Correlation of Electrons in a Narrow s Band

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The ground-state wave function for the electrons in a narrow s band is investigated for arbitrary density of electrons and arbitrary strength of interaction. An approximation is proposed which limits all the calculations to counting certain types of configurations and attaching the proper weights. The expectation values of the one-particle and two-particle density matrix are computed for the ferromagnetic and for the nonferromagnetic case. The ground-state energy is obtained under the assumption that only the intra-atomic Coulomb interaction is of importance. Ferromagnetism is found to occur if the density of states is large at the band edges rather than in the center, and if the intra-atomic Coulomb repulsion is sufficiently strong. The relation of this approximation to certain exact results for one-dimensional models is discussed.

INTRODUCTION

IN order to understand transition metals as well as certain insulating crystals with unfilled d shells a ground-state wave function has to be found for the situation which was described particularly by Van Vleck.[1] Its main feature is the localization of the $3d$ wave functions around the nuclei. The Hamiltonian becomes, therefore, different from the one commonly used for metals. The single-particle terms correspond more closely to a tight-binding picture and the two-particle terms describe a very short-range interaction rather than the long-range Coulomb interaction which is studied in the ordinary theory of electron correlation in metals. The discussion of such a Hamiltonian has been taken up recently by a number of authors,[2] each using a different approach and obtaining qualitatively different results. These results are mainly concerned with the occupation probabilities for the electrons in reciprocal space, and with a comparison of the ground-state energies for a ferromagnetic and for a paramagnetic ground state.

The present work attempts to break away from the limitation of low particle density which was inherent in the diagrammatic analysis of GI and GII,[2] although the wave function which was proposed therein is believed to be a good approximation at all densities. The success of the present attempt depends on a relatively simple proposition to which this paper is dedicated and which seems to hold at least in the case of a narrow s band with a strong intra-atomic Coulomb repulsion (cf. GI and HI). This proposition states the following: The main features of the behavior of spin-up electrons, such as their occupation probability in reciprocal space, can be understood qualitatively if it is assumed that the spin-down electrons occupy a band of zero width; and vice versa.

Unfortunately, it is not clear to what extent this proposition is true, except that the domain of validity is larger than one might expect at first. In the present paper, the main argument in favor of this claim comes from an exact result about the occupation probabilities in reciprocal space for the wave function of GI. This result states that for very strong interaction the occupation probability is constant inside the Fermi surface and depends only on the total number of electrons of opposite spin. A very simple approximate treatment of this result is given, in addition to the exact derivation, in the Appendix, and is generalized to the case of intra-atomic Coulomb repulsion of arbitrary strength. The computation of any specific expectation value depends then directly on the number of contributing configurations and their relative weights.

Section 1 states the problem and defines the terms. Section 2 discusses the manner in which various configurations in the lattice contribute to the various density functions, in order to show the reasonableness of our main proposition. Section 3 gives precise rules for calculating the various expectation values for arbitrary numbers of electrons and arbitrary strength of interaction. These rules are illustrated on some examples. Section 4 applies the method to the computation of the energy and goes on to find a criterion for the occurrence of ferromagnetism. The final section is devoted to a discussion of the present results in the light of some exact results in one dimension.

1. GENERAL WAVE FUNCTION FOR THE NARROW s BAND

The case of one narrow s band is described exactly as in GI. There are L lattice sites numbered by a small latin index f, g, h, or j. To each site there belongs, for a given spin, only one orbital $\varphi(x-g)$ of the Wannier type, i.e.,

$$\int \varphi^*(x-f)\varphi(x-h)dx=\delta_{fh}. \tag{1}$$

Bloch waves $\psi_k(x)$, with wave vectors called k or l, are constructed by forming

$$\psi_k(x)=L^{-1/2}\sum_g \exp(ikg)\varphi(x-g). \tag{2}$$

Each of these wave functions is to be multiplied by a

[1] J. H. Van Vleck, Rev. Mod. Phys. **25**, 220 (1953).
[2] Martin C. Gutzwiller, Phys. Rev. Letters **10**, 159 (1963); and Phys. Rev. **134**, A923 (1964), to be referred to as GI and GII; J. Hubbard, Proc. Roy. Soc. (London) **A276**, 238 (1963); **277**, 238 (1964), to be referred to as HI and HII; J. Kanamori, Progr. Theoret. Phys. (Kyoto) **30**, 275 (1963).

