Moment-Generated Solution to the Hubbard Narrow-Energy-Band Model*†

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A solution to the Hubbard model is presented which invokes the *single* assumption that the low-energy peak in the spectral weight function can be well approximated by a function which duplicates its zeroth, first, and second moments to a given order in the bandwidth. The solution takes advantage of the rigorous moment relations of Harris and Lange. A simple, exact, and unambiguous technique to evaluate the correlation functions, required for the moment relations, in the atomic limit is developed. These functions are used to calculate the moments which in turn generate a spectral weight function with no restriction on the electron density. The ground-state energy for the paramagnetic and ferromagnetic configurations are calculated and compared. The model is found to be ferromagnetic for moderate densities.

I. INTRODUCTION

The vast preponderance of literature on magnetism starts from either the Heisenberg-model or the Stoner–Hartree–Fock-model approximation.[1] Both of these approaches have certain drawbacks. The Heisenberg model, in its traditional form, assumes well-defined localized moments. This is in contradiction with mobility measurements in most ferromagnets. The Stoner–Hartree–Fock approach begins with the correct itinerant-electron picture. However, the approach predicts magnetic order only for strongly interacting electrons. Since the Hartree–Fock approximation is only valid for weakly interacting electrons, we would like to have an approach that starts from the itinerant-electron picture but which treats the correlations between electrons in a more careful manner. The Hubbard model[2] can be such an alternative. As we shall see, conceptually it is an extremely simple model. It is a single-band model which includes the Coulomb interaction between electrons on the same site, but neglects interatomic interactions and (in the form we use here) orbital degeneracy. However, as we point out in Sec. II, good solutions to even this simplified model are difficult to obtain. Clearly we should treat the simple model before generalizing.

It is the aim of this paper to present a solution to the Hubbard model which is based on a minimum of well-established assumptions. In the region of interest, the spectral weight function (SWF) consists of two separated peaks.[3] In essence our only assumption is to approximate each of the peaks by a function which is generated from the known zeroth, first, and second moments of the given peak. Finite lifetime effects are included by considering the second moment. Including effects up to, but not beyond, a finite lifetime is consonant with the majority of literature on the many-body problem. Indeed, much of the literature stops at the quasiparticle approximation which neglects lifetime effects.

One may rightly ask whether it is meaningful to seek magnetic order for such a simplified model. The Heisenberg model includes only interatomic interactions and does not even treat intra-atomic interactions. We neglect these interactions and in addition neglect orbital degeneracy. Nevertheless, we will answer the question "Can magnetic ordering occur in the Hubbard model for some values of its parameters?" in the affirmative.

Section II reviews past solution attempts for the Hubbard model. It is emphasized that one major difficulty is that it has not been recognized what one should properly mean by a "solution" to the Hubbard model. Section III presents some definitions and a formalism. Section IV outlines the solution approach, while the results and concluding remarks are given in Sec. V.

II. SOLUTIONS TO MODEL–SYNOPSIS

In the following, we present a somewhat longer than usual review of proposed solutions to the Hubbard model. The purpose is twofold. First, a comprehensive review is needed, but is unavailable, for this particular problem. The following is offered in lieu of such a review. No attempt is made to cover all contributions by all authors. However, we tried to critically analyze representatives of the various modes of attack in a somewhat synoptic fashion. Second, it is the aim of this paper to present a systematic approach to the Hubbard model that is based on a minimum of well-established assumptions. This will be contrasted with some earlier approaches based on an uncertain, and sometimes incorrect, foundation. We should point out that because of the nature of this review it will be necessary to focus mainly on the negative aspects of the various theories, and many of the positive aspects will not

be treated in as much depth.

The Hubbard model is a cell model describing electrons hopping in a lattice, interacting only when two electrons are on the same site. We postpone the complexities of interatomic interactions, orbital degeneracy, and interband effects to a later work. The Hamiltonian is

$$H = \Delta \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \tfrac{1}{2} I \sum_{i,\sigma} n_{i\sigma} n_{i\sigma} \quad . \tag{1}$$

Here, $c_{i\sigma}^{\dagger}$ creates an electron in a Wannier state associated with site i and with spin σ ($=\pm 1$); $n_{i\sigma}$ is the number operator for site i, spin σ; t_{ij} are geometric factors describing the hopping ($t_{ii}=0$); and Δ and I are measures of the bandwidth and intra-atomic interactions, respectively.

The physically interesting region for the Hubbard model is $kT \ll \Delta \ll I$, where T is the temperature, Δ is a measure of the bandwidth or hopping strength, and I is the intra-atomic Coulomb interaction (interatomic interactions are neglected in the model). One reason for interest in this region is that the other limiting cases can be easily handled. In addition, even at room temperature $kT \approx 0.03$ eV is usually much less than Δ. But more importantly, this is the region of interest in reference to magnetic order. Hartree–Fock (HF) predicts magnetic order for $I \gtrsim \Delta$. Because HF neglects correlations between antiparallel electrons, then magnetic order (*if* it exists at all within the context of this model) must occur in the region $I \gg \Delta$.

