *SUM32*,9X, *U* )
384         PRINT 385, DIRECT,NDIV2N,EXCHANG,T,SUM31,SUM32,U
385         FORMAT (1HO,14X, 7(F10.3,4X))
            GO TO 9999
387         PRINT 388
388         FORMAT (1HO, *FERROMAGNETIC*, 9X, *K*,9X, *N/2N*,9X, *J*,9X, *T*,
            1*SUM31*,9X,*SUM32*,9X,*U*)
389         PRINT 385, DIRECT,NDIV2N,EXCHANG,T,SUM31,SUM32,U
            GO TO 9999
C-------END OF ETOT STRADDLE ROUTINE     ------------------------------------------
C-----BEGINNING OF FTOT COMPUTATION    ------------------------------------------
400         DO 430 IC=1,NARR
            FTOTI=0.0
            ZIM=(1.+EXP(E1(IC)))**(-1)
            ZAMM=(1.+EXP(E2(IC)))**(-1)
426         FTOTI=(240./48000.)*(E1(IC)*ZIM+E2(IC)*ZAMM)-
            1  U240./48000.)*(NDIV2N*(1.+X)*NDIV2N*(1.-X))-
            2  5.*.001*KB*T*(ZIM*ALOG(ZIM)+ZAMM*ALOG(ZAMM)+
            3  U1.-ZIM)*ALOG(1.-ZIM)+(1.-ZAMM)*ALOG(1.-ZAMM))
            FTOTI=FTOTI*R(IC)
428         FTOT(IX)=FTOT(IX)+FTOTI
C------COMMENT-------------------------WEIGHING
430         CONTINUE
500         PRINT 501
501         FORMAT(*FTOT*,5X,*NDIV2N*,5X,*DIRECT*,5X,*EXCHANG*,5X,
            1*T*,5X,*X*,5X,*U*)
```

Table 6 (cont'd.)

```
502         PRINT 503,FTOT,NDIV2N,DIRECT,EXCHANG,T,X,U
503         FORMAT(*F7.4,5X,F7.4,5X,F7.4,5X,F7.4,5X,F7.4,5X,F7.4,5X,F7.4*)
505         CONTINUE
C--------COMMENT-X=0.0,0.01 LOOP FOR STRADDLE ROUTINE    --------------------------
C--------END OF FTOT  COMPUTATION-----------------------------------------------------
C--------BEGINNING OF FTOT STRADDLE ROUTING-------------------------------------------
600         FTOT2=FTOT(1)
C-------COMMENT-------FTOT2=FTOT(X=0.0)
604         FTOT1=FTOT(2)
C--------FTOT1=FTOT(X=0.01)
605         FSLOPE=(FTOT2-FTOT1)/0.1
610         IF (FSLOPE  .GT. 0.0) GO TO 645
620         IF (FSLOPE .LT. 0.0) GO TO 653
640         PRINT 641
641         FORMAT (*FTOT HAS ZERO SLOPE FOR THIS NDIV2N BAND FILLING VALUE*)
            GO TO 9999
645         PRINT 646
646         FORMAT (*PARAMAGNETIC*,5X,*K*,5X,*N/2N*,5X,*J*,5X,*T*)
650         PRINT 651,DIRECT,NDIV2N,EXCHANG,T
651         FORMAT(*15X,F7.4,5X,F7.4,5X,F7.4,5X,F7.4*)
            GO TO 9999
653         PRINT 654
654         FORMAT (*FERROMAGNETIC*,5X,*K*,5X,*N/2N*,5X,*J*,5X,*T*)
655         PRINT 656,DIRECT,NDIV2N,EXCHANG,T
656         FORMAT (*15X,F7.4,5X,F7.4,5X,F7.4,5X,F7.4*)
            GO TO 9999
C--------END OF FTOT STRADDLE ROUTINE-------------------------------------------------
9700        PRINT 9701
9701        FORMAT (* TOO MANY U LOOPS--MORE THAN TWENTY*)
9999        CONTINUE
8888        CONTINUE
            END
'
'
```

case. We need only heuristically prove why this was so in his calculation to show that it will also be true of our phase diagram at any temperature and for any J/4T value. The Hubbard-Hamiltonian contains, in the interaction term, the two-body operator product $a^+a\ a^+a$, which becomes $\langle a^+a\rangle a^+a$ after Gorkov factorization. These may be written in number operator form, since $n = a^+a$, as n n and $\langle n\rangle n$ respectively. Whichever we choose to consider, we know that the number of d-type particles, be they electrons (to the left of 1/2 n/N) or holes (to the right of 1/2 n/N = 1/2), enter as n^2. Now, the number of electrons added to the number of holes is unity. Calling n the number of electrons and h the number of holes:

$$n + h = 1 \qquad (3.184)$$

Thus:

$$n^2 = (1-h)^2 \qquad (3.185)$$

which becomes:

$$n^2 = 1 - 2h + h^2 \qquad (3.186)$$

Now the factor "1" is a constant and can be absorbed in $H_{Hubbard}$ by redefining our origin of energy when we calculate the eigenvalues of $H_{Hubbard}$, the $E_{\underline{k}}$'s. The "-2h" factor is linear in the number of holes, while all interaction terms are quadratic in the number operator, be it n for electrons or h for holes. Thus, "-2h" is absorbed in the definition of $\epsilon_{\underline{k}}$ in the kinetic energy term and

$$n^2 = h^2 \qquad (3.187)$$

as far as the interaction term goes. So the 1/2 n/N > 1/2 and 1/2 n/N < 1/2 halves of the phase diagram as symmetric about the half-filled band, 1/2 n/N , 1/2, ordinate, for any k/4T, J/4T, or temperature T/4T. The utilization of five-fold degenerate electrons has no bearing on this: In Penn's diagram we have:

$$(3.188) \quad n_s^2 = h_s^2;$$

in ours, we will have:

$$(3.189) \quad n_d^2 = h_d^2.$$

A further simple result will help us eliminate the number of iterations necessary to calculate the chemical potential as a function of temperature/4T[67]. Kittel plots chemical potential/E_F as a function of k_BT/E_F for a free electron gas in three dimensions. Since our Gorkov factorization reduced our d-electron system to a system of quasi-d-electrons, we can use Kittel's diagram, reproduced here, to help us select a best first guess for the chemical potential in our programs.

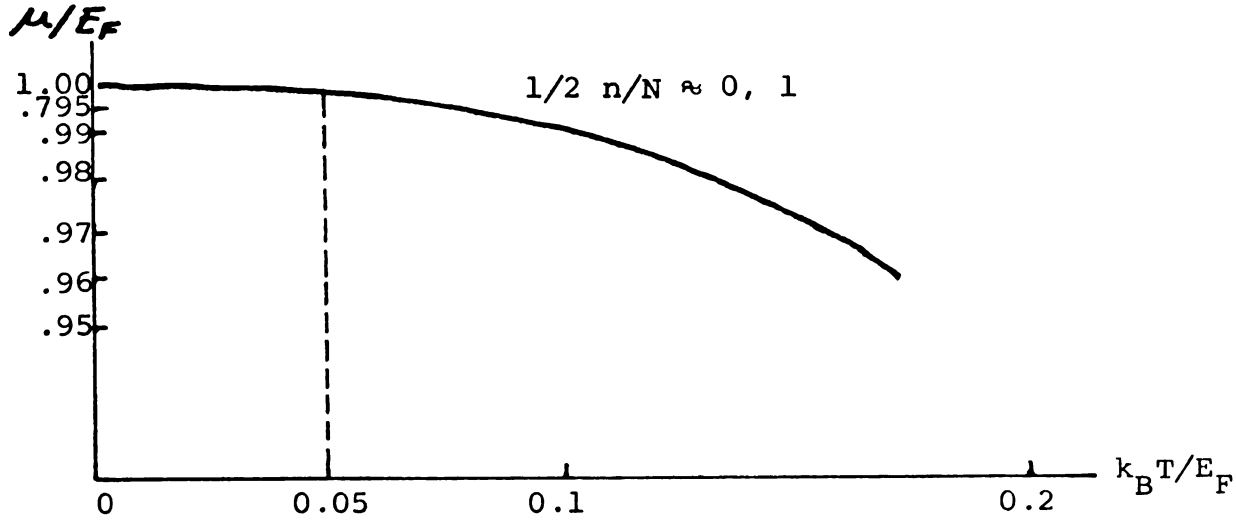


Figure 20. Variation in Chemical Potential as a Function of Temperature.

From this we can read off some interesting results. At zero temperature $\mu = \epsilon_F$ since $\mu/\epsilon_F = 1.00$. Now $\epsilon_F \approx 40{,}000°K$, so $k_BT/\epsilon_F = 0.2$ corresponds to 8,000°K. Thus $k_BT/\epsilon_F = 0.1$ corresponds to 4,000°K. Our highest Currie or Neel temperature is of the order of 1,800°K, so that we are always going to be working at $k_BT/\epsilon_F<0.005$. The ordinate value of $\mu/\epsilon_F = 0.99$ and is probably above $\mu/\epsilon_F = 0.995$. Thus, for our highest temperature, say $\approx$ 1,800"K, $\mu = 0.995\ \epsilon_F$, is an excellent first guess for the chemical potential. Only, at most, four iterations will be needed to achieve the best μ to the nearest thousandth. For low temperatures, a guess of $\mu = \epsilon_F$ will yield quick results and similarly.

There is one difficulty with this approach. Kittel's "free electron gas" means just that; $n/2N \approx 0$ (or ≈ 1, since a free hole gas should behave just as a free electron gas, as we have argued before), and we must correct his curve, Fig. 20, as 1/2 n/N approaches 1/2, the half-filled band case. For the half-filled band case, $\mu = \epsilon_F$. Thus, we have a family of curves as in Figure 21.

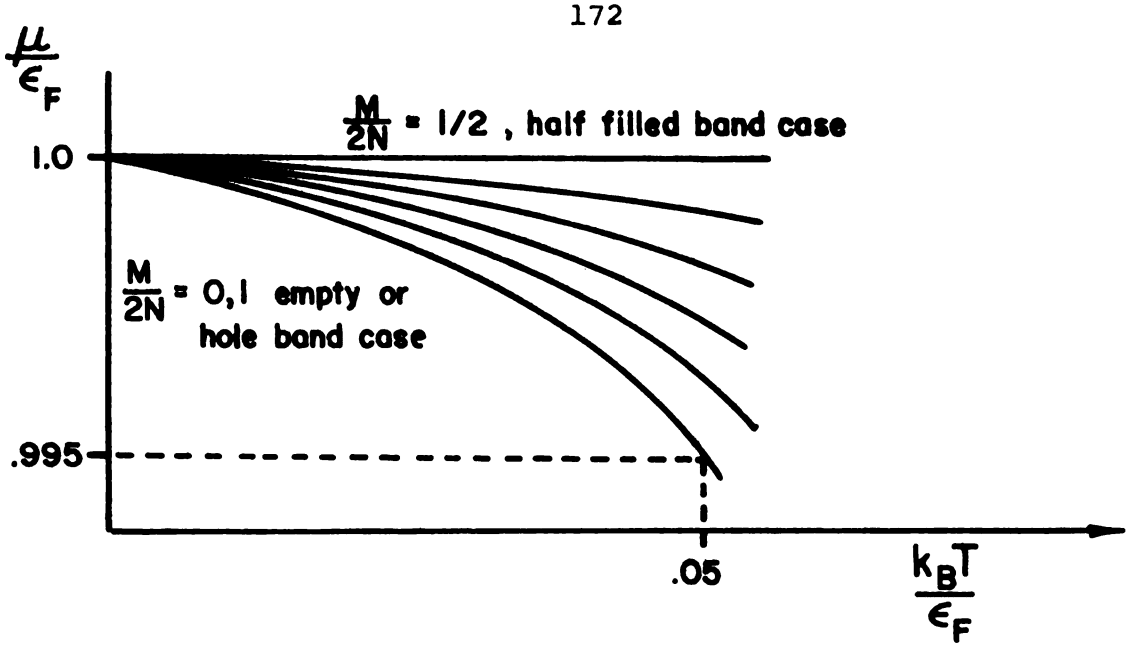
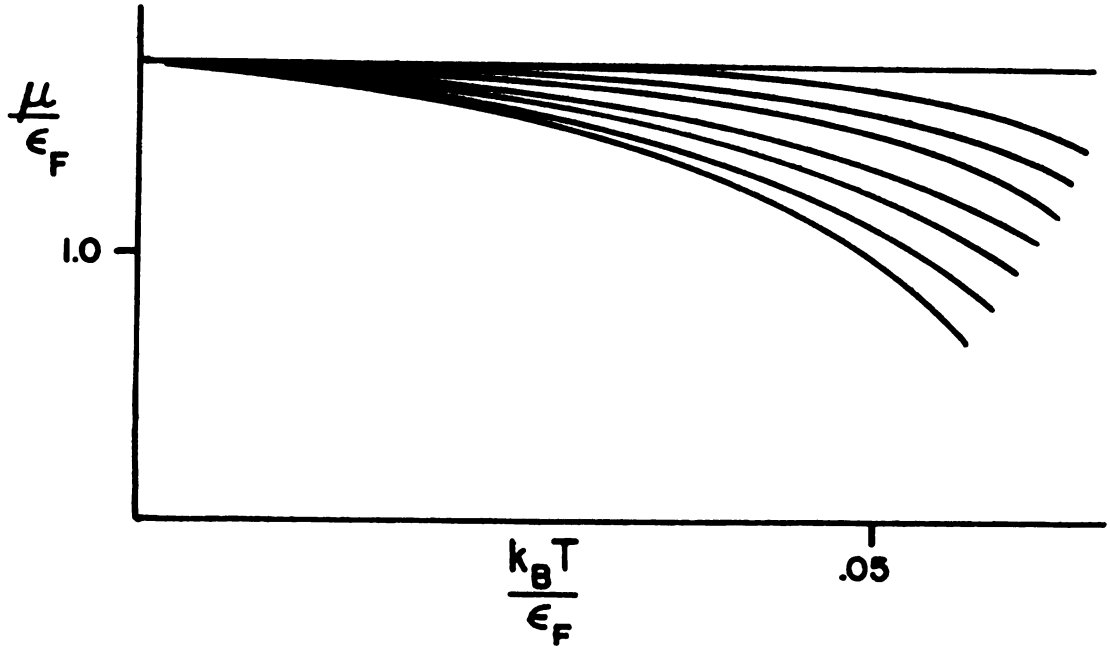


Figure 21. Spread in Chemical Potential Versus Temperature as a Function of Band Filling.

