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t-Matrix Analysis of the Magnetic Phases of a Narrow Energy Band

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Previous calculations of a t-matrix approximation to Hubbard's model of a half-filled narrow energy band are extended to cover all possible occupancies. The method is exact in the low-density limit. The paramagnetic state is found to be more stable than in the Kanamori approximation. The nearly half-filled band, infinite-repulsion limit is also consistent with Nagaoka's prediction. The resulting phase transitions between paramagnetic, ferromagnetic, and antiferromagnetic states occur at smaller bandwidth/potential-energy ratios than those of Penn's Hartree-Fock approach.

I. INTRODUCTION

The authors have previously investigated the ground state of a half-filled nondegenerate narrow energy band using second-order perturbation theory.[1] This was compared to a t-matrix approximation. The electronic Hamiltonian used was that of Hubbard,[2] and the calculations were performed assuming a simple-cubic lattice in the tight-binding limit.

In the weak-interaction limit, an expansion in the bare interaction or the reaction matrix is convergent. Such expansions are, however, generally known to be unreliable for a paramagnetic state at larger carrier densities and for a strong electronic interaction. These considerations are fully expanded on in our earlier paper.[1] But it turns out that, for the half-filled band in the Hubbard model, the paramagnetic state becomes unstable in favor of an antiferromagnetic state before the strength of the interaction can invalidate either approximations. Most of the correlation is already included in this long-range-ordered state since opposite-spin electrons effectively stay out of each other's way. Although it was found that a t-matrix approximation is uncalled for in the half-filled-band case, it is necessary in the low-carrier-density limit. As shown by Day[3] the t-matrix approximation is the first term in a power-series expansion in the density and thus exact at low electron or hole occupancies. It then appears worthwhile at this stage to extend the t-matrix calculations to cover all band densities. The resulting paramagnetic, ferromagnetic, and antiferromagnetic phase study will be accurate at low density or larger bandwidths. The only questionable results would be those for large occupancies and large repulsion.

All calculations will again be performed for a simple-cubic structure in the tight-binding limit at absolute zero of temperature. The interatomic distance is normalized to 1.

II. t-MATRIX

The basic Hamiltonian is Hubbard's[1]

$$H = -T\sum_{ij}^{nn}\sum_{\sigma} C_{i\sigma}^{\dagger} C_{j\sigma} + I\sum_{i} N_{i+}N_{i-} . \tag{2.1}$$

The unperturbed single-particle wave functions on which to build the t-matrix approximation are those of the following Hamiltonian:

$$H_0 = -T\sum_{ij}^{nn}\sum_{\sigma} C_{i\sigma}^{\dagger} C_{j\sigma} + I\sum_{i}\sum_{\sigma} \Delta_{i\sigma} N_{i\sigma} . \tag{2.2}$$

For the paramagnetic and ferromagnetic states we choose

$$\Delta_{i+} = \Delta_{i-} = 0, \tag{2.3}$$

while for the antiferromagnetic state

$$\Delta_{i\pm} = \pm \tfrac{1}{2}\Delta e^{i\vec{\pi}\cdot\vec{R}_i}, \tag{2.4}$$

where

$$\vec{\pi} = \pi(\hat{X} + \hat{Y} + \hat{Z}). \tag{2.5}$$

The unperturbed wave functions and their energies are

$$\Phi_{\vec{k}\pm}(\vec{R}) = N^{-1/2} e^{i\vec{k}\cdot\vec{R}}, \tag{2.6}$$

$$E_{\vec{k}}^{\circ} = \epsilon_{\vec{k}} = -2T(\cos k_x + \cos k_y + \cos k_z) \tag{2.7}$$

for the paramagnetic and ferromagnetic states, and

$$\Phi_{\vec{k}\pm}(\vec{R}) = N^{-1/2} e^{i\vec{k}\cdot\vec{R}} (A_{\vec{k}} \mp B_{\vec{k}} e^{i\vec{\pi}\cdot\vec{R}}), \tag{2.8}$$

$$E_{\vec{k}}^{\circ} = -\tfrac{1}{2} S_{\vec{k}}^{\circ} (\Delta^2 + 4\epsilon_{\vec{k}}^{\,2})^{1/2}, \tag{2.9}$$