spin-wave function, indicated by an arrow, ↑ or ↓, as index. Corresponding to $\varphi(x-g)$, there is a Fermion creation operator $a_g^\dagger$, in the usual manner; and corresponding to $\psi_k(x)$, there is a Fermion creation operator $a_k^\dagger$, with the relation (2) now becoming

$$a_k^\dagger = L^{-1/2}\sum_g \exp(ikg)a_g^\dagger. \tag{3}$$

Let $G=(g_1,\cdots g_m)$ denote a set of lattice sites to be occupied by ↑ particles, and $\Gamma=(\gamma_1,\cdots,\gamma_\mu)$ a set of lattice sites to be occupied by ↓ particles; a configuration $\Phi_{G\Gamma}$ belongs to these two sets, namely,

$$\Phi_{G\Gamma}=\prod_G a_{g\uparrow}^\dagger \prod_\Gamma a_{\gamma\downarrow}^\dagger \Phi_0, \tag{4}$$

where Φ_0 is the vacuum state. The correlated state Ψ is expressed in terms of the amplitudes $A_{G\Gamma}$ by the expansion

$$\Psi=\sum_{G\Gamma} A_{G\Gamma}\Phi_{G\Gamma}, \tag{5}$$

where the summation goes over all different sets G and Γ.

The amplitudes $A_{G\Gamma}$ can be chosen arbitrarily, as real or even complex numbers. In order to compute the energy expectation values for Ψ, only the first- and second-order density functions, ρ_1 and ρ_2, are needed. But, quite generally, it is of interest to examine the nth-order density function ρ_n in terms of its arguments, which we now choose to be the lattice sites and the spin directions, e.g.,

$$\rho_n(h_1\uparrow,\cdots,h_n\uparrow;f_1\uparrow,\cdots,f_n\uparrow) = (n!)^{-1}(\Psi|a_{h_n\uparrow}^\dagger\cdots a_{h_n\uparrow}^\dagger a_{f_1\uparrow}\cdots a_{f_n\uparrow}|\Psi). \tag{6}$$

The calculation of the diagonal elements of ρ_n, where the set $(h_1,\cdots,h_n)$ coincides with the set $(f_1,\cdots,f_n)$, involves only the absolute value of the amplitudes $A_{G\Gamma}$. However, in computing the off-diagonal elements of ρ_n, where the set $(h_1,\cdots,h_n)$ does not coincide with the set $(f_1,\cdots,f_n)$, it is necessary to know something about the "relative phases between adjacent configurations." This expression refers to the complex number $\exp(i\alpha)$ of absolute value 1 by which the amplitudes of two configurations differ, if their sets G and Γ coincide, except that one configuration contains $(f_1\uparrow,\cdots,f_n\uparrow)$, where the other contains $(h_1\uparrow,\cdots,h_n\uparrow)$.

The requirement of antisymmetry imposes very strong restrictions on the choice of the relative phases. These restrictions are not easy to enforce. Therefore, it is reasonable to take one particular set of relative phases which has proven its value in a related problem and stick to that set all through the development. The domain of variation for the variational ansatz (5) is thereby drastically reduced, but it is felt that it would lead into too many complications to proceed differently.

The set of phases to be adopted arises from some uncorrelated wave function Φ which is the antisymmetrized product of Bloch functions. In the case of a simple s band, let this uncorrelated function Φ be given by

$$\Phi=\prod_{(k)} a_{k\uparrow}^\dagger \prod_{(\kappa)} a_{\kappa\downarrow}^\dagger \Phi_0. \tag{7}$$

The set (k) is supposed to be the volume contained inside some Fermi surface S, and similarly the set (κ) is the inside of some Fermi surface Σ in reciprocal space. The coefficients in an expansion of the type (5) are given by the product of two determinants[3]:

$$\left(L^{-1/2}e^{ikg}\begin{vmatrix}k_1\cdots k_m\\ g_1\cdots g_m\end{vmatrix}\right)\left(L^{-1/2}e^{i\kappa\gamma}\begin{vmatrix}\kappa_1\cdots\kappa_\mu\\ \gamma_1\cdots\gamma_\mu\end{vmatrix}\right).$$

If the sets (k) and (κ) are chosen in such a way as to include always k and $-k$ simultaneously, and similarly with κ and $-\kappa$, each of the two determinants is easily shown to be a real number times some fixed power of i. This power depends on the order in which k and $-k$ appear in the set $(k_1\cdots k_m)$ and on some other conventions which are irrelevant to the further discussion.