being bounded by a constant curve for the half-filled band. The curve for largest possible variation of μ with temperature occurs when the band is almost empty or almost full. In the anti-ferromagnetic state the curves will uniformly shift up or down the μ/E_F axis as Δ varies.



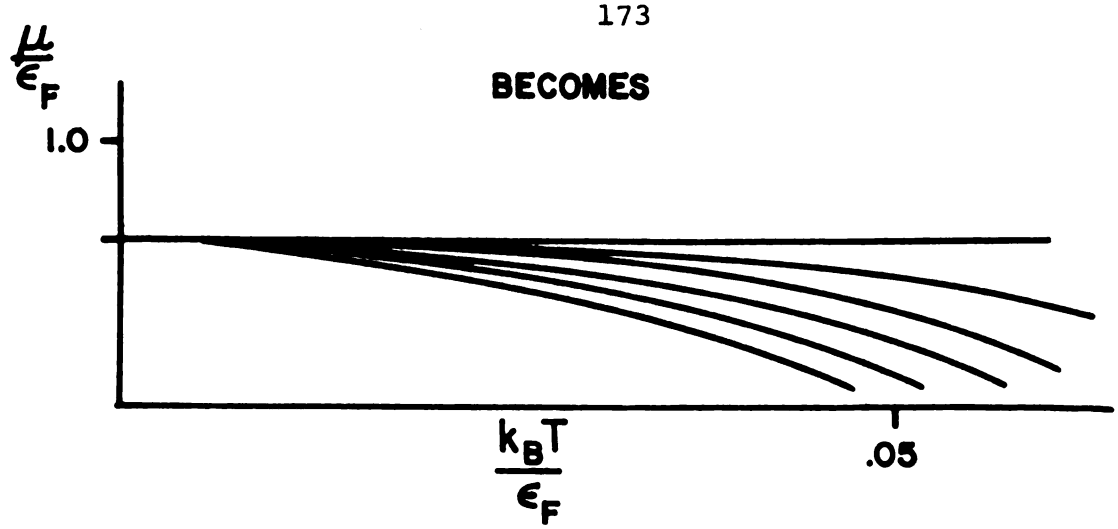


Figure 22. Variation of Chemical Potential Versus Temperature for Various Band Fillings as a Function of the AFM Gap Parameter.

We must derive these results rigorously so that an idea of $\mu = \mu(T,n/2N,\Delta)$, the explicit functional dependence, is gotton. Certainly for any fixed n/2N value and for any temperature, the $n/2N \approx 0, 1$ curve is the largest $\mu(T)$ variation so that a guess of $\mu \approx 0.995\ \epsilon_F$-$1.00\ \epsilon_F$ is an excellent first guess and will minimize the number of self-consistent iterations needed to find μ.

In the paramagnetic and ferromagnetic states, the quasi-free electron or hole energy band is parabolic for low $|\underline{k}|$ and high $|\underline{k}|$, so that

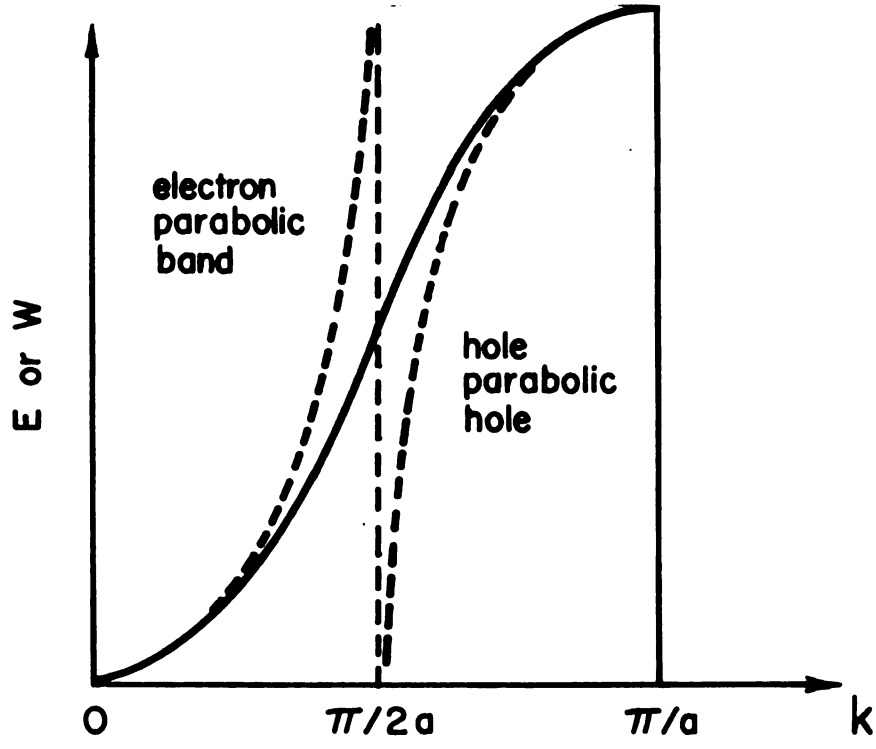


Figure 23. Electron and Hole Parabolic Band Approximation Near k = 0 and π/a Respectively.

the only region in question is for filling of $n/2N \approx 1/2$ for $k \approx \pi/2a$. In this region, this question for the paramagnetic and ferromagnetic states does not really arise since Penn's phase diagram, and Kemeny and Caron, have shown that the antiferromagnetic state will be most stable for $n/2N \approx 1/2$, the half-filled band case. For low Co (in an s-electron calculation like Penn's) the half-filled band case is paramagnetic. Here we simply note that the curve of μ versus T will be within the family of curves so that $\mu = 0.995\ \epsilon_F - 1.000\ \epsilon_F$ will be an excellent first guess. To prove this, aside from our knowledge that $n^2 = h^2$ which we proved before, we note that:

$$(3.190) \quad f(\epsilon_{\underline{k}}) = [1+ \exp((\epsilon_{\underline{k}}/4T - \mu/4T)/k_B T)]^{-1}$$

where

$$(3.191) \quad \epsilon_{\underline{k}}/4T = -1/2(\cos k_x a + \cos k_y a + \cos k_z a)$$

$$= -1/2(\cos \varphi_x + \cos \varphi_y + \cos \varphi_z)$$

if $\varphi_i = k_i a$ for a tight binding d electron. Near the botton of the band, we expand the cosines about $\varphi = 0$ and

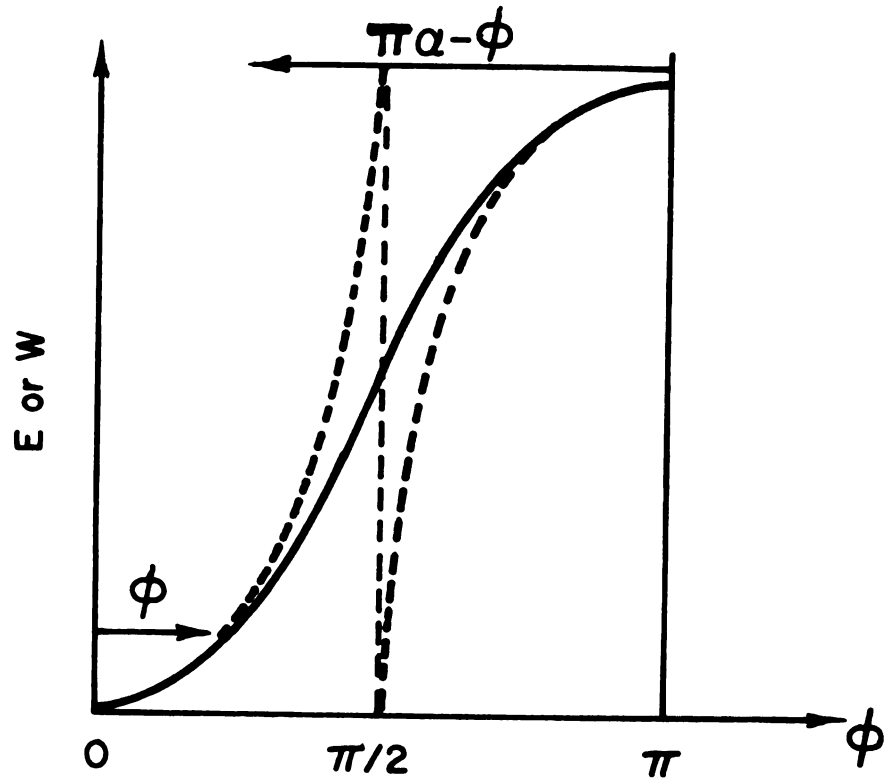


Figure 24. Parabolic Band Approximations Reexpressed in Terms of $\emptyset = ka$.

near the top of the band we expand the cosine about $\pi a - \varphi = 0$. We see:

$$(3.192) \quad (\cos \varphi_i)_{\varphi=0} \approx 1 - \varphi_i^2(0)\ \partial^2 \varphi_i/\partial^2 \varphi_i(0)$$

$$(3.193)\quad (\cos\varphi_i)_{\varphi=a} \approx 1-[\pi a-\varphi_i(0)]^2\ \partial^2[\pi a-\varphi_i]/\partial^2[\pi a-\varphi_i(0)]$$
$$\approx 1-(\pi^2a^2-2a\varphi_i(0)+\varphi_i^2(0))\,(\pi a-\partial^2\varphi_i/\partial^2[\pi a-\varphi(0)])$$

which is approximately of the same form as the first equation so that holes behave just as electrons and have the same $f(\epsilon_{\underline{k}})$.

Now:

$$(3.194)\quad \epsilon_{\underline{k}}/4T = -1/2(\cos\varphi_x+\cos\varphi_y+\cos\varphi_z)$$
$$= -1/2\ (3-3\varphi_x^2(0)\ \partial^2\varphi_x/\partial\varphi_x(0)^2)$$

since $\varphi_x = \varphi_y = \varphi_z$ in a simple cubic lattice. We know $\epsilon_{\underline{k}} = \hbar^2\underline{k}^2/2m^*$ so that $\epsilon_k/4T = \hbar^2\underline{k}^2/8Tm^*$. Thus:

$$(3.195)\quad -1/2(3-3\varphi_x^2(0)\ \partial^2\varphi_x/\partial\varphi_x^2(0)) = \hbar^2\underline{k}^2/8Tm^*$$

Resubstituting $\varphi_x = k_x a \equiv ka$

$$(3.196)\quad -1/2(3-3(ka)^2\partial^2(ka)/\partial[(ka)(ka)]^2 = \hbar^2\underline{k}^2/8Tm^*$$
$$= 3/2\ (1-a^2\partial^2 ka/\partial[(ka)(ka)]^2)k^2 = \hbar^2\underline{k}^2/8Tm^*$$

So

$$(3.197)\quad k^2\left(\frac{\hbar^2}{8Tm^*} - \frac{3}{2}\,a^2\,\frac{\partial^2(ka)}{\partial[(ka)(ka)]^2}\right) = -\frac{3}{2}$$

For small k, say $k = \pi/100a$

$$(3.198)\quad \left(\frac{1}{m^*}\right)_{k=\pi/100a} = \left(-3/2 + 3/2\,\frac{\partial^2(ka)}{\partial[(ka)(ka)]^2}\,\frac{\pi^2}{10^4}\right)\frac{8T}{\hbar^2}$$

For large k, say $k = \pi/3a$, but still in the parabolic region,

$$(3.199)\quad \left(\frac{1}{m^*}\right)_{k=\pi/3a} = \left(-3/2 + 3/2\,\frac{\partial^2(ka)}{\partial[(ka)(ka)]^2}\,\frac{\pi^2}{9}\right)\frac{8T}{\hbar^2}$$

The difference in both of these effective mass values is small, as $\partial^2(ka)/\partial[(ka)(ka)]^2$ is much larger at $k = \pi/100a$ than at $k = \pi/3a$ so that the 10^4 factor in one denominator is not grossly different in its effect from the 9 factor. We know m* (k small or large) > m* (middle of band), so there is some discrepancy since curvature depends on m* and is small at the center of the band. Thus m* still has meaning near the middle of the band.