with

$$A_{\vec{k}} = (\tfrac{1}{2})^{1/2}[1 - 2S_{\vec{k}}^{\circ}\epsilon_{\vec{k}}/(\Delta^2 + 4\epsilon_{\vec{k}}^{\,2})^{1/2}]^{1/2}, \tag{2.10}$$

$$B_{\vec{k}} = (\tfrac{1}{2})^{1/2} S_{\vec{k}}^{\circ}[1 + 2S_{\vec{k}}^{\circ}\epsilon_{\vec{k}}/(\Delta^2 + 4\epsilon_{\vec{k}}^{\,2})^{1/2}]^{1/2}, \tag{2.11}$$

$$S_{\vec{k}}^{\circ} = -\epsilon_{\vec{k}}/|\epsilon_{\vec{k}}| \tag{2.12}$$

for the antiferromagnetic state.

Following Appendix B of our earlier paper,[1] the energy in the t-matrix approximation is

$$E_t = -T\sum_{\sigma}\sum_{\vec{k}<\vec{k}_{F\sigma}}\sum_{ij}^{nn} \Phi_{\vec{k}\sigma}^{*}(\vec{R}_i)\Phi_{\vec{k}\sigma}(\vec{R}_j) + I\sum_{\vec{k}_1<\vec{k}_{F+}}\sum_{\vec{k}_2<\vec{k}_{F-}}\sum_{i} \psi_{\vec{k}_1\vec{k}_2}(\vec{R}_i\vec{R}_i)\Phi_{\vec{k}_{1+}}(\vec{R}_i)\,\Phi_{\vec{k}_{2-}}(\vec{R}_i), \tag{2.13}$$

where the pair wave function defined in Day[3] is

$$\psi_{\vec{k}_1\vec{k}_2}(\vec{R}_1\vec{R}_2) = \Phi_{\vec{k}_{1+}}(\vec{R}_1)\Phi_{\vec{k}_{2-}}(\vec{R}_2) - I\sum_{\vec{k}_1'>\vec{k}_{F+}}\sum_{\vec{k}_2'>\vec{k}_{F-}} \Phi_{\vec{k}_{1+}'}(\vec{R}_1)\Phi_{\vec{k}_{2-}'}(\vec{R}_2) \times\sum_{i}\Phi_{\vec{k}_{1+}'}^{*}(\vec{R}_i)\Phi_{\vec{k}_{2-}'}^{*}(\vec{R}_i)\psi_{\vec{k}_1\vec{k}_2}(\vec{R}_i\vec{R}_i)/ (E_{\vec{k}_1'} + E_{\vec{k}_2'} - E_{\vec{k}_1} - E_{\vec{k}_2}). \tag{2.14}$$

The formal solution of Eq. (2.13) is easy once the unperturbed single-particle wave functions are substituted. In each of the paramagnetic, ferromagnetic, and antiferromagnetic states one has to choose spin-dependent Fermi surfaces, as characterized by the Fermi momenta $\vec{k}_{F\pm}$, consistent with the electronic occupancy and the spin polarization of the band. For the ferromagnetic state the degree of magnetization was used as a variational parameter with which to minimize the energy. In the antiferromagnetic solution, it is the parameter Δ which was used variationally. The stability of these vari-