Before proceeding to the various proposed solutions, it would be well to recall some rigorous results of relevance to this section. (Some additional exact properties of the model will be discussed in later sections.) They are the following: (i) the Harris–Lange sum rules[3] which give the moments of the spectral weight function to a given order in Δ/I in terms of certain equal-time correlation functions; (ii) Bari's exact solution[4] of the two-electron N-site Hubbard model; (iii) certain rigorous relations among the correlation functions in the atomic limit which will be derived below; and (iv) the observation of Esterling[5]—any solution to the Hubbard model which is "correct to lowest order in Δ" would be equivalent to an exact solution to a dynamical excluded volume problem. Since we are some distance from a complete exact solution of even the static excluded volume problem, it follows from (iv) that any proposed solution to the Hubbard model which claims to be correct to lowest order in Δ is most probably in error.

Most solutions to the Hubbard model employ some sort of Green's-function decoupling. They fall into two categories. First, there are those which are equivalent to a Hartree–Fock–like solution, such as that used by Langer, Plischke, and Mattis.[6] These are invalid for any discussion of magnetic order since such approximations are only valid for $\Delta \gg I$. They all have the property that the self-energy diverges as $I \to \infty$. The second category factors some higher-order correlation function, separating operators referring to different lattice sites, claiming this procedure is correct to lowest order in Δ. This is the original approach by Hubbard[2] as well as by Tahir-Kheli and Jarrett,[7] Roth,[8] Kishore and Joshi,[9] and Arai and Parrinello.[10] This violates property (iv), they do not in general preserve the sum rules [property (i)], and the simple factoring is incorrect to zeroth order in Δ as we will show below [property (iii)].

Another set of solutions employs some sort of perturbation expansion. Expansions in I/Δ have been employed by Kanamori,[11] Hubbard,[12] and others. Kanamori (who used the model before it was "invented" by Hubbard) developed a T-matrix approximation which is limited to, but certainly valid for, low enough densities. This has been applied to spin waves by Edwards and by Callaway.[13] Any other such expansion (e.g., Hubbard's) for arbitrary densities is clearly divergent in our region of interest. Esterling and Lange[14] derived a mass operator perturbation expansion in Δ/I. This preserved the sum rules of Harris and Lange. However, they also claimed a solution correct to Δ/I. In fact, the series did not converge. For example, the second-order terms in Δ for the mass operator $\Sigma(\omega)$ included both terms like Δ^2/I and terms like Δ^2/ω. Since the frequencies (ω) of interest are of order Δ, the latter class of terms is not small. This was demonstrated explicitly by Bari [property (ii)].

Another approach to the Hubbard model has been taken by Sokoloff[15] and by Brinkman and Rice[16] based on Nagaoka's path formulation.[17] This consists of calculating the quantity of interest (e.g., partition function) by following the path of a single hole in an otherwise half-filled band. The generalizations by Sokoloff (ferromagnetic path approximation) and Brinkman and Rice (self-retracing paths only) to multiple holes at best can only be trusted near the half-filled band case. The latter technique is further restricted to nearest-neighbor hopping only. While this approach seems to work well (within the above restrictions, at least in the sense of good agreement with the calculated moments) for the simple cubic lattice, recent calculations by Sokoloff[18] indicate a deterioration of the technique for other Bravais lattices such as fcc. We would also like to question the use of a "random" spin configuration by these authors as one of the states of the system. This corresponds to a simple average over all possible spin configurations. This will be valid for high

temperatures, i.e., $kT \gg \Delta$, but is not valid in the region explored by these authors. The interesting state—paramagnetic—has equal not arbitrary numbers of spin-up and spin-down electrons. One might argue that the difference between a random and paramagnetic configuration is unimportant. But if that is so, then we may equally argue that the difference between, say, a ferromagnetic and paramagnetic state is unimportant as well, since the ferromagnetic state is one state that is averaged into the random configuration. However, this is precisely the difference of interest. Most likely, the random configuration will tend to be intermediate between the strictly paramagnetic and ferromagnetic configurations. Finally, the mobility calculation by Brinkman and Rice has serious difficulties. They require a two-particle correlation function. They assume that this factors into a simple product of single-particle correlation functions. As we shall see, this factoring is incorrect to zeroth order in the bandwidth.

A variational approach has been used by Kaplan and Bari[19] and has more recently been applied by Kaplan[20] to a two-band Hubbard-like model proposed by Falicov and Kimball.[21] Kaplan considers extended (Bloch) states as well as localized (Wannier) states as possible states for the valence band in the variational calculation of an approximate free energy. It is shown that the conclusion of Falicov and Kimball (localization of valence electrons) is not valid at low temperatures. However, both of the sets used by Kaplan are approximations to the exact correlated states. While their use is probably justified at low temperatures (when there are few valence holes and hence a small probability for two holes being close enough to correlate), correlation effects must certainly become important at moderate temperatures or hole densities. Even for low hole densities we should be cautious—again referring to the small energy differences discussed above for this limit. These small effects could be vital in obtaining good expressions for the approximate free energy.