It remains to see how $\mu = \mu$(Temperature, Δ (Temperature), n/2N) for the antiferromagnetic state. We know

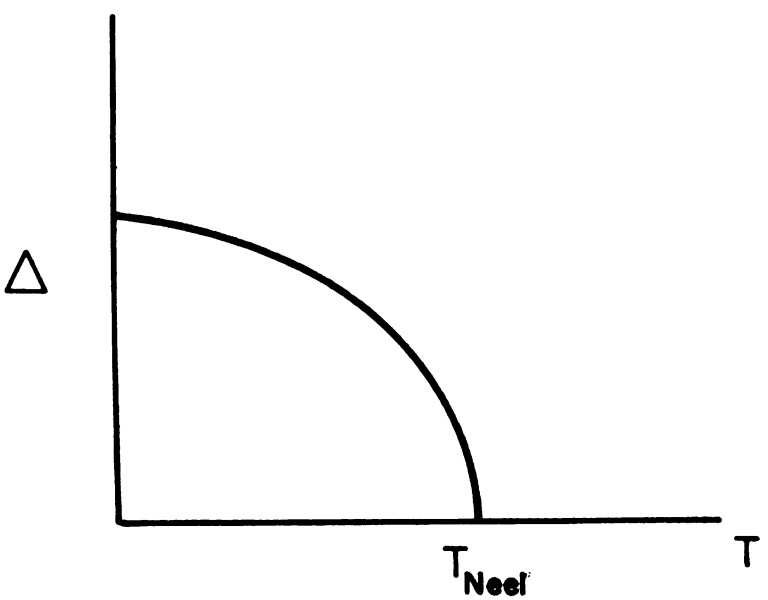


Figure 25. AFM Gap Paramater Dependence on Temperature.

the Δ(Temperature) dependence. This is seen[64] as:

$$(3.200)\quad \Delta = \frac{(9K-4J)}{N} \sum_{\underline{k}} \left[\frac{\Delta}{\sqrt{\Delta^2+(\epsilon_{\underline{k}}-\epsilon_{\underline{k}+\underline{Q}})^2}} \left(\frac{1}{e^{\alpha+\beta E_s(\underline{k})}+1} - \frac{1}{e^{\alpha+\beta E_A(\underline{k})}+1} \right) \right]$$

where $E_s(\underline{k})$ and $E_A(\underline{k})$ are the split lower and upper bands respectively, and α and β are constants, α being determined by Matsubara and Yokota's equation (10) (that the sum of Fermi factors over all $\underline{k}$ states for the upper and lower split bands equals half the number of electrons in the system), and is thus a chemical potential, and $\beta = 1/k_B T$ as usual.

The band splitting is 2Δ,

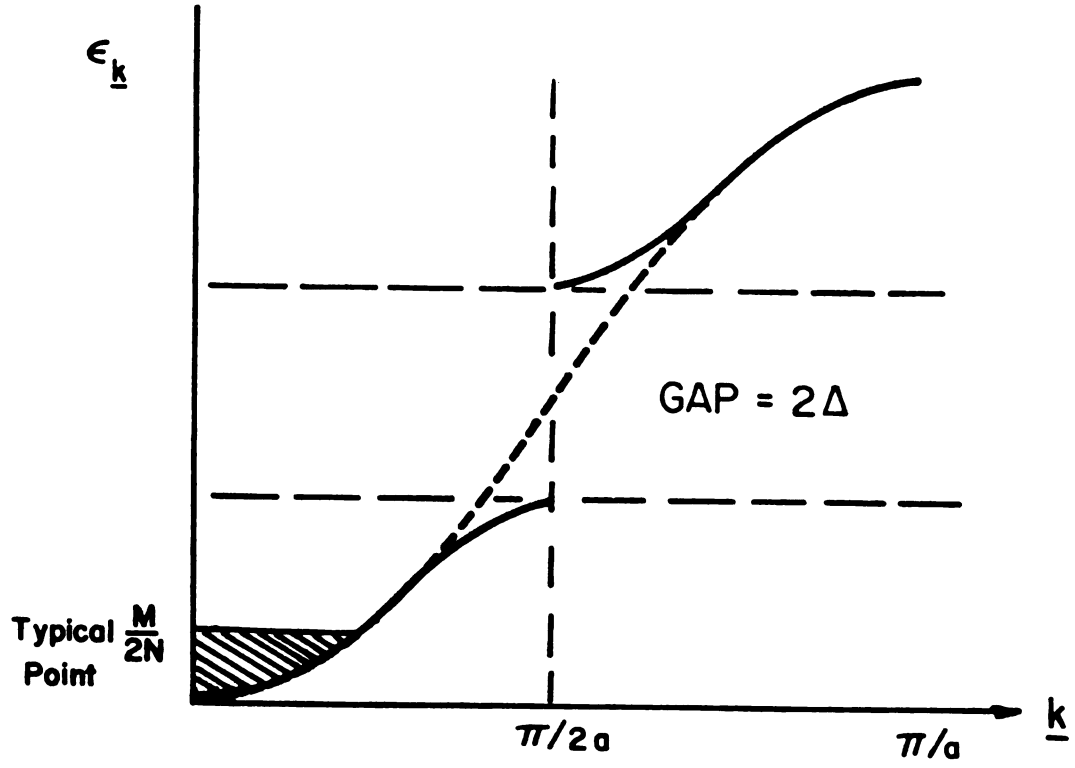


Figure 26. AFM Gap in Dispersion Relation.

so that the $\epsilon_{\underline{k}}$ value at $k = \pi/2a$ depends on temperature. As the temperature rises, the gap narrows and the origin about which we expanded cos ka in $E_{\underline{k}}$ in the hole expression, $k \approx \pi/2a$, shifts.

What has this to do with band filling? For $n/2N < 1/2$, $n/2N > 1/2$, there is hardly any effect. But for $n/2N \approx 1/2$, there may be a large effect. Now we know $\mu = 1.0\ \epsilon_F$ at $n/2N = 1/2$ (i.e. at $k = \pi/2a$) so that μ must look like Figure 27.

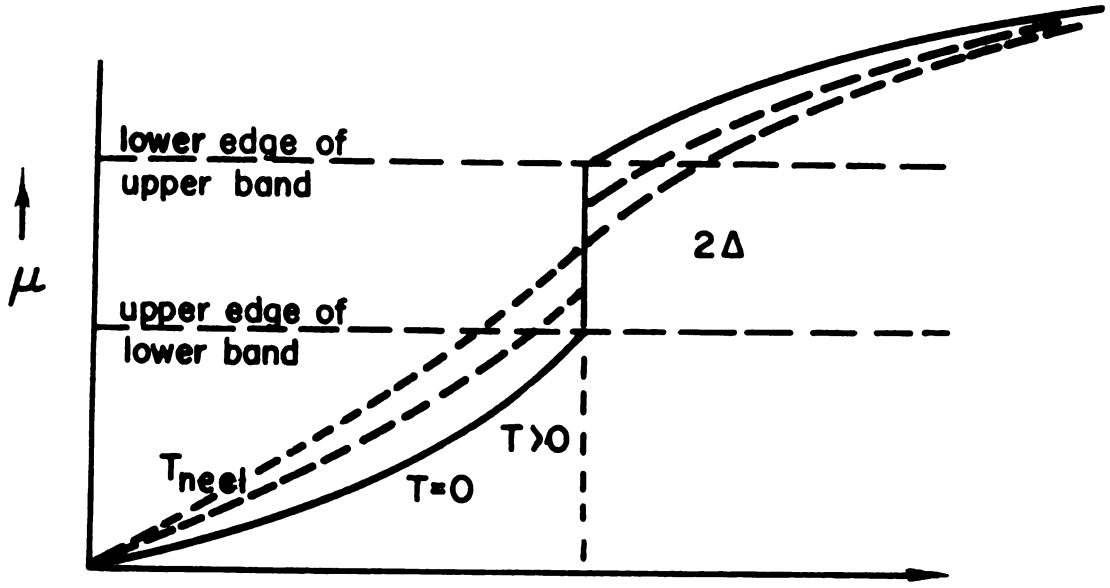


Figure 27. Jump in Chemical Potential at AFM Gap.

as a function of n/2N; with a jump of 2Δ between n/2N slightly less than 1/2 and n/2N slightly greater than 1/2. If μ were a single value, continuous function of n/2N, we could plot:

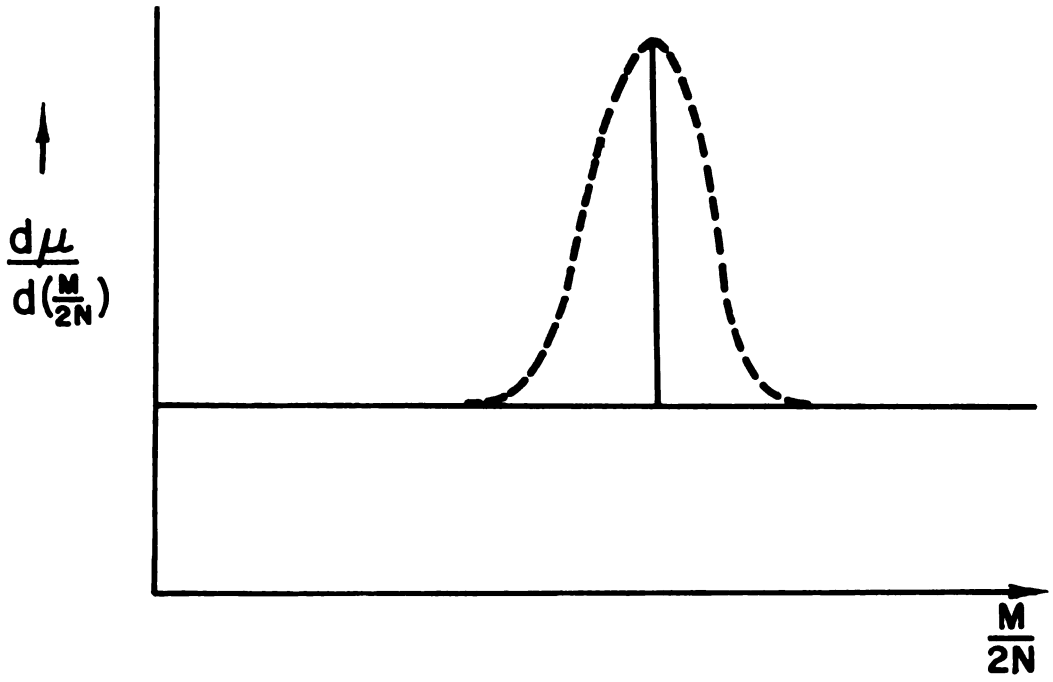


Figure 28. Peak in Derivitive of Chemical Potential with Respect to Band Filling Versus Band Filling at Low Temperature Around AFM Gap (n/2N = 0.5).

Since this cannot be true at n/2N, we represent its derivitive by a maximum at n/2N (dotted curve). Thus the n/2N = 1/2 case corresponds to the lower curve (the most deviation from $\mu \equiv E_F$) for T = 0 in Figure 22. As T > 0, the n/2N = 1/2 curve goes into the family of curves along with all the other n/2N curve, since Δ decreases as T increases. Therefore, an excellent range to choose our initial μ from is μ = 0.995 - 1.000 E_F.

DISCUSSION AND CONCLUSIONS

The FM-PM phase boundary straddeling program was run on the C.D.C.-6500 computer at Michigan State University. Only single precision arithmetic was used to evaluate the sign change of the energy difference (at low temperature) or the free energy difference (at high temperature) between the two magnetic phases.