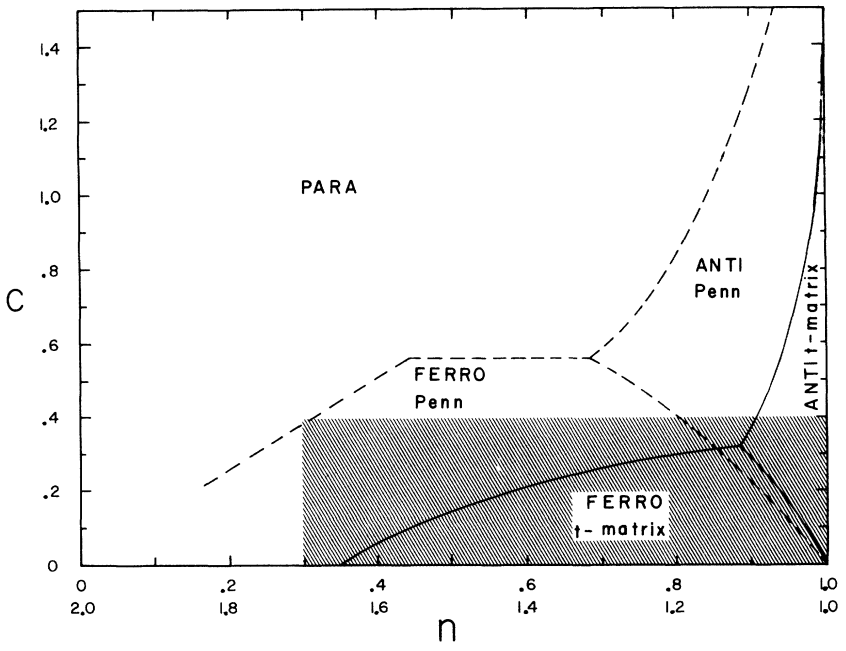

FIG. 1. Phase diagram of the paramagnetic, ferromagnetic, and antiferromagnetic states in the t-matrix approximation (solid line) compared to Penn's one-body Hartree approach (dashed line). The hatched area represents the region in which the t-matrix phase boundaries are inconclusive. The electronic occupancy loops back because of electron-hole symmetry. The bandwidth/potential-energy ratio is $3c$.

TABLE I. Ratio of the energy correction from the Kanamori approximation to that of the t matrix for the paramagnetic state at infinite repulsion. n is the electronic occupancy per site and E_F is the Fermi energy.

n	E_F/NT	$\Delta E_{\text{Kanamori}}/\Delta E_{t\text{ matrix}}$
0	−6.0	1.00
0.1	−4.2	1.01
0.2	−3.35	1.10
0.3	−2.6	1.28
0.4	−2.1	1.32
0.5	−1.75	1.37
0.6	−1.4	1.36
0.7	−1.05	1.32
0.8	−0.7	1.26
0.9	−0.35	1.18
1.	0	1.06

ous phases is decided on a minimal-energy basis.

III. RESULTS

The phase diagram of the paramagnetic, ferromagnetic, and antiferromagnetic states resulting from the t-matrix analysis is shown in Fig. 1. We have used the dimensionless parameter

$$C = 4T/I \tag{3.1}$$

as a measure of bandwidth. Because of the close similarity with the results of Penn,[4] we have also plotted them on the same figure. Note, however, the inverted appearance of the diagram of Penn, who used the variable $2/c$ on his vertical axis. The effect of short-range correlations on the Hartree-Fock approximation of Penn is to push the phase transitions to considerably smaller bandwidths. The reason is that correlation effects are more intense on a Hartree-Fock paramagnetic state than on a spin-polarized state which already has some correlations built in. The numerical inaccuracy in the calculations translates into a 10% uncertainty in the bandwidth at the phase boundaries.

It would surely be of interest to compare these results with those obtained from Kanamori's[5] approximation to the t matrix. He replaced the pair wave-function correction in Eq. (2.14) by an approximate average which he chose to be the value at zero pair momentum,

$$\psi_{\vec{k}_1\vec{k}_2}(\vec{R}_1\vec{R}_2) \approx \Phi_{\vec{k}_{1+}}(\vec{R}_1)\Phi_{\vec{k}_{2-}}(\vec{R}_2) - I \sum_{\vec{k}_1' > \vec{k}_{F+}} \sum_{\vec{k}_2' > \vec{k}_{F-}} \Phi_{\vec{k}_{1+}'}(\vec{R}_1)\Phi_{\vec{k}_{2-}'}(\vec{R}_2) \times \sum_i \Phi^*_{\vec{k}_{1+}'}(\vec{R}_i)\Phi^*_{\vec{k}_{2-}'}(\vec{R}_i)\psi_{00}(\vec{R}_i\vec{R}_i)/(E_{\vec{k}_1'} + E_{\vec{k}_2'} - 2E_0). \tag{3.2}$$