Finally, there is the recent functional integral (FI) approach by Kimball and Schrieffer.[22] The details of the calculation are as yet unpublished. However, one should regard any results of this technique with extreme caution. The technique is known to break down for trivial problems. This is indicated by Keiter,[23] in particular, by the discussion of his Eq. (64). [This is for the random-phase approximation (RPA), which is a generalization of the static approximation used by Kimball and Schrieffer.] Recently, Bari[24] has shown that this technique (the static approximation) gives incorrect behavior for the specific heat in the zero-bandwidth case. Finally, one of us (D. M. E.) in collaboration with Hassing[25] has shown that the static approximation yields incorrect predictions for the ground-state energy of the Anderson model in the zero-mixing limit (analogous to the Hubbard atomic limit), if the impurity energy level ϵ_d is in the range $0 \geq \epsilon_d \geq \frac{1}{4}I$ or $\frac{3}{4}I \geq \epsilon_d \geq -\infty$. (The chemical potential is chosen to be zero.) The discrepancy is equal to $\frac{1}{4}I$ and should persist for finite mixing. The nature of the FI approximations involved for a general model are in an unsettled state. This particular approach only discusses the exactly half-filled band case. There are some simplifications which prevail in this limit. The ground state does not exhibit the extreme degeneracy discussed by Harris and Lange,[3] Esterling and Lange,[26] and Esterling.[5] Hence the difficulties discussed therein do not arise. Any generalization of this treatment for arbitrary densities must grapple with the ambiguities that arise when $\Delta \to 0$, but $\Delta/kT \gg 1$.

III. MODEL AND SOME FORMALISM

In this section we introduce the model, define some quantities of interest (Green's function, spectral weight function), and present some exact properties (equation of motion, moment relations). In this particular work, we restrict ourselves to zero temperature (hence $\Delta/kT \gg 1$ even for $\Delta \to 0$ in the atomic limit).

The following Green's functions will be of interest:

$$G_{11'\sigma} \equiv -i\langle (c_{1\sigma} c^{\dagger}_{1'\sigma})_+ \rangle \ , \tag{2a}$$

$$\Gamma_{11'\sigma} \equiv -i\langle (n_{1-\sigma} c_{1\sigma} c^{\dagger}_{1'\sigma})_+ \rangle \ , \tag{2b}$$

$$G^{\sigma\sigma'}_{121'2'} \equiv (-i)^2 \langle (c_{1\sigma} c_{2\sigma'} c^{\dagger}_{2'\sigma'} c^{\dagger}_{1'\sigma})_+ \rangle \ , \tag{2c}$$

$$\Gamma^{\sigma\sigma'}_{121'2'} \equiv (-i)^2 \langle (n_{1-\sigma} c_{1\sigma} c_{2\sigma'} c^{\dagger}_{2'\sigma'} c^{\dagger}_{1'\sigma})_+ \rangle \ . \tag{2d}$$

Here 1 refers to (R_1, t_1) and $(\ )_+$ refers to positive time ordering. Higher-order Green's functions will be defined analogously. The Green's functions defined in Eqs. (2a) and (2c) will be referred to as G_1 and G_2, respectively. G_1 has the following spectral representation:

$$G_{k\sigma}(\omega) = \int \frac{d\bar{\omega}}{2\pi} \frac{A_{k\sigma}(\bar{\omega})}{\omega - \bar{\omega} + i\delta \operatorname{sgn}(\omega - \mu)} \ , \tag{3}$$

where we have Fourier transformed G_1. This is one definition of $A_{k\sigma}(\omega)$—the spectral weight function (SWF). An equivalent expression for its Fourier transform is[3]

$$A_{11'\sigma} = \langle \{c_{1\sigma}, c^{\dagger}_{1'\sigma}\} \rangle \ , \tag{4}$$

where the curly brackets denote anticommutation.

The moment relations follow immediately from Eq. (4) (see Ref. 3):

$$m^{(0)}_{11'\sigma} \equiv \int \frac{d\omega}{2\pi} A_{11'\sigma}(\omega) = \langle \{c_{1\sigma}, c^{\dagger}_{1'\sigma}\} \rangle \big|_{t_1 = t_{1'}} \ , \tag{5a}$$

$$m^{(1)}_{11',\sigma} \equiv \int \frac{d\omega}{2\pi} A_{11',\sigma}(\omega)\omega = \langle\{[c_{1\sigma}, H], c^\dagger_{1',\sigma}\}\rangle\big|_{t_1=t_{1'}} , \tag{5b}$$

$$m^{(2)}_{11',\sigma} \equiv \int \frac{d\omega}{2\pi} A_{11',\sigma}(\omega)\omega^2 = \langle\{[[c_{1\sigma}, H], H], c^\dagger_{1',\sigma}\}\rangle\big|_{t_1=t_1} \tag{5c}$$

Finally we derive some equations of motion in a form suitable for Sec. IV. The equation of motion for G_1 is (there is an implied sum and/or integration over repeated indices)

$$(G^0_{12})^{-1} G_{21',\sigma} = \delta_{11'} + \Delta t_{12} G_{21',\sigma} + I\,\Gamma_{11',\sigma} , \tag{6}$$

where

$$(G^0_{12})^{-1} = i\frac{\partial}{\partial t_1}\delta_{12} . \tag{7}$$

The equation of motion for G_2 is

$$(G^0_{13})^{-1} G^{\sigma\sigma'}_{321'2'} = \delta_{11'} G_{22',\sigma'} - \delta_{12'} G_{21',\sigma}\delta_{\sigma\sigma'} + \Delta t_{13} G^{\sigma\sigma'}_{321'2'} + I\,\Gamma^{\sigma\sigma'}_{121'2'} . \tag{8}$$