Three sets of phase boundaries at three different temperatures were calculated with an error of about 5%. The variables used in the program for temperature was TT, defined as temperature/ 1/3 x d-bandwidth x k_B, a form chosen so that temperature was normalized similarly to the direct and exchange coupling constants, K and J. This is in the dimensionless form.

At T = 1.1609°K. (TT = 10^{-4}), we calculated the difference between E_{TOT} for spin polarization equal to zero and for spin polarization equal to 0.1. This was done for J/4T = 0.0, J/4T = 1/2 K/4T, and J/4T = K/4T, the maximum value the ratio (exchange coupling/1/3 bandwidth) can attain.

At T = 300°K. (TT = 2.584 x 10^{-2}) and T = 1000°K. (TT = 8.614 x 10^{-2}), we calculated the difference between F_{TOT} for spin polar-

ization equal to zero and for spin polarization equal to 0.1. This was also done for the same three ratios (exchange coupling/ 1/3 bandwidth) ratios as the low temperature case.

The results of these calculations are shown in Figures 29 to 41. In Figure 29 we see the low temperature phase boundary at the three (exchange coupling/1/3 bandwidth) ratios. It is evident that there is a progressive increase of the ferromagnetic region at the expense of the paramagnetic as exchange coupling increases. Our zero exchange coupling phase boundary does not coincide with Penn's because we have an extra coefficient of 5 multiplying the potential term in the five-fold degenerate case. There is one electron in each of five d-shells as opposed to one electron in Penn's only s-shell.

In Figure 30 we illustrate the results of Figure 29 in a three-dimensional phase diagram. This is done to illustrate that the ratios J/4T = 1/2 K/4T and J/4T = K/4T do not lie on planes parallel to that of the J/4T = 0.0 calculation. We will denote these planes as (100) for J/4T = 0.0, (102) for J/4T = 1/2 K/4T, and (101) for J/4T = K/4T. These should not be confused with crystal lattice planes; they are planes in the parameter space of the phase diagram. Thus, all the two-dimensional phase boundary diagrams are projections of phase boundaries from the (101) and (102) planes onto the (100) plane in which the J/4T =

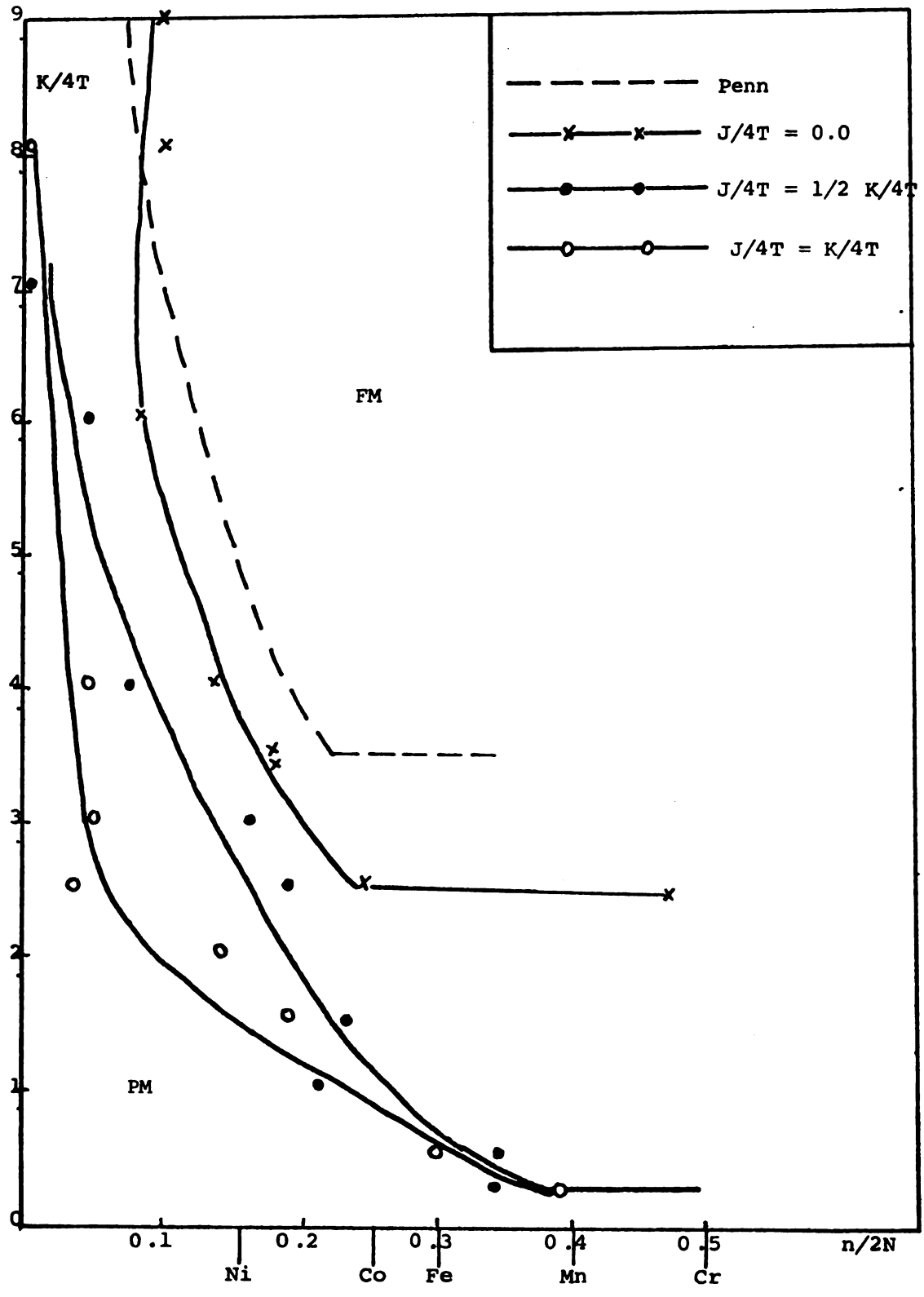


Figure 29. T=1.1609 K. FM-PM Phase Boundary.

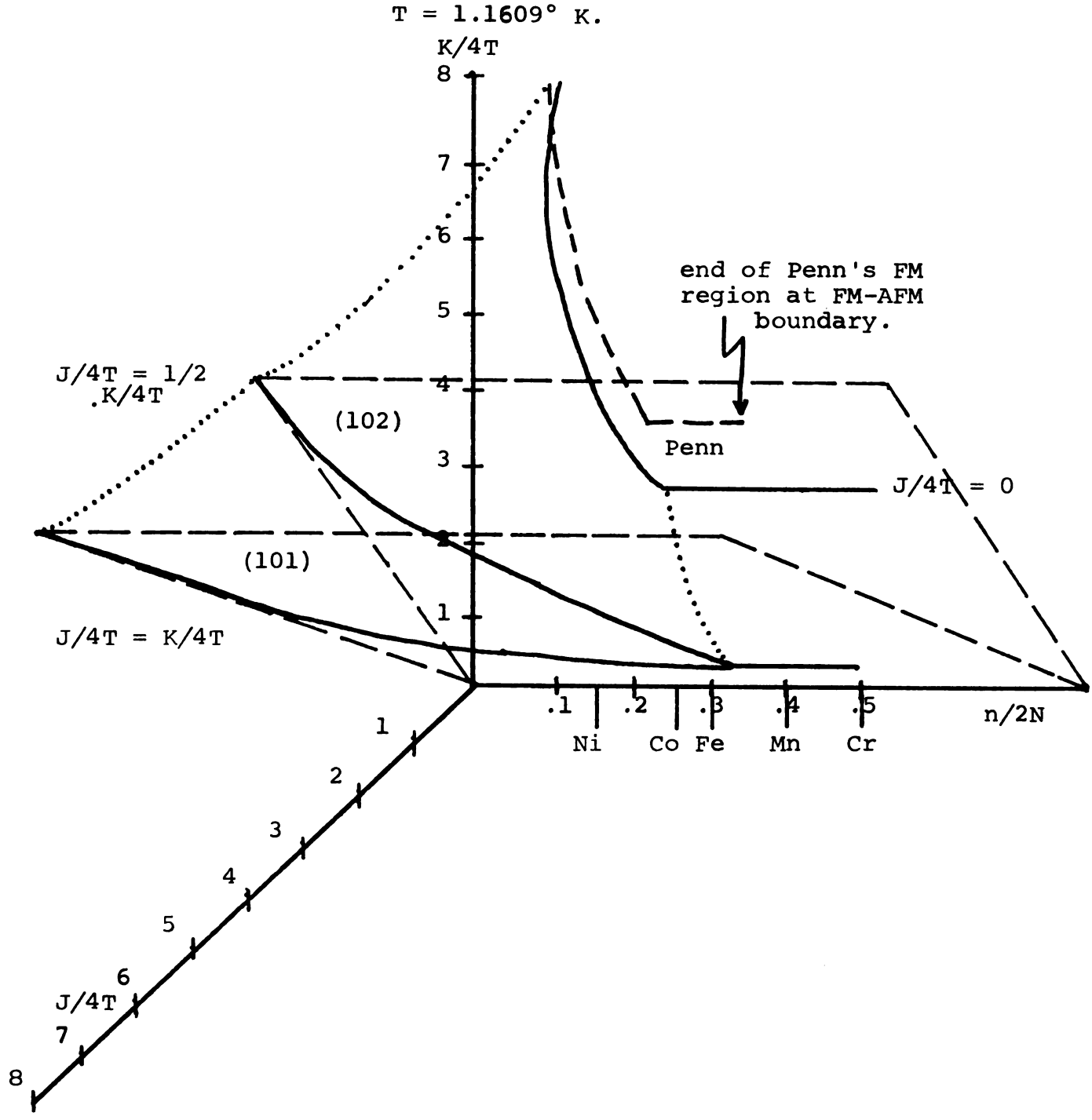


Figure 30. Isometric View of Isothermal Phase Surface in (K/4T, J/4T, n/2N) Parameter Space. The phase surface looks similar at higher temperatures in this projection.

0.0 boundary is plotted. The convergence of the two $J/4T \neq 0.0$ boundaries in Figure 29 at low values of $K/4T$ is simply because they are on (101) and (102) planes which merge at $K/4T = 0.0$.

In Figure 31 we see that at $T = 300°K.$, all boundaries have been shifted so as to decrease the ferromagnetic region at the expense of the paramagnetic. The same reverse trend on increase of $J/4T$ is seen as in the low temperature case. Figure 32 illustrates both of these trends at 1000°K. The scatter of computed points seems to decrease as the temperature of the calculation increases. Penn's work did not include any data points, so we must assume that his smooth phase boundary curves are best fits to some data point scatter. Anyway, only trends are really important, as the Hubbard model itself is only a rough approximation.

Figures 33, 34, and 35 are the results illustrated in Figures 29, 31, and 32 respectively, only with the $K/4T$ ratio inverted so as to superimpose the curves on those of Kemeny and Caron, as we saw in Chapter 2. Because this inverted phase diagram exaggerates the low $K/4T$ region of the previous phase diagrams, the trend toward increasing the ferromagnetic region at the expense of the paramamagnetic region is very evident. At higher temperatures, this trend is still evident, but it is offset by

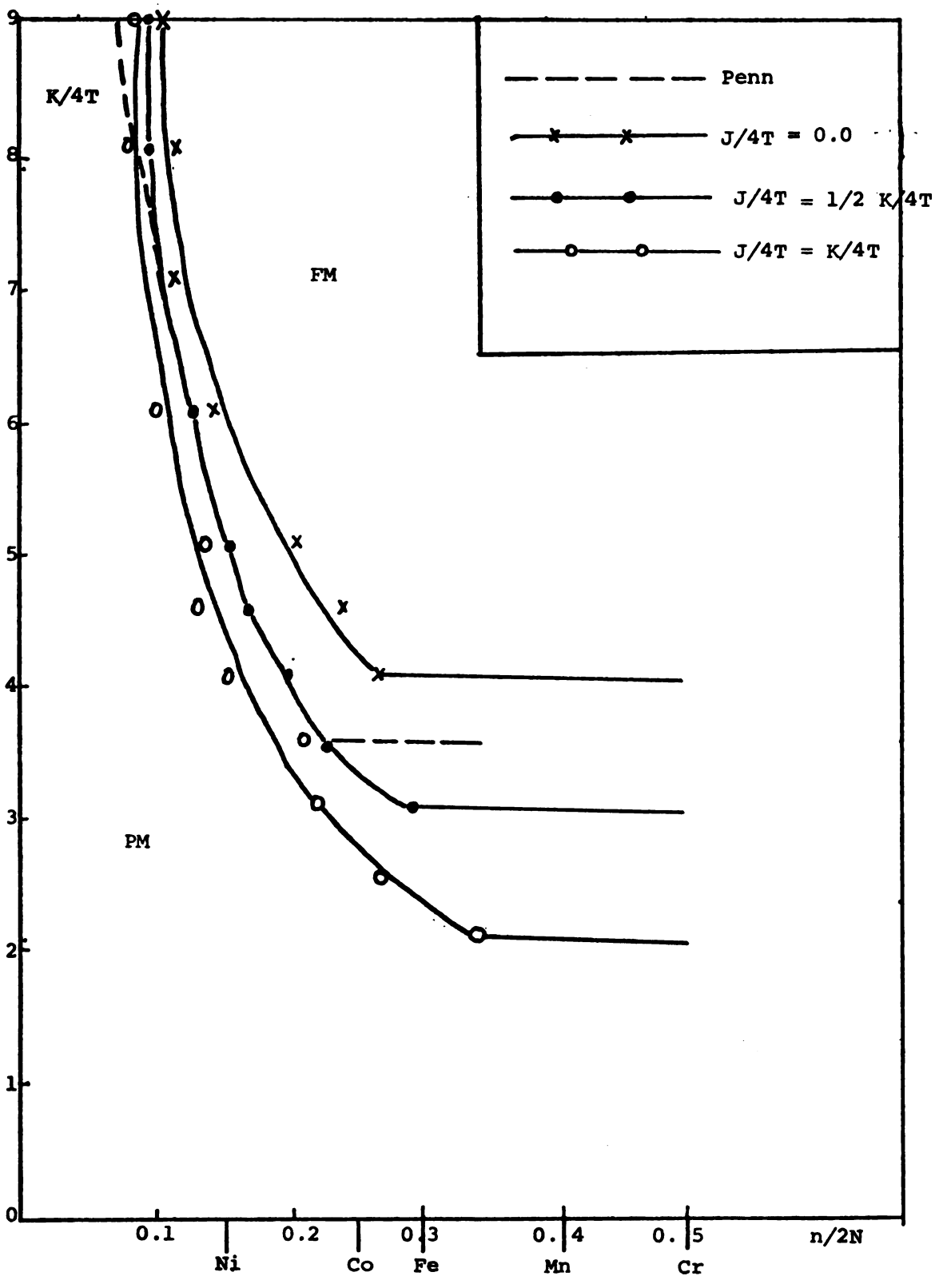


Figure 31. T=300 K. FM-PM Phase Boundary.