He reasoned this approximation would be excellent at small electron occupancy since most of the particles have nearly zero momentum anyway. He also estimated the error would be small for a constant density of state. In Table I we calculated the ratio of the energy correction from the Kanamori approximation to that of the t matrix for the paramagnetic state in the infinite-repulsion limit. The excellence of the Kanamori approximation is verified at low electron density. But there is a rather large discrepancy at intermediate densities with a comeback at the half-filled-band limit. It would appear the Kanamori approximation overemphasizes the energy correction whenever the Fermi level falls in a nonlinear region of the density of states. This can be deduced from the position of the Fermi level relative to the density of states which is plotted in Fig. 2. This would explain why Kanamori found a small error for a constant density of states. In Table II

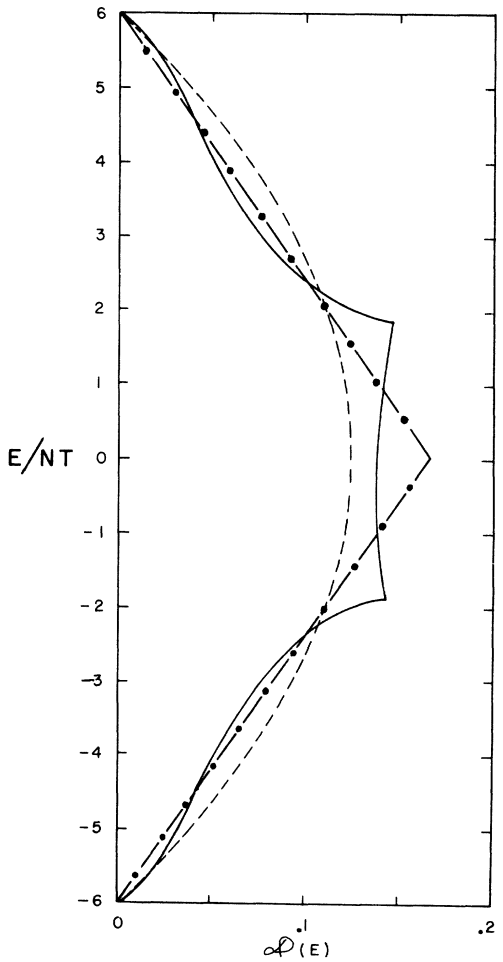

FIG. 2. Density of states as a function of the energy per site in units of temperature for the simple-cubic lattice in the tight-binding limit (solid line), the parabolic distribution (dashed line), and the triangular distribution (dot-dashed line).

TABLE II. Comparison of critical values for the ferro-paramagnetic phase transition with those using the Kanamori approximation. n is the electronic occupancy per site and $3C$ is the bandwidth/potential-energy ratio.

Approximation	$n_{cr}(c=0)$	$n_{cr}(c=\frac{1}{6})$	$C_{cr}(n=1)$
t matrix			
Simple-cubic lattice, tight-binding limit	0.35	0.54	0.33
Kanamori			
Simple-cubic lattice, tight-binding limit	0.24	0.42	0.37
Parabolic density of states	0.208	0.367	0.375
Triangular density of states	0.214	0.395	0.538

we compare the t-matrix results for the ferromagnet-paramagnet transition to those obtained by the Kanamori approximation. We have included Kanamori's own results for parabolic and triangular densities of states which are also plotted in Fig. 2. One notices the rather large difference between the t-matrix and the Kanamori approximations again at intermediate densities. The half-filled-band case is very close to the Kanamori estimate even using a parabolic density of states. The effect of a full t-matrix approximation is then to further stabilize the paramagnetic state at the expense of ferromagnetism, the more so at intermediate densities. The consistency between the Kanamori estimates using various densities of states assures us of the accuracy of our computations.

It is also reassuring to note that Nagaoka's[6] conclusion is verified. For infinite repulsion, the addition or removal of a few electrons from the half-filled band results in a transition to the ferromagnetic state. The t-matrix approximation, however, will be shown to be invalid for the ferromagnetic state near the half-filled-band limit. Any conclusions are then purely academic.