We next multiply both sides of Eq. (8) by G_1 and obtain

$$(\delta_{13} + I\,\Gamma_{13\sigma}) G^{\sigma\sigma'}_{321'2'} = G_{11',\sigma} G_{22',\sigma'} - \delta_{\sigma\sigma'} G_{12',\sigma} G_{21',\sigma} + I\,G_{13\sigma}\Gamma^{\sigma\sigma'}_{321'2'} . \tag{9}$$

It is to be noted that there are no explicit Δ's in Eq. (9). This will be useful in Sec. IV.

IV. SOLUTION

In Sec. II, we critically reviewed previous solution schemes for the Hubbard model. Although there were many approaches, there were also many difficulties. Further, the viable solutions were limited to special values of the density. In this section we present a solution in the physically interesting region $kT \ll \Delta \ll I$. In this particular paper we will only work at zero temperature. We assert the solution has the following two characteristics: (i) it is based on a minimum of well-established assumptions and (ii) it is not limited to any density region. Indeed we make only one assumption—that the spectral weight function can be approximated by a function (a Gaussian in this case) which has the same zeroth, first, and second moments, to lowest order in Δ. (We include finite lifetime effects.) More precisely, the SWF splits into two peaks in the region of interest and we approximate each of the subpeaks by a Gaussian using the first three moments of each subpeak. Further, the moments will be expressed (exactly) in terms of the momentum distribution in the atomic limit. This distribution (and hence the moments) will finally be determined self-consistently from the approximate SWF. One may view this self-consistency condition as an additional assumption. The technique may be generalized to include higher-order moments and to include expressions for the moments to higher order in Δ/I. In summary, we generate an expression for the SWF, for arbitrary density, using the moments of the SWF to a given order in Δ/I. These moments involve equal-time correlation functions expressed in terms of the self-consistently determined atomic-limit momentum distribution. We do not determine the SWF to a given order in Δ/I.

The first step will be to generate expressions for the moments of each subpeak of the SWF to a given order in Δ/I. The technique has already been derived by Harris and Lange.[3] The first two moments are as follows (the third moment is given in the Appendix):

$$m^{(0)}_{k\sigma} = (1 - n_{-\sigma}) + O(\Delta/I) , \tag{10a}$$

$$m^{(1)}_{k\sigma} = (1 - n_{-\sigma})^2 \Delta\epsilon_k - \tau_{-\sigma} + L_{k,-\sigma} + O(\Delta^2/I) , \tag{10b}$$

where $\Delta\epsilon_k$ (the Bloch energy) is the Fourier transform of Δt_{ij}, τ_σ is the average kinetic energy of electrons of spin σ,

$$\tau_\sigma = \frac{\Delta}{N}\sum_{i,j} t_{ij}\langle c^\dagger_{i\sigma} c_{j\sigma}\rangle , \tag{11}$$

and $L_{k,\sigma}$ is the Fourier transform of

$$L_{ij,\sigma} = \Delta t_{ij}(\langle n_{i-\sigma} n_{j-\sigma}\rangle - n^2_{-\sigma} + \langle c^\dagger_{j\sigma} c_{j-\sigma} c^\dagger_{i-\sigma} c_{i\sigma}\rangle) . \tag{12}$$

The important point is that to lowest order in Δ, the nth moment involves up to an $(n+1)$-order correlation function (see the expression for $m^{(2)}$ in the Appendix). We appear to be heading for the same trap as the Green's-function decouplers. The further we go, the higher the order of the required correlation function. However, we make the observation that *if* we could evaluate the required equal-time correlation functions to zeroth order in Δ (i.e., in the atomic limit), then we could have our required moment expressions to lowest order in Δ. The atomic limit is *not* a trivial limit as has been emphasized by Esterling and Lange,[26] and by Esterling.[5] What we will do, however, is derive expressions for the various higher-order atomic-limit correlation functions in terms of the atomic-limit single-particle correlation function (or, equivalently, the momentum distribution function). These expressions will be *exact* (in contrast to usual factoring schemes).

Hence the second step in the solution will be to derive the required expressions for the higher-order correlation functions in terms of the single-particle correlation function. We first present the Fourier transform of the single-particle Green's function $G_{11',\sigma}$ in the atomic limit,

$$G_{k\sigma}(\omega)=\left(\frac{1-n_{-\sigma}}{\omega+i\delta}+\frac{n_{-\sigma}}{\omega-I+i\delta}\right)+2\pi i\delta(\omega)n_{k\sigma}\,, \tag{13}$$

where $n_{k\sigma}$ is the Fourier transform of $\lim\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle$ as $\Delta\to 0$. The last term has been neglected by many authors, but is responsible for the nonlocal nature of G_1 in the atomic limit. The nonlocality property is central to an understanding of the atomic limit. There is no way to further specify $n_{k\sigma}$ without specifying how the limit is taken, i.e., without specifying the coefficients t_{ij}. Some may find the nonlocality surprising for vanishing hopping, but a similar term may be easily found for the free-electron gas G_1 in the atomic limit.[5]