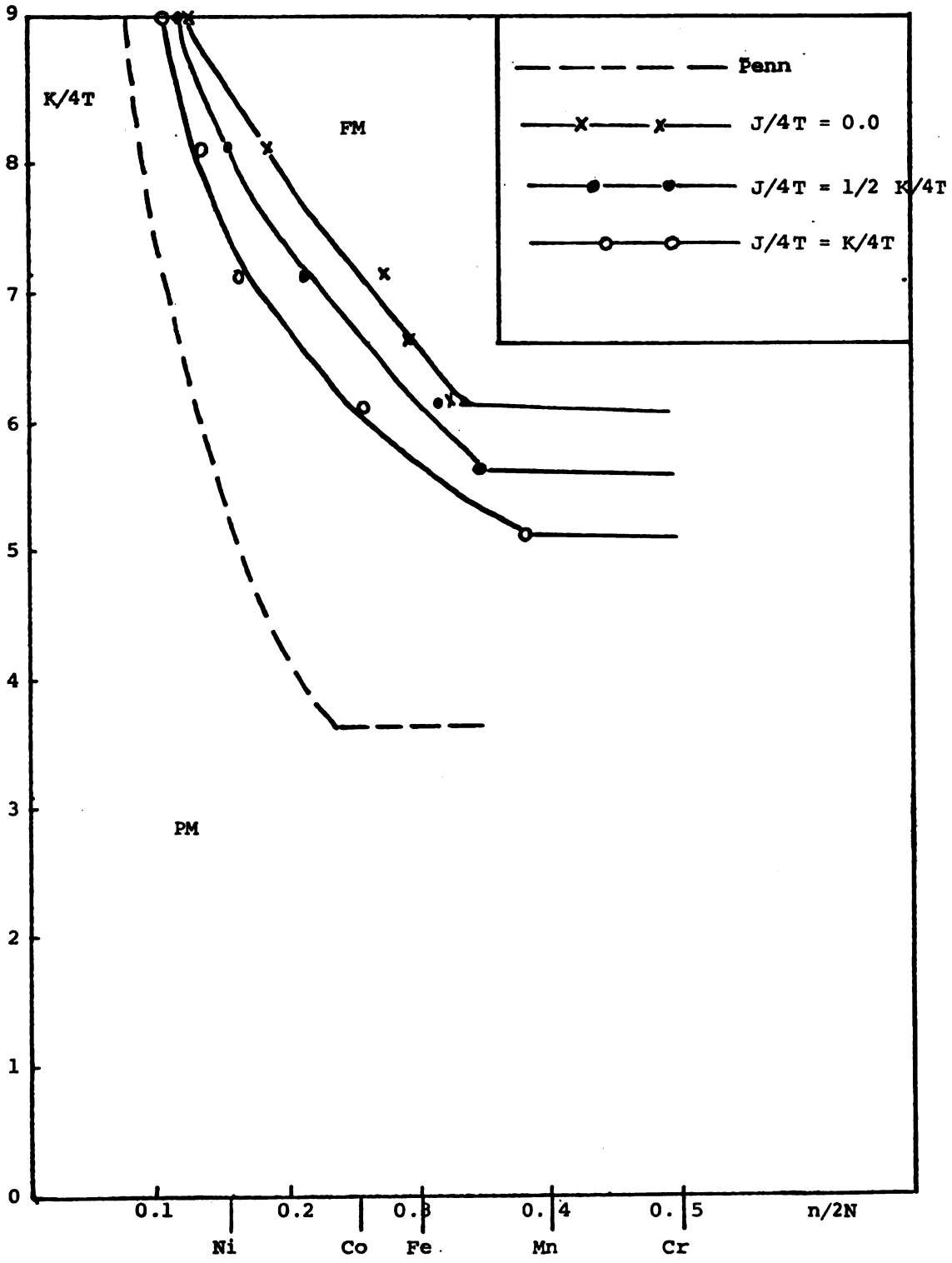


Figure 32. T=1000 K. FM-PM Phase Boundary.

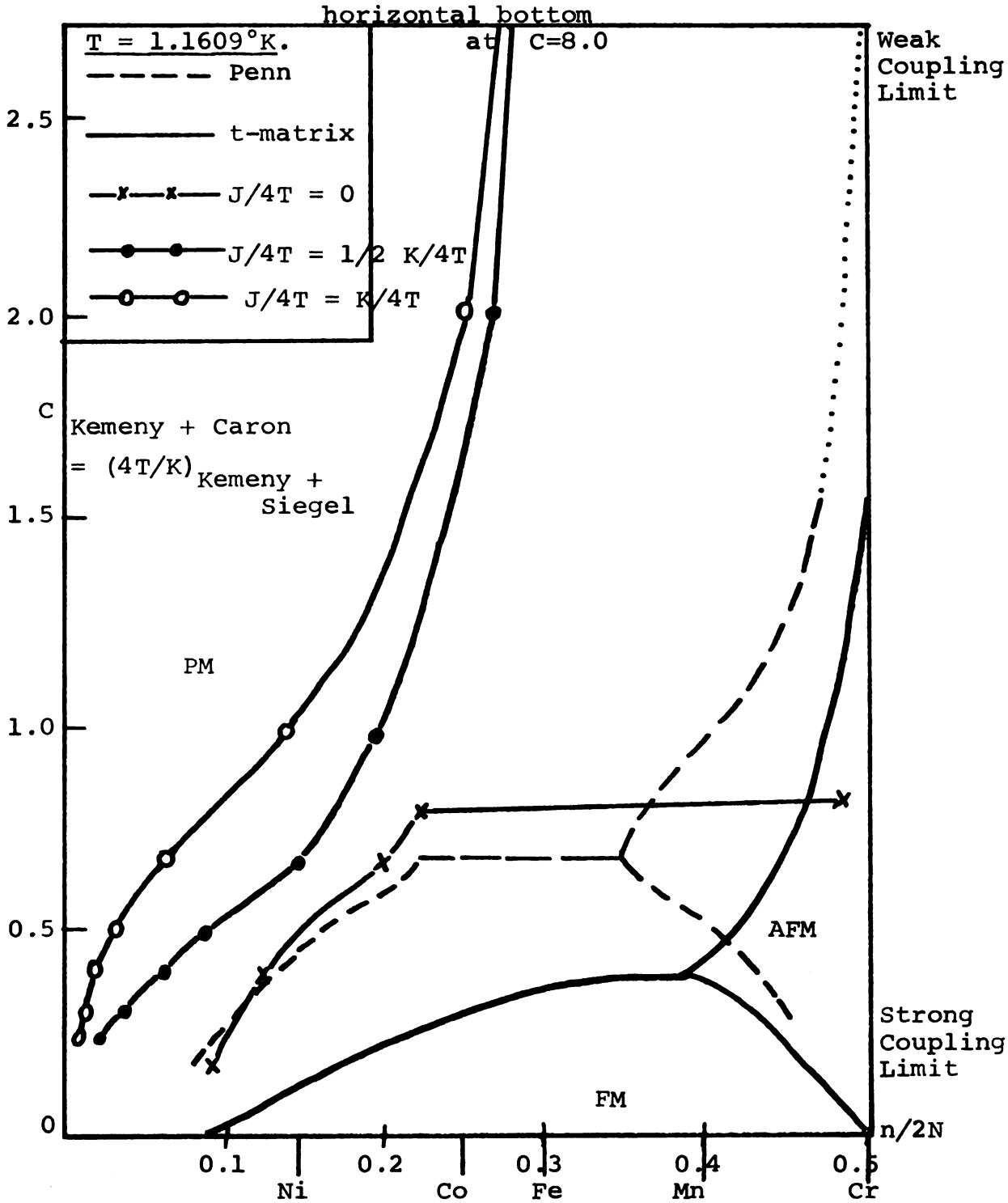


Figure 33. Inverted T = 1.1609°K. FM-PM Phase Boundary.

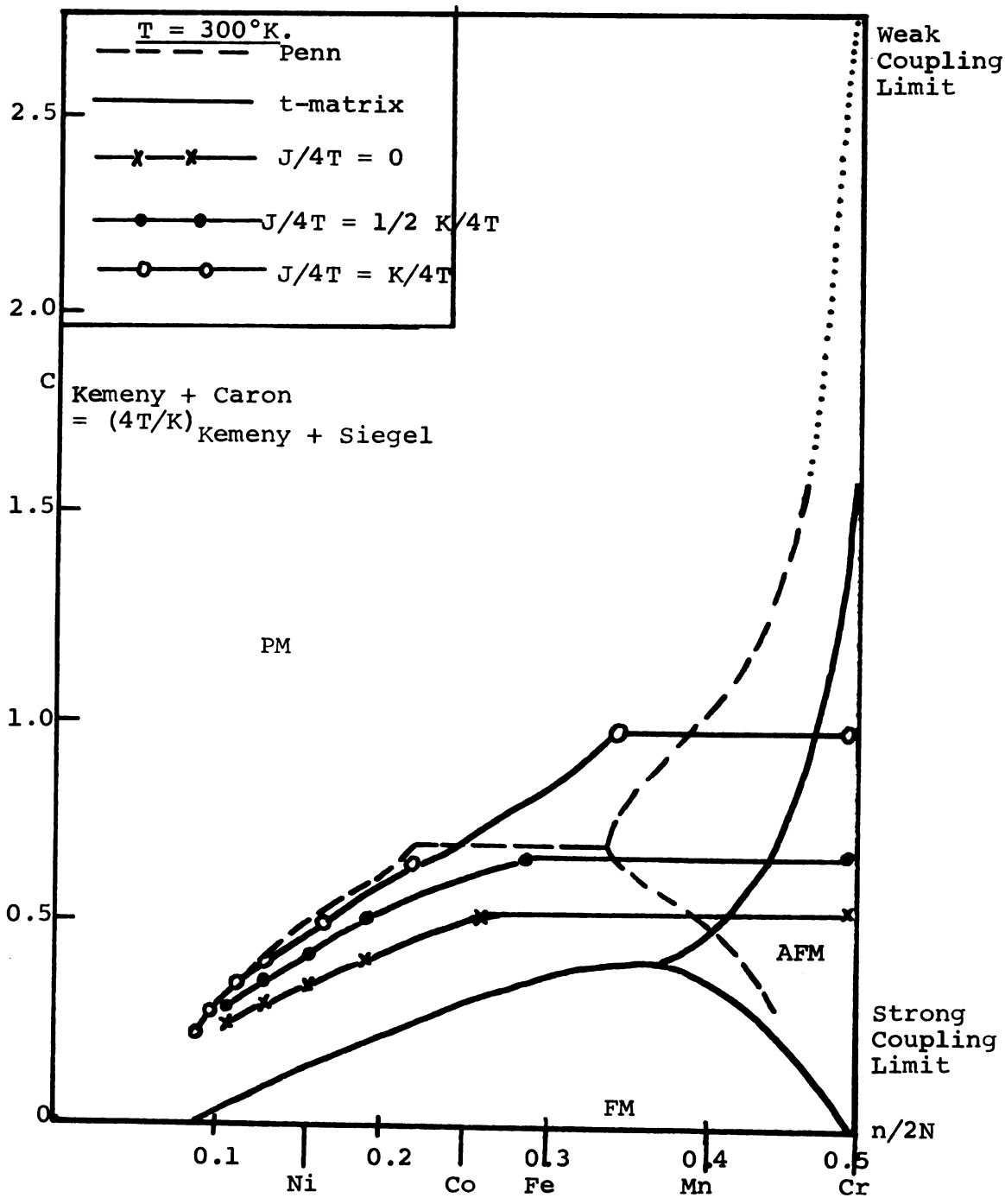


Figure 34. Inverted T = 300°K. FM-PM Phase Boundary.