One significant difference with Penn's results other than at the small-density limit is at an average site occupancy of 1. This was the outcome of our earlier paper. We find a transition from the antiferromagnetic state to a paramagnetic state contrary to the Hartree expectations for nearest-neighbor hopping only.

We have not indulged in any discussion of the order of the phase transitions because our numerical inaccuracy makes such a determination inconclusive.

IV. VALIDITY OF t-MATRIX APPROXIMATION

In order to assess the credibility of the t-matrix results one must examine the validity of the approximation. The t-matrix approximation is justified whenever (i) an expansion in the reaction matrix is convergent, or (ii) an expansion in the number of hole lines is convergent.

In both cases the t matrix is the first term in the expansion. An example of the first type of convergence is for small interactions, while the small-density limit represents the second type. In our preceding paper[1] we had examined the convergence of the reaction-matrix expansion in the half-filled-band case and found it good for

$$C \gtrsim 0.4. \tag{4.1}$$

On the other hand, Day[3] deduced that an expansion in the number of hole lines is sensitive to the particle density. In fact, the convergence parameter ζ as defined in our earlier paper is proportional to the electronic occupancy per site n_σ. One would expect convergence of such a series for

$$n_\sigma \lesssim 0.3, \tag{4.2a}$$

i.e.,

$$n \lesssim \begin{cases} 0.6 \text{ for a paramagnetic state} & (4.2b) \\ 0.3 \text{ for a ferromagnetic state}. & (4.2c) \end{cases}$$

From both these convergence criteria, one deduces that a t-matrix approximation is unjustifiable in the highly correlated high-density region. This occurs in the ferromagnetic phase and the small-bandwidth part of the antiferromagnetic phase. The only exception is in the half-filled antiferromagnetic phase when the Fermi level falls in the antiferromagnetic energy gap. We deduced in Ref. 1 that a bare-interaction expansion, and more so a reaction-matrix expansion, would then be convergent for all bandwidths.

That a t matrix is unjustifiable in the ferromagnetic and part of the antiferromagnetic phases does not mean these are not the true phases of the model Hamiltonian. It simply means one cannot use arguments based on the t-matrix analysis to deduce the nature of the phases. It also implies that the position of their boundaries is somewhat uncertain.

As mentioned in our earlier paper, [1] Kohn and Luttinger[7] found an additional contribution to the Goldstone expansion for nonspherical Fermi surfaces. We will show that this additional contribution is negligible within the region of validity of a t-matrix approximation, i.e., at low carrier density or for larger bandwidths.

At low electron or hole density, the t-matrix term is the first-order correction in a density expansion. Kohn and Luttinger have shown that there is no correction to first order in the perturbation. This is true whether the perturbation is the interaction potential strength or the density.

At larger bandwidths, the t-matrix approximation is almost equivalent to a second-order one (see

Ref. 1). To second order in the interaction, the energy correction to the Goldstone series depends on the second-order anomalous correction and the derivative with respect to the chemical potential of the first-order correction to the thermodynamic potential.[7] If, as was shown in Appendix D of Ref. 1, we choose the zero-order Hamiltonian to be the Hartree one, we find a vanishing derivative of the first-order correction to the thermodynamic potential and no anomalous diagrams. This is a consequence of the Hubbard model which does not contain any interaction between like-spin particles. There is then no second-order correction to the Goldstone series for the energy. But the Goldstone series is independent of any one-body potential that may be added to the unperturbed Hamiltonian and subtracted from the interaction part as long as the Fermi surface remains the same. As this is the case for the paramagnetic and antiferromagnetic states, the previous conclusions also hold when using the unperturbed Hamiltonian in zero order on these states. This is not so for the ferromagnetic state, but since the t-matrix approximation has been found unreliable for the ferromagnetic state, it all becomes academic.

V. CONCLUSION

The t-matrix approximation further stabilizes the paramagnetic state. Except for crucial behavior at low density and in the half-filled-band case it leads qualitatively to the same conclusions as a Hartree-Fock approach, and suffers from the same inaptness in the densely populated limit of the ferromagnetic phase. One would have to call on a more powerful approximation to deal with this phase. Roth's[8] extension of the two-pole theory is surely more appropriate for a saturated or nearly saturated ferromagnet.

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