Next we consider the atomic limit G_2. Equation (9) is in a useful form since it has no explicit Δ's. The form of the equation remains the same in the atomic limit. We note that the usual equation [Eq. (8)] is not in a useful form since, among other items, it contains a factor $(G^0)^{-1}$. This factor Fourier transforms into a frequency factor which when multiplying G_2 could annihilate important terms in G_2 which are analogous to the last term in G_1. We have G_2 in terms of G_1 and Γ_2. The latter is a three-particle Green's function [see Eq. (2d)]. Our goal is to express G_2 in terms of G_1 (exactly). This has been done for the general G_2, but for simplicity we present the approach for the specific two-particle correlation functions required for our $m^{(1)}$. In particular, we will express Γ_2 in terms of G_2. We may then find G_2 in terms of G_1.

We first illustrate the reduction process for Γ_1. The steps for Γ_2 are similar but more complex. The following is restricted to the atomic limit. Further, with no loss in generality (we have electron-hole symmetry), we may assume that the number of electrons is less than or equal to the number of sites. Expectation values are taken over the ground state which then has no doubly occupied sites. We will often use the condition

$$n_{1\sigma}n_{1-\sigma}|0\rangle=0\,, \tag{14}$$

where $|0\rangle$ denotes the atomic-limit ground state. Further, it has been shown earlier[26] that in the atomic limit, the c operators obey the following anticommutation relations even for unequal times:

$$\{c_{1\sigma},c_{1'\sigma'}^{\dagger}\}=\delta_{R_1R_{1'}}\delta_{\sigma\sigma'}\,, \tag{15a}$$

$$\{c_{1\sigma},c_{1'\sigma'}\}=0\,. \tag{15b}$$

We are now prepared for the formal manipulations:

$$\begin{aligned}\Gamma_{11'\sigma}&=-i\langle(n_{1-\sigma}c_{1\sigma}c_{1'\sigma}^{\dagger})_{+}\rangle\\&=-i\theta(t_1-t_{1'})\langle n_{1-\sigma}c_{1\sigma}c_{1'\sigma}^{\dagger}\rangle+i\theta(t_{1'}-t_1)\langle c_{1'\sigma}^{\dagger}n_{1-\sigma}c_{1\sigma}\rangle\\&=-i\theta(t_1-t_{1'})\langle n_{1-\sigma}c_{1\sigma}c_{1'\sigma}^{\dagger}\rangle\\&=-i\theta(t_1-t_{1'})\delta_{R_1R_{1'}}\langle n_{1-\sigma}c_{1\sigma}c_{1'\sigma}^{\dagger}\rangle\,.\end{aligned} \tag{16}$$

In the third equality we used the fact that the ground state has no doubly occupied sites, and in the last equality we used, in addition, the fact that the c operators obey unequal-time anticommutation relations of the same form as equal-time relations, when the c's refer to different sites.[26] By putting in a complete set of states we obtain for $R_1=R_{1'}$

$$\begin{aligned}\langle n_{1-\sigma}c_{1\sigma}c_{1'\sigma}^{\dagger}\rangle&=\textstyle\sum_a\langle 0|n_{-\sigma}c_{\sigma}|a\rangle\langle a|c_{\sigma}^{\dagger}|0\rangle e^{-iE_a(t_1-t_{1'})}\\&=\textstyle\sum_a\langle 0|n_{-\sigma}c_{\sigma}|a\rangle\langle a|c_{\sigma}^{\dagger}|0\rangle e^{-iI(t_1-t_{1'})}\\&=\langle 0|n_{-\sigma}c_{\sigma}c_{\sigma}^{\dagger}|0\rangle e^{-iI(t_1-t_{1'})}\\&=n_{-\sigma}e^{-iI(t_1-t_{1'})}\,,\end{aligned} \tag{17}$$

where in the second equality we used that fact that either $E_a=I$ or the first factor vanished. Hence

$$\Gamma_{11'\sigma}=-i\theta(t_1-t_{1'})\delta_{R_1R_{1'}}e^{-iI(t_1-t_{1'})}n_{-\sigma}\,. \tag{18}$$

We now outline the reduction procedure for Γ_2. The required G_2's are

$$D_{12,\sigma}\equiv\langle n_{1\sigma}n_{2\sigma}\rangle-n_{\sigma}^2=-G_{121^+2^+}^{\sigma\sigma}\,, \tag{19}$$

$$S_{12,\sigma}\equiv\langle c_{1-\sigma}^{\dagger}c_{1\sigma}c_{2\sigma}^{\dagger}c_{2-\sigma}\rangle=G_{122^+1^+}^{\sigma-\sigma}\,, \tag{20}$$

where the atomic limit is implied. Putting in complete sets of states again and using the condition that the atomic-limit ground state has no doubly occupied sites, the corresponding Γ_2's become (for $R_1\neq R_2$)