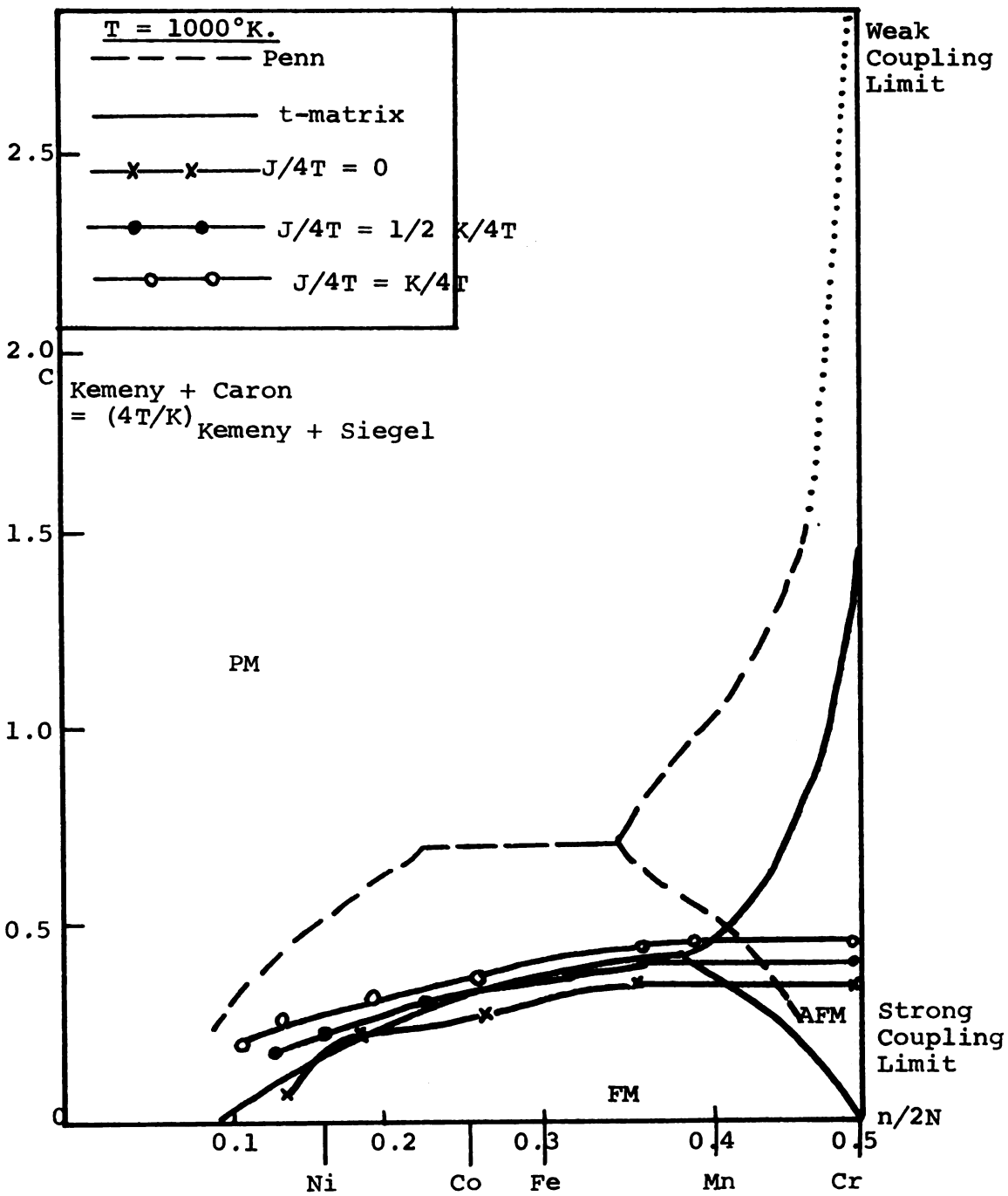


Figure 35. Inverted T = 1000°K. FM-PM Phase Boundary.

the effect of the higher temperature as seen in Figures 34 and 35. The important trend that emerges is that increasing J/4T yields results opposite to Kemeny and Caron's t-matrix calculation.

In Figures 36, 37, and 38, we have plotted for constant J/4T, the motion of the phase boundary as temperature increases. Again, the trend of reduced ferromagnetism as temperature increases is evident.

In Figures 39, 40, and 41 we have plotted, on the inverted phase diagram, the phase boundaries at constant J/4T as temperature increases. There, we can see that the trend toward a reduced ferromagnetic region as temperature increases, seeming to parallel the result of the t-matrix calculation at T = 0°K., that of a reduced tendency toward ferromagnetism for most band fillings as compared to Penn's prediction.

The AFM-PM program was never run due to a lack of funds for computer time. These self-consistent calculations require long running time programs with even longer, more expensive debugging periods.

The conclusions of the FM-PM program runs can be qualitatively compared with experiment in a way to bring out the trends of

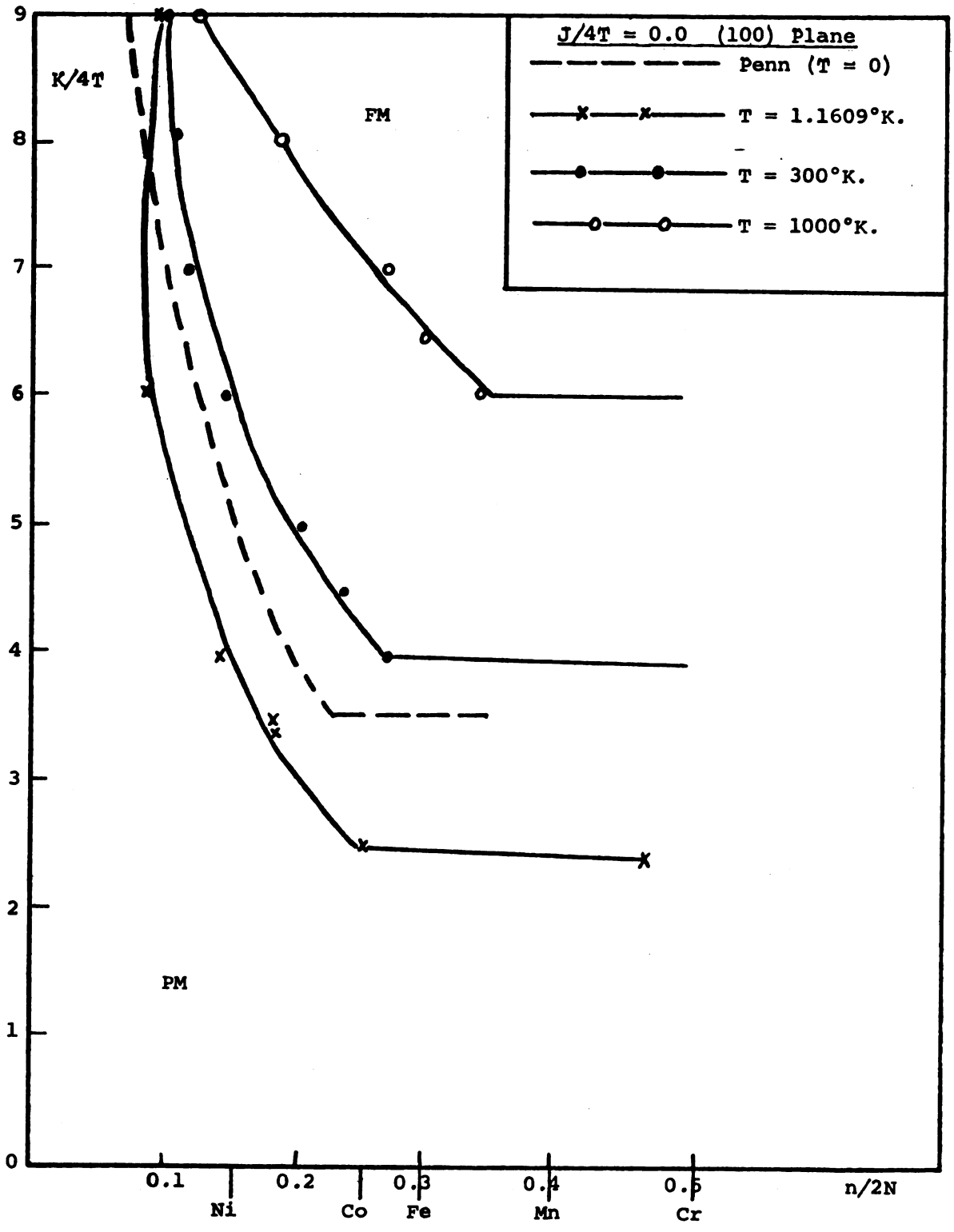


Figure 36. J/4T = 0.0 FM-PM Phase Boundary.

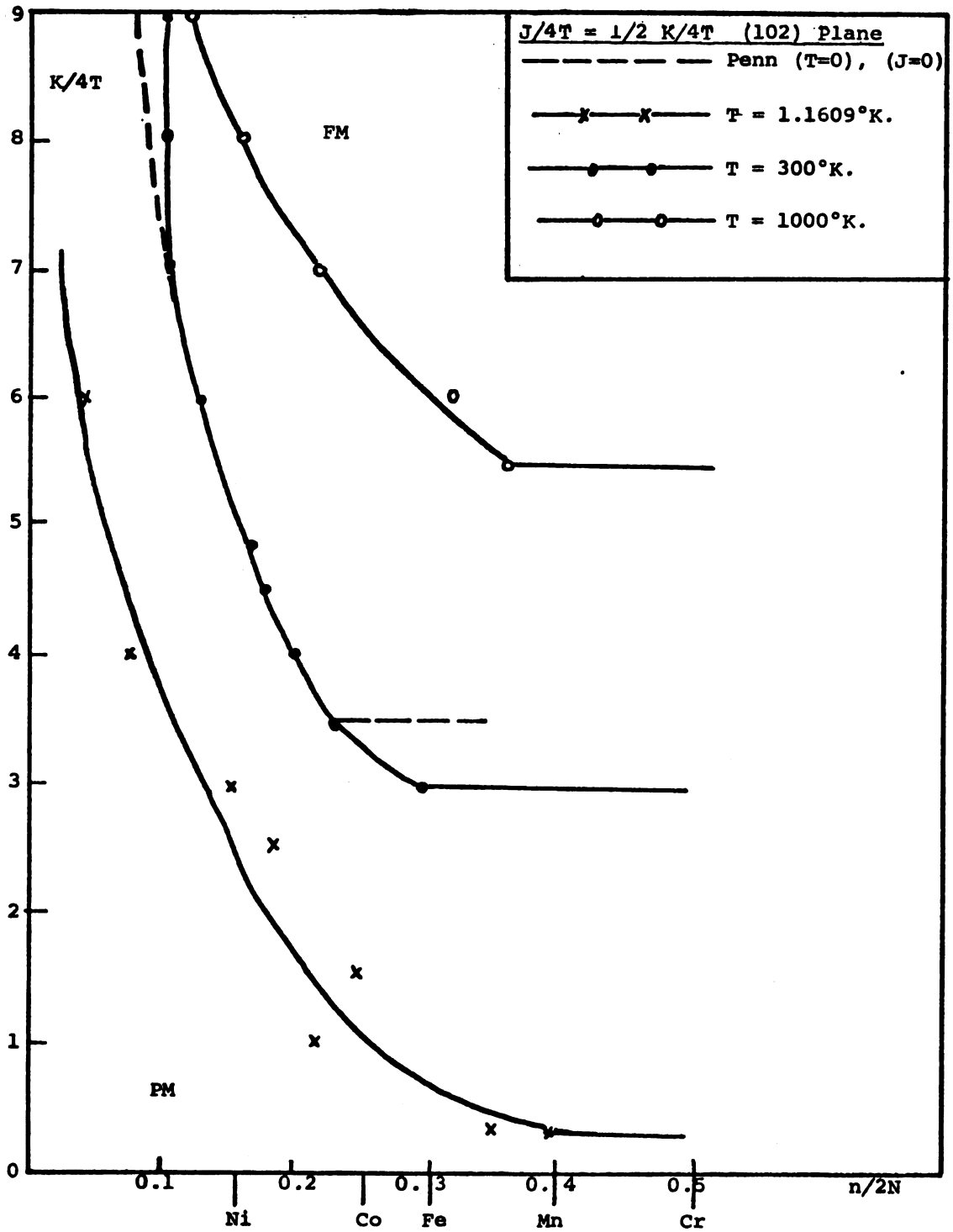


Figure 37. J/4T = 1/2 K/4T FM-PM Phase Boundary.