The amplitudes $A_{G\Gamma}$ of the correlated wave function Ψ are now written as

$$A_{G\Gamma}=B_{G\Gamma}\eta^\nu\left(L^{-1/2}e^{ikg}\begin{vmatrix}k_1\cdots k_m\\ g_1\cdots g_m\end{vmatrix}\right)\times\left(L^{-1/2}e^{i\kappa\gamma}\begin{vmatrix}\kappa_1\cdots\kappa_\mu\\ \gamma_1\cdots\gamma_\mu\end{vmatrix}\right), \tag{8}$$

where ν is the number of identical lattice sites among the sets $(g_1,\cdots g_m)$ and $(\gamma_1,\cdots,\gamma_\mu)$. $B_{G\Gamma}$ is assumed to be real and positive. The parameter η gives a weight to each configuration depending on the amount of crowding. Obviously, the uncorrelated wave function Φ is obtained by setting $B=1$ and $\eta=1$. The correlated wave function Ψ of GI is obtained by setting $B=1$ but $\eta<1$. By letting B differ from one, the diagonal and the off-diagonal elements of ρ_n can be given certain simple properties, which may not follow from setting $B=1$.

2. CASE FOR INFINITELY HEAVY SPIN-DOWN ELECTRONS

The probability for finding the electrons in a configuration G and Γ is given by

$$|A_{G\Gamma}|^2=B_{G\Gamma}{}^2\eta^{2\nu}\left(w(g'-g'')\begin{vmatrix}g_1\cdots g_m\\ g_1\cdots g_m\end{vmatrix}\right)\times\left(\omega(\gamma'-\gamma'')\begin{vmatrix}\gamma_1\cdots\gamma_\mu\\ \gamma_1\cdots\gamma_\mu\end{vmatrix}\right), \tag{9}$$

[3] Determinants are written, where possible, using the following abbreviation:

$$\left(f(x,y)\begin{vmatrix}x_1\cdots x_n\\ y_1\cdots y_n\end{vmatrix}\right)=\begin{vmatrix}f(x_1,y_1)&f(x_1,y_2)&\cdots&f(x_1,y_n)\\ f(x_2,y_1)&f(x_2,y_2)&\cdots&f(x_2,y_n)\\ \vdots&\vdots&&\vdots\\ f(x_n,y_1)&f(x_n,y_2)&\cdots&f(x_n,y_n)\end{vmatrix}.$$

where $w(g'-g'')$ and $\omega(\gamma'-\gamma'')$ are the propagation functions

$$w(h-f)=(1/L)\sum_{(k)}\exp(ikh-ikf),$$
$$\omega(h-f)=L^{-1}\sum_{(\kappa)}\exp(i\kappa h-i\kappa f). \tag{10}$$

Apart from contributing a sign to $A_{G\Gamma}$, the determinants in (8) contribute to the absolute value of the amplitude of the determinants appearing in (9). The latter describe the effect of the so-called exchange hole. Their value is small if the sites $(g_1,\cdots,g_m)$ or $(\gamma_1,\cdots,\gamma_\mu)$ are close to one another.

The correlation tends to magnify this effect, if it is not compensated by a judicious choice of the coefficients $B_{G\Gamma}$. For instance consider the case $B_{G\Gamma}=1$ and $\eta=0$. If Eq. (9) is summed over all sets Γ, it follows that

$$\sum_\Gamma |A_{G\Gamma}|^2=\begin{pmatrix} w(g'-g'') & \Big| & g_1\cdots g_m \\ & & g_1\cdots g_m\end{pmatrix}$$
$$\times\begin{pmatrix} \delta_{\gamma'\gamma''}-\omega(\gamma'-\gamma'') & \Big| & g_1\cdots g_m \\ & & g_1\cdots g_m\end{pmatrix}. \tag{11}$$

The second determinant gives simply the probability of not finding any of the $\downarrow$ particles in $g_1,\cdots,g_m$. This probability shows exactly the same effect of the exchange hole, in that it is small for a set of sites $(g_1,\cdots,g_m)$ close to one another. The probability of finding $\uparrow$ particles at $(g_1,\cdots,g_m)$ independently of the location of the $\downarrow$ particles, provided there is no crowding, shows therefore an enhanced effect of the exchange hole.