$$\begin{aligned}\Gamma_{121'2^+}^{\sigma\sigma'}&=\langle(n_{1-\sigma}c_{1\sigma}n_{2\sigma'}c_{1'\sigma}^{\dagger})_{+}\rangle\\&=\delta_{R_1R_2}\,\theta(t_1-t_{1'})e^{-iI(t_1-t_{1'})}\langle(n_{1\sigma}n_{2\sigma'})_{+}\rangle\end{aligned} \tag{21}$$

and

$$\begin{aligned}\Gamma_{122^+2'}^{\sigma-\sigma}&=-\langle(n_{1-\sigma}c_{1\sigma}c_{2\sigma}^{\dagger}c_{2-\sigma}c_{2'-\sigma}^{\dagger})_{+}\rangle\\&=-\delta_{R_1R_{2'}}\theta(t_1-t_{2'})e^{-iI(t_1-t_{2'})}\\&\quad\times\langle(c_{1\sigma}c_{2'-\sigma}^{\dagger}c_{2\sigma}^{\dagger}c_{2-\sigma})_{+}\rangle\,.\end{aligned} \tag{22}$$

Finally, doing similar manipulations on the right-hand side of Eq. (9), we obtain (integrating over t_3)

$$\begin{aligned}(\delta_{13}+I\Gamma_{13\sigma})G_{321^+2^+}^{\sigma\sigma'}&=-\langle n_{1\sigma}n_{2\sigma'}\rangle\\&\quad\times[1+(-i)I\theta(t_1-t_3)e^{-iI(t_1-t_3)}n_{-\sigma}]\\&=-(1-n_{-\sigma})\langle n_{1\sigma}n_{2\sigma'}\rangle\end{aligned} \tag{23}$$

and

$$(\delta_{13}+I\Gamma_{13\sigma})G_{322^+1^+}^{\sigma-\sigma}=(1-n_{-\sigma})\langle c_{1-\sigma}^{\dagger}c_{1\sigma}c_{2\sigma}^{\dagger}c_{2-\sigma}\rangle\,. \tag{24}$$

For simplicity we consider the paramagnetic case ($n_{\sigma}=n_{-\sigma}=n$, $D^{\sigma\sigma}=D^{-\sigma-\sigma}$, etc.). The operators

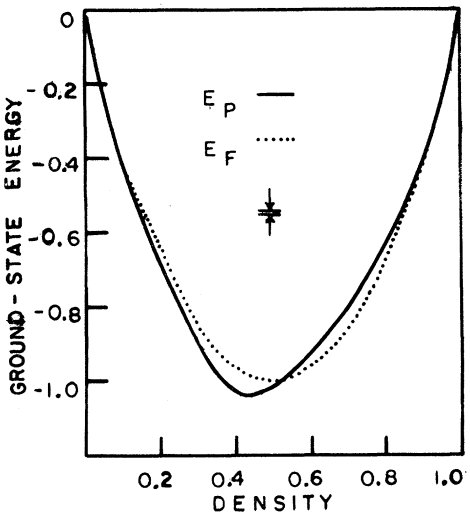

FIG. 1. Ground-state energy vs total electron density for paramagnetic (solid line) and ferromagnetic (dashed line) configurations in a simple cubic lattice with nearest-neighbor hopping. The scale of energy is chosen so that the hopping parameter for nearest neighbors is unity.

$n_{1\sigma}$ and $c_{1\sigma}c_{1-\sigma}^{\dagger}$ are time independent since they commute with the atomic-limit Hamiltonian, and hence D and S are time independent. It follows from the above equations that for $R_1 \neq R_2$,

$$D_{12}^{\sigma\sigma} = -\frac{1-n}{1-2n} g_{12\sigma} g_{21\sigma} \quad , \tag{25}$$

$$D_{12}^{\sigma,-\sigma} = \frac{n}{1-2n} g_{12\sigma} g_{21\sigma} \quad , \tag{26}$$

$$S_{12,\sigma} = -\frac{1}{1-2n} g_{12\sigma} g_{21\sigma} \quad , \tag{27}$$

where 1 refers to R_1 and 2 refers to R_2. Here $g_{12\sigma} = \langle c_{1\sigma}^{\dagger} c_{2\sigma} \rangle$ is the Fourier transform of $n_{k\sigma}$. Similar manipulations were required in order to obtain the expressions for G_3 in terms of G_1 (required for $m^{(2)}$). Note that although the above expressions for D and S are fairly simple, they are not the expressions one would obtain in a usual factoring scheme. Furthermore, in the sort of factoring approach used by Hubbard and others, these correlation functions are assumed to vanish if $R_1 \neq R_2$ and $\Delta \to 0$. Finally, the full two-particle correlation function has a very complicated dependence on g_{12} and could not be obtained from almost any conceivable factoring scheme.