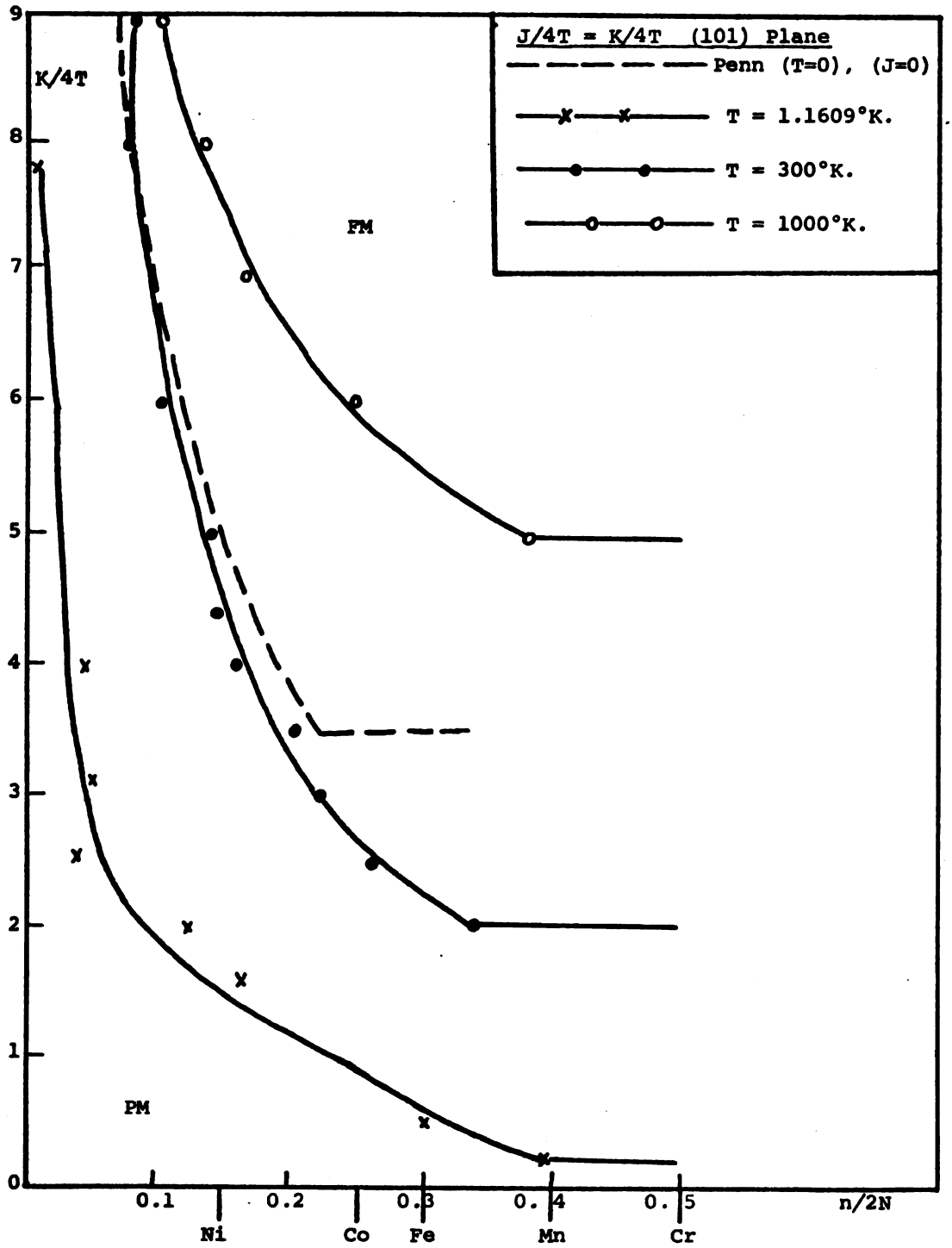


Figure 38. J/4T = K/4T FM-PM Phase Boundary.

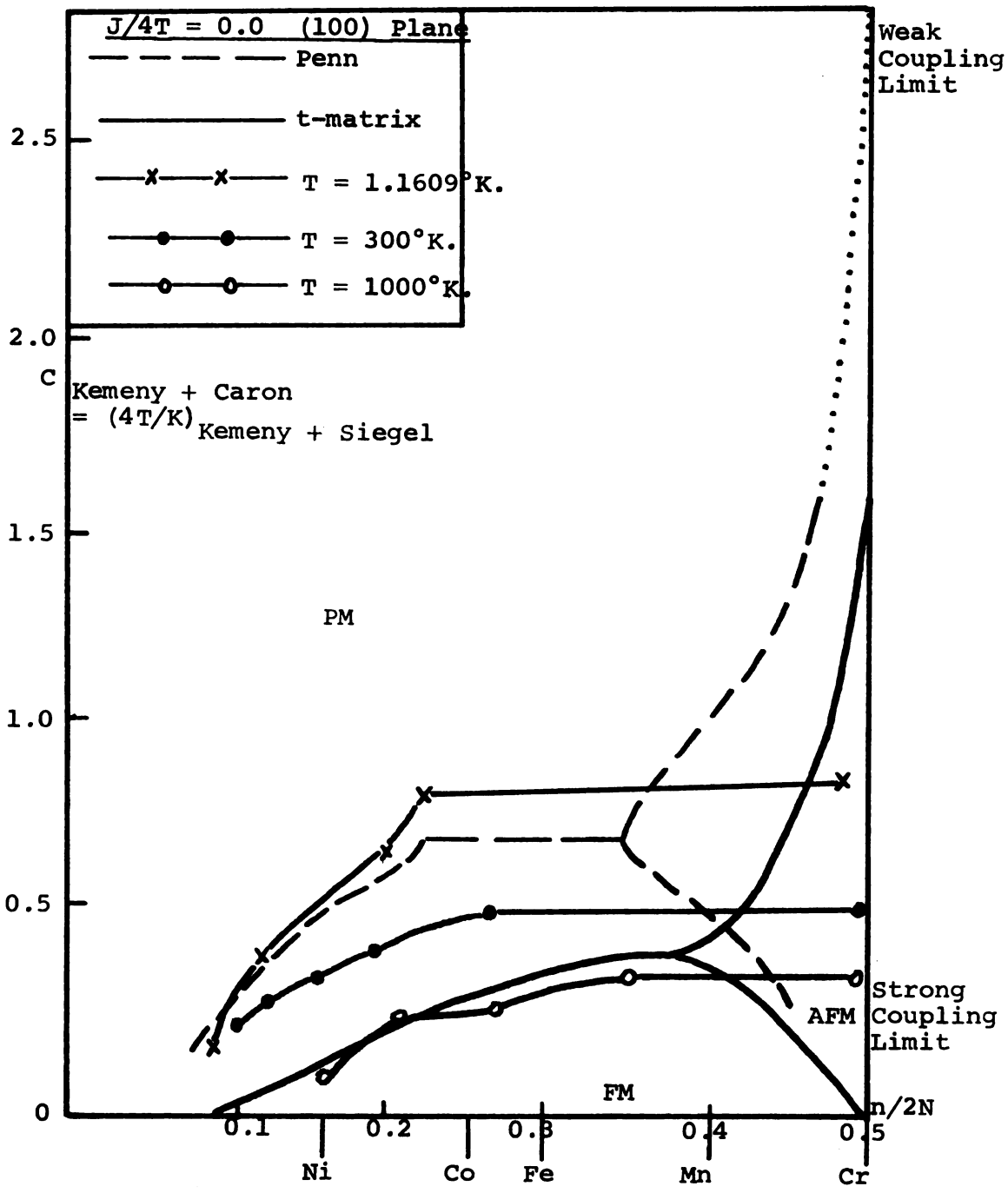


Figure 39. Inverted J/4T = 0.0 (100) Plane. FM-PM Phase Boundary.

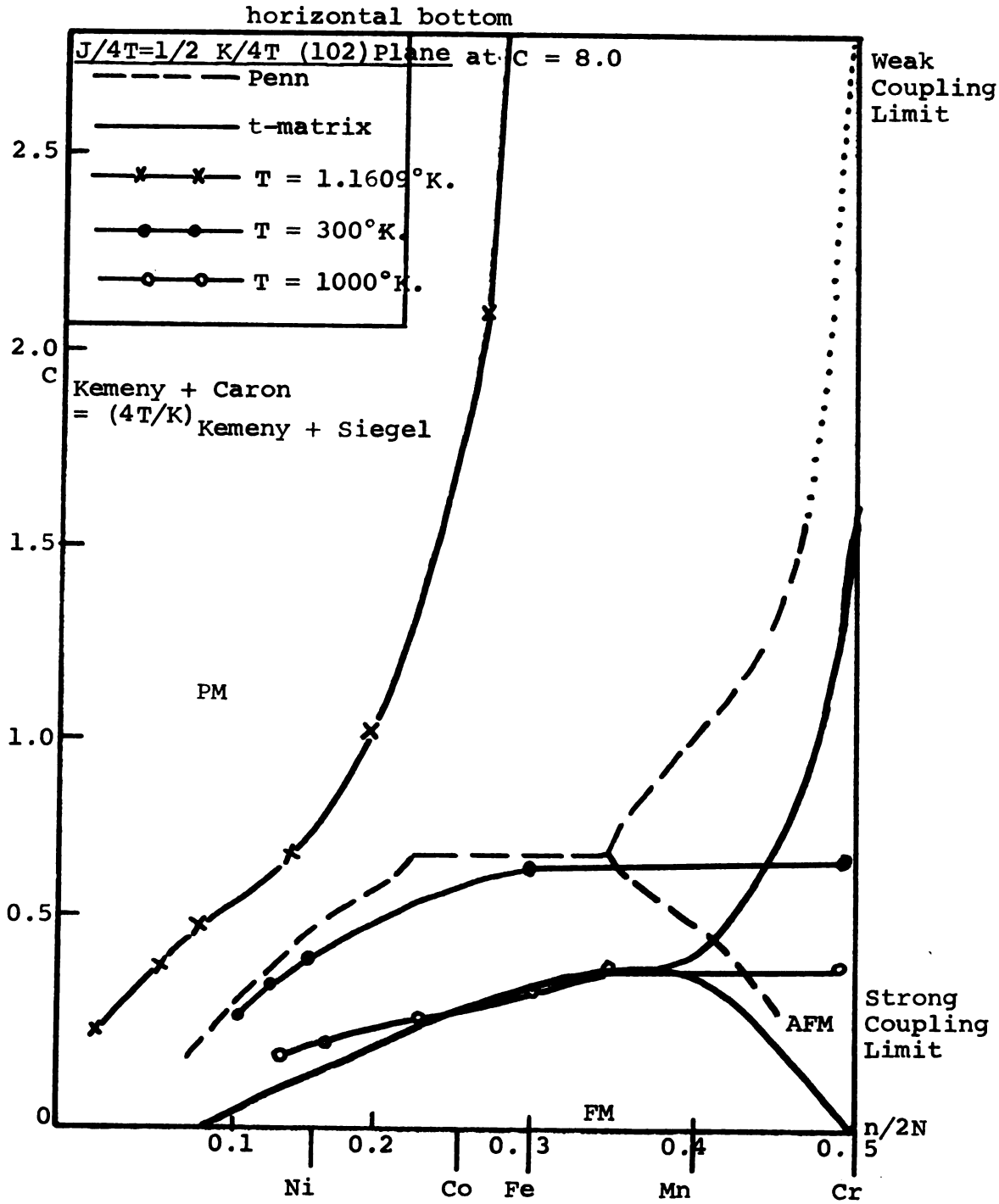


Figure 40. Inverted J/4T = 1/2 K/4T (102) Plane. FM-PM Phase Boundary.