We now have $m^{(0)}$, $m^{(1)}$, and $m^{(2)}$ as functions of the atomic limit $n_{k\sigma}$. The next step is to use these moments to approximate the SWF. The functional form for the SWF was taken as follows:

$$A_{k\sigma}(\omega) = \frac{(2\pi)^{1/2} m_{k\sigma}^{(0)}}{\sigma_{k\sigma}} e^{-(\omega - E_{k\sigma})^2 / 2\sigma_k^2} \quad , \tag{28}$$

where

$$E_{k\sigma} = m_{k\sigma}^{(1)} / m_{k\sigma}^{(0)} \quad , \tag{29}$$

$$\sigma_{k\sigma}^2 = m_{k\sigma}^{(2)} / m_{k\sigma}^{(0)} - E_{k\sigma}^2 \quad . \tag{30}$$

This gives the SWF as a functional of $n_{k\sigma}$. Finally the momentum distribution may be obtained from the SWF in the usual way,

$$n_{k\sigma} = \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A_{k\sigma}(\omega) \quad , \tag{31}$$

where the chemical potential μ is determined in the usual way by the requirement that it correspond to a given number of electrons N_e:

$$N_e = \sum_{k,\sigma} n_{k\sigma} \quad . \tag{32}$$

We now have a closed set of equations. In Sec. V we will discuss the results. In particular, we will use the SWF to calculate ground-state energies in the ferromagnetic-versus-paramagnetic configurations and discuss the question of magnetic stability.

V. RESULTS: APPLICATION TO MAGNETIC ORDER

In this section we will use a result derived by Bari and Lange[27] in order to obtain ground-state energies for the paramagnetic and ferromagnetic configurations. The result, which follows from coupling-constant differentiation, is

$$E(\Delta) = \int_{0^+}^{\Delta} d\alpha \sum_{k\sigma} \epsilon_k n_{k\sigma}(\alpha)$$
$$= \Delta \sum_{k,\sigma} \epsilon_k n_{k\sigma}(0^+) + O(\Delta^2/I) \quad , \tag{33}$$

where $E(\Delta)$ is the ground-state energy for a given bandwidth Δ, ϵ_k is the Fourier transform to t_{ij}, and $n_{k\sigma}(\alpha)$ is the momentum distribution when the bandwidth is equal to α. Since $n_{k\sigma}$ is dimensionless, it can be expressed in a power series in Δ/I. The second equality gives the required result which is consistent with the accuracy pursued in this paper.

Given a total density and an energy dispersion (ϵ_k) we may use the equations in Sec. IV to obtain an expression for the SWF and for the momentum distribution. This was done for nearest-neighbor hopping on a simple cubic lattice. In Fig. 1, we plot the total energy of the paramagnetic and the ferromagnetic ground states, assuming nearest-neighbor hopping. As is well known, the ferromagnetic state is exactly soluble. Since we employed a Monte Carlo approach in the self-consistent evaluation of $n_{k\sigma}$, there is some lack of internal precision in the results. This is indicated by the error bar in the figure. The error estimate was obtained by comparing successive solutions. It is roughly the same for both curves.

Although the two curves are very close, it is reasonable to conclude that if we restrict our-

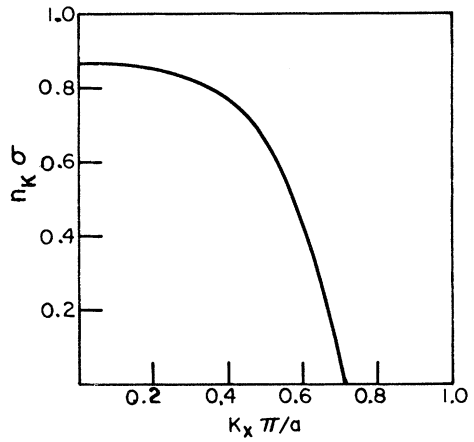

FIG. 2. Momentum distribution $n_{k,\sigma}$ in [100] direction for a total electron density of 0.2. The lower peak in the SWF has a total weight of $1-n_{-\sigma}$ or 0.9 in this case. It follows that $n_{k\sigma} \leq 1-n_{-\sigma}$.

selves to spatially uniform solutions (paramagnetic or ferromagnetic), then the model is ferromagnetic for $0.5 \lesssim n \lesssim 1.5$ (we extend the results for $n > 1.0$ using electron-hole symmetry) and is paramagnetic for $n \lesssim 0.5$. For $n < 0.2$ or $0.8 < n < 1.0$, the data are not sufficiently accurate to distinguish between the two unambiguously. Clearly, we need to calculate each energy more accurately by sampling more points in our Monte Carlo calculations. Alternatively, we may take advantage of some additional approximations which are valid in the low-density and half-filled band limits such as those discussed in Sec. II. These results are in agreement with the conclusions of Nagaoka[17] that the model is ferromagnetic for one electron less than a half-filled band. We have not considered spatially nonuniform (e.g., antiferromagnetic) solutions in this work and so we do not obtain the usual antiferromagnetic solution for an exactly half-filled band.

We can understand the behavior of the two curves by looking at the corresponding momentum distributions. In Fig. 2 we give the momentum distribution along the [100] direction at a moderately low total density (0.2). Already there is considerable smearing out owing to the electron scattering. The model is ferromagnetic at moderate densities since the broad momentum distribution in the paramagnetic case forces the k summation in Eq. (33) to include high-energy states with significant weight. Although the ferromagnetic momentum distribution must contain more volume in k space than the corresponding paramagnetic distribution for a given spin, it still does not sample the very high energy levels because it has a sharp cutoff. This argument breaks down at very low (or very high) electron density. There is less scattering and the paramagnetic distribution is sharper.

In future work we hope to generalize to other Bloch energy dispersions. However, the general behavior of the momentum distribution should be similar and yield similar ordering as a function of the density. We have calculated a curve similar to Fig. 1, but for the one-dimensional case. This case is important because of an exact theorem by Lieb and Mattis[28] that a system with a symmetric potential cannot exhibit ferromagnetic order in one dimension (see also Ghosh[29]). They argue that this should serve as a very strong constraint on any theory of magnetism—theories that predict magnetic order in three dimensions generally predict (incorrectly) order in one dimension. The theorem applies here and our results in one dimension are depicted in Fig. 3. It may be observed that the paramagnetic state has significantly lower energy for all densities.

We hope to extend these results to finite temperatures in a later publication. We replace expectation values over the ground state by thermal averages. However, as long as kT is very small compared to I, then excited states with double occupancies will have negligible weight and the expressions for the moments in terms of the momentum distribution remain valid. Hence the generalization should be straightforward. In addition, it would be of interest to calculate the magnetic susceptibility and the specific heat.

We have not discussed spin-density waves. Since the SWF is not in general positive definite for this case, then the approach taken here is not immediately amenable. However, we would like to point out the somewhat neglected result that the Hubbard model is exactly soluble for any spin

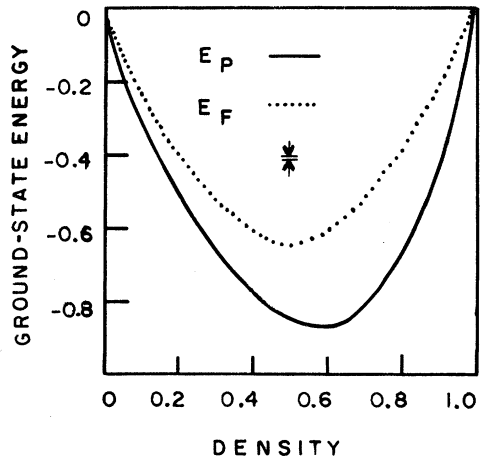

FIG. 3. Ground-state energies in a one-dimensional lattice for paramagnetic (solid line) and ferromagnetic (dashed line) configurations.

wave of unit amplitude. This follows from a perusal of Eq. (6) in a paper by Morris and Cornwell.[30] The ferromagnetic situation is only a special case of this more general result. Hence comparison may still be made with systems with spin-wave states including antiferromagnetic ordering.

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APPENDIX

The techniques developed by Harris and Lange and described in Sec. IV may be used to obtain the following expression for the second moment of the low-energy peak of the spectral weight function in the Wannier representation:

$$
\begin{aligned}
m^{(2)}_{ij,\sigma} = \Delta^2 t_{il}\, t_{lj} [& \langle (1-n_{i-\sigma})(1-n_{l-\sigma})(1-n_{j-\sigma})\rangle \\
& + \langle a^\dagger_{j\sigma} a_{j-\sigma} a^\dagger_{l-\sigma} a_{l\sigma} (1-n_{i-\sigma})\rangle \\
& + \langle a^\dagger_{i-\sigma} a_{i\sigma} a^\dagger_{j\sigma} a_{j-\sigma} (1-n_{l\sigma})\rangle \\
& + \langle a^\dagger_{l\sigma} a_{l-\sigma} (1-n_{j-\sigma}) a^\dagger_{i-\sigma} a_{i\sigma}\rangle] \\
& + \Delta^2 t_{ij}\, t_{lj} \langle (1-n_{i-\sigma}) a_{j-\sigma} a^\dagger_{l-\sigma}\rangle \\
& - \Delta^2 t_{il}\, t_{ij} \langle a^\dagger_{i-\sigma} a_{l-\sigma} (1-n_{j-\sigma})\rangle \\
& + \Delta^2 t_{ij}\, t_{lj} \langle a^\dagger_{l\sigma} a^\dagger_{i-\sigma} a_{i\sigma} a_{j-\sigma}\rangle \\
& + \Delta^2 t_{il}\, t_{ij} \langle a^\dagger_{j\sigma} a_{j-\sigma} a^\dagger_{i-\sigma} a_{l\sigma}\rangle \\
& + \delta_{ij} \Delta^2 t_{il}\, t_{li} \langle [n_{i\sigma} - n_{i-\sigma}] n_{l-\sigma}\rangle \\
& + \delta_{ij} \Delta^2 t_{il}\, t_{mi} \langle a_{l\sigma} a^\dagger_{j\sigma} a_{j-\sigma} a^\dagger_{m-\sigma}\rangle \\
& + \delta_{ij} \Delta^2 t_{il}\, t_{mi} \langle a^\dagger_{i-\sigma} a_{i\sigma} a_{l-\sigma} a^\dagger_{m\sigma}\rangle \quad ,
\end{aligned}
$$

where $a_{i\sigma} \equiv (1-n_{i-\sigma}) c_{i\sigma}$ and we implicitly sum over repeated indices (except i and j). These expressions may be further simplified if we restrict ourselves to no doubly occupied sites. In particular, if we introduce the convention that—with the exception of the first four terms in the bracket above—each of the site indices is restricted to be different from any other index in the same term (i.e., we restrict our sums), then we may replace the a's by simple c's.

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