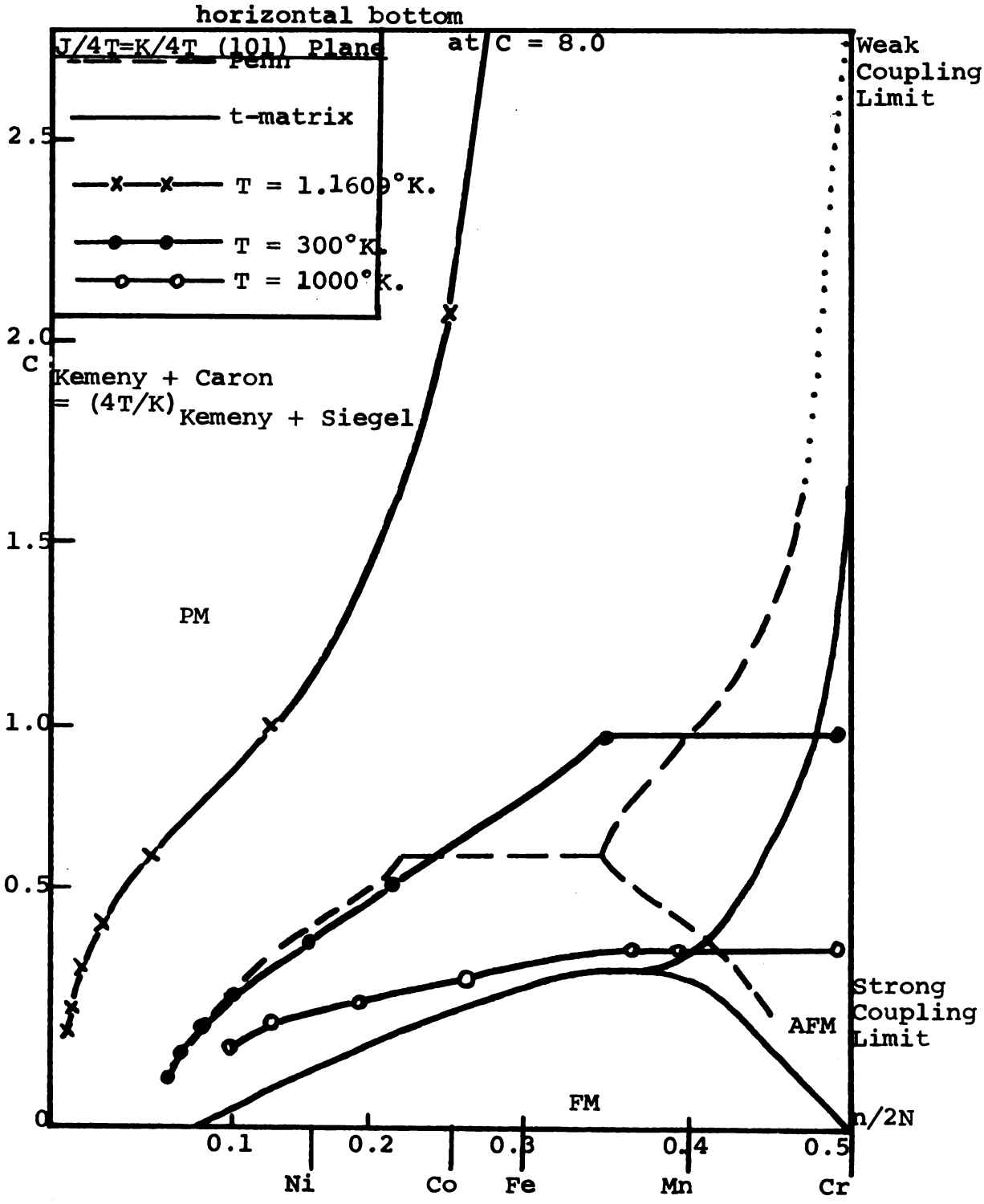


Figure 41. Inverted J/4T = K/4T (101) Plane. FM-PM Phase Boundary.

phase transitions in the 3d series transition metals. A survey of the experimental literature indicates the following Curie and Neel points:

Table 7. Properties of Transition Metals.

Metal	Atomic Spin Moment (μ_B)	Number of d-holes	Number of d-electrons	Transition	Transition Temperature (°K.)
Cr	0.6	5.0	5.0	AFM-PM	312
α- Mn	0.5	4.0	6.0	AFM-PM	95-100
γ- Mn	---	4.0	6.0	AFM-PM	500
Fe	2.0	3.0	7.0	FM-PM	1043
Ni	0.5	1.5	8.5	FM-PM	627-631
Co	1.5	2.5	7.5	FM-PM	1400

There is no recorded AFM-FM transition in transition metals. The number of d-electrons is the numerator of our n/2N abscissa in the phase diagrams. As we have shown, the electron-hole symmetry in terms of what magnetic state their intrinsic spin angular momenta will produce when coupled, we can pinpoint the abscissa corresponding to a given transition metal. For the FM-PM transition, we can place Fe, Co, and Ni at 3.0 holes per d-band, 2.5 holes per d-band, and 1.5 holes per d-band, respectvely. Chromium has 5.0 holes per d-band $\equiv$ 5.0 electrons per

d-band. Thus Cr occurs at the $n/2N \approx 5.0$ abscissa, (at the very center of the AFM central phase region), a value which we would not expect to be altered if a FM-AFM program with the full five-fold d-electron orbital degeneracy had been run. Next, in decreasing hole band filling, comes Mn, with approximately $n/2N = 4.0$ holes per d-band, still fairly near the half-filled band. This band filling places Mn in the antiferromagnetic region of Penn's diagram, and the addition of the five-fold degeneracy should not alter its tendency to an AFM state either.

On our final phase diagrams, we labeled the band fillings for Cr, Mn, Fe, Co, Ni, at which the three temperatures the calculation was performed. The direct and exchange interaction constants have not been separated experimentally as yet for the transition metals, so the K/4T and J/4T intercepts for any of the transition metals are unknown.

We should emphasize that we have not included the variation in crystal lattice structure between the transition metals. The energy difference between the crystal structures should dominate that between the magnetic phases.

As mentioned previously, the non-isomorphic mapping makes a unique choice of a finite number of $\underline{q}$ values impossible so that a unique $\psi_{\underline{k}}^{MAG}$ or $\gamma_{\underline{k}}^{+}$ cannot be written in the F.C.C., B.C.C.,

and H.C.P. lattices. Nevertheless, our calculation has shown the enhanced FM phase region at the expense of the PM phase region as the ratio (exchange interaction energy/1/3 bandwidth) increases, and the increase in the PM phase region at the expense of the FM phase region as temperature rises. An explicit experimental knowledge of K, J, and the bandwidth in Cr, Mn, Fe, Co, and Ni would help fix the J/4T and K/4T intercepts for each of these particular metals. There is some doubt, however, that such K/4T, J/4T, and n/2N values would be temperature independent, so that any high temperature conclusions would involve a shift in the point (K/4T, J/4T, n/2N) in the three parameter space of the phase diagram, in addition to the shift of phase boundary we have calculated.

For a comparison of Cr, Mn, Fe, Co, Ni, we illustrate a Slater-Pauling curve of magnetic moment per atom versus atomic number for the first transition period in Figure 42. There, it is seen that the magnetic moment per atom rises, peaks, and falls with atomic number quite linearly. Metals to the left of the center line tend to be B.C.C.; those to the right, tend to be F.C.C.-H.C.P.

We see that $\bar{\mu}/\mu_B$ is a maximum at the quarter-filled band near Fe, which corresponds with the fact (found by both Penn and us) that Fe has the largest FM region at its band filling, n/2N

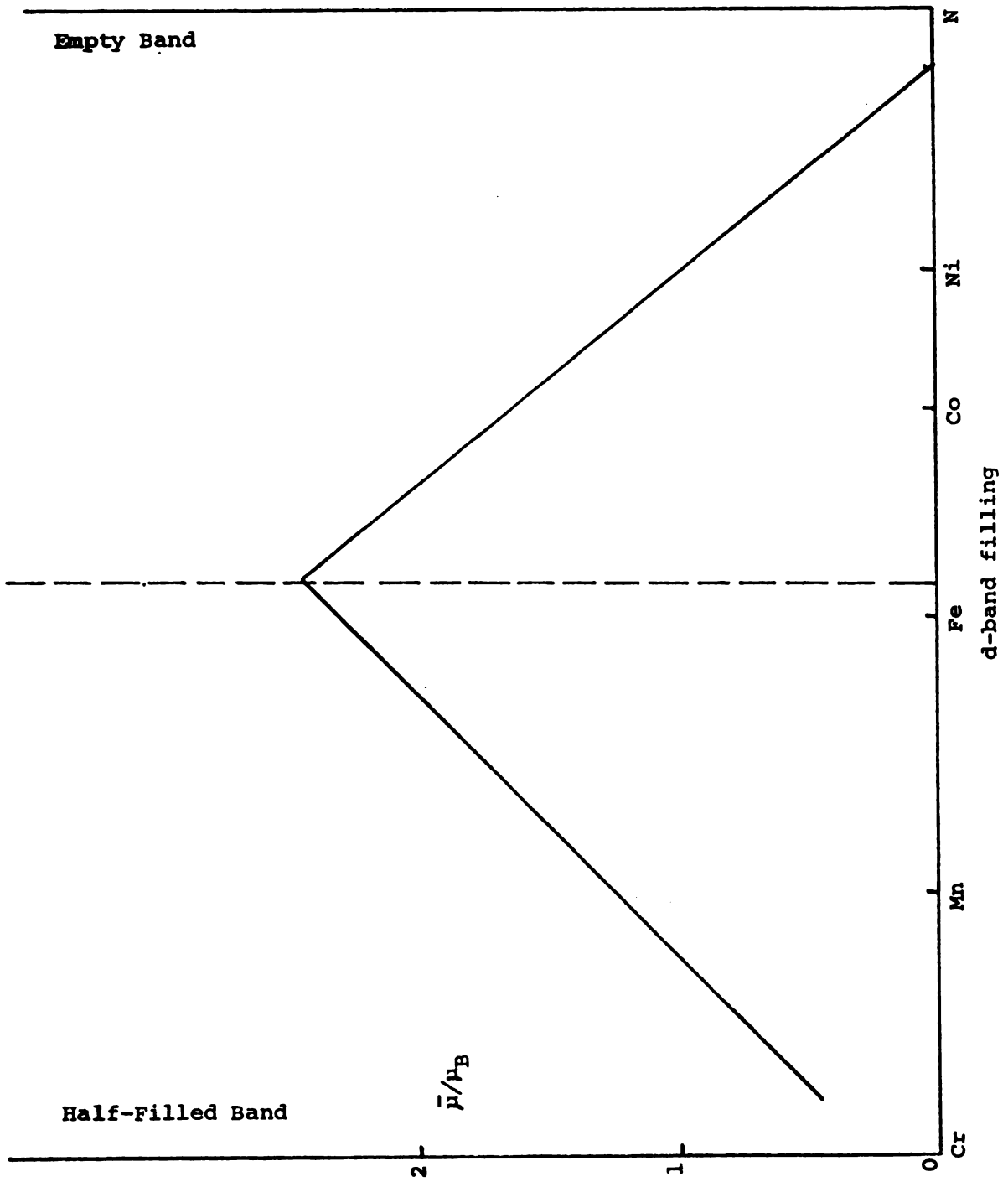


Figure 42. Slater-Pauling Curve for 3d Transition Metals.

value (= 3.0), while AFM Cr and Mn have no net $\bar{\mu}/\mu_B$, and the $\bar{\mu}/\mu_B$ per atom is smaller. The Slater-Pauling curve thus, qualitatively, upholds our result of a PM region near the empty band (with consequent low $\bar{u}/u_B$ values), and a strong FM region near the quarter-filled band (with very high $\bar{u}/u_B$ values). As band filling proceeds, the AFM-FM question needs to be solved by comparing results of the AFM-PM calculation and the FM-PM calculation.

The utilization of this technique also has again demonstrated the power and applicability of Kemeny's and Mattuck and Johansson's momentum space correlation function approach to ordered magnetic phases as opposed to the configuration space correlation function approach originally taken by Hubbard.

In conclusion, we see that a full five-fold degenerate Hartree-Fock treatment shifts the FM-PM phase transition curve in a direction opposite to the many-body (t-matrix) nondegenerate s-electron calculation of Kemeny and Caron, with Penn's non-degenerate s-electron Hartree-Fock approach lying somewhere inbetween. This could have been expected since a Hartree-Fock treatment of the Hubbard model, even without exchange, is certain to enhance ferromagnetism, perhaps unnaturally so. As a result, without knowing K/4T and J/4T experimentally for Fe, Ni, Co, Cr, and Mn, we cannot conclusively say whether Kemeny and Caron's

or our own improvement over Penn's simplified model is superior. At present, we only know the plane defined by the n/2N (bandfilling) for each of these metals. Such a decision must await the accurate experimental measurements of d-electron bandwidths, direct interaction constant, and exchange interaction constant in order to pin down the K/4T and J/4T intercepts for a particular transition metal.

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