As long as the Hamiltonian does not contain any Coulomb interaction terms between atomic orbitals of different lattice sites, as happens to be the case for (35), there seems to be no reason *a priori* for reducing this enhanced effect of the exchange hole. Also, the enhanced exchange hole has a simple explanation: Since a $\downarrow$ particle cannot share a lattice site with a $\uparrow$ particle, there is a tendency to have unlike neighbors ($\uparrow$ and $\downarrow$) rather than like ones ($\uparrow$ and $\uparrow$). Two spin-up electrons tend to stay away from each other. This situation would change, of course, if we introduce some terms into the Hamiltonian which tend to favor parallel alignment of spins on neighboring atoms.

It would seem, however, that this enhanced exchange hole effect has a bad influence on the kinetic energy and crystal potential terms which are determined by $\rho_1(h\uparrow,f\uparrow)$. To make this more evident, compare the expression for $\eta=1$ and $B_{G\Gamma}=1$, viz.,

$$\rho_1(h\uparrow,f\uparrow)=\sum_{(g_2\cdots g_m)}\begin{pmatrix} w(g'-g'') & \Big| & hg_2\cdots g_m \\ & & fg_2\cdots g_m\end{pmatrix}=w(h-f), \tag{12}$$

with the expression for $\eta=0$, *viz.*,

$$\rho_1(h\uparrow,f\uparrow)=\sum_{(g_2\cdots g_m)}\begin{pmatrix} w(g'-g'') & \Big| & hg_2\cdots g_m \\ & & fg_2\cdots g_m\end{pmatrix}$$
$$\times\sum_{\Gamma\neq(fGh)}B_{fG\Gamma}B_{hG\Gamma}\begin{pmatrix} \omega(\gamma'-\gamma'') & \Big| & \gamma_1\cdots\gamma_\mu \\ & & \gamma_1\cdots\gamma_\mu\end{pmatrix}, \tag{13}$$

where the summation over Γ includes only such sets of lattices sites $\gamma_1,\cdots,\gamma_\mu$ which do not coincide with any of the sites $f, g_2,\cdots,g_m, h$. First, observe that the sum over Γ has $\binom{L-m-1}{\mu}$ terms when $h\neq f$, and $\binom{L-m}{\mu}$ when $h=f$. The value of $\rho_1(f\uparrow,f\uparrow)$ is fixed by the normalization to $m/L=w(f-f)$. The value of $\rho_1(h\uparrow,f\uparrow)$ will usually be smaller than $w(h-f)$, if $h\neq f$, because the sum over Γ has fewer terms, namely, by a factor $(L-m-\mu)/(L-m)$, as a consequence of $\eta=0$. The correlation affects the transfer of electrons between lattice sites more than their chance of being at any particular lattice site. Second, note that the sum over Γ in (13) has the least harmful effect on ρ_1 if it does not depend on G, because then the sum over G approximates most closely the formula (12). The coefficients $B_{G\Gamma}$ should, therefore, be chosen so as to compensate at least partially the exchange hole effect which is inherent in the last determinant of (13). In this manner, the particular features of the spin-down electrons are completely smeared out in the sum over Γ, and the specific choice of the coefficients $B_{G\Gamma}$ does not have to be described in detail in order to obtain a reasonable result for the summation over Γ. (For additional discussion of the best values for $B_{G\Gamma}$, cf. Sec. 5.)

It is then conceivable that $\rho_1(h\uparrow,f\uparrow)$ becomes largely independent of the particular choice of the wave vectors κ appearing in ω, i.e., independent of the region in reciprocal space occupied by spin-down electrons, and that a typical value of $\rho_1(h\uparrow,f\uparrow)$ is obtained by putting

$$\sum_{\Gamma\neq G}|B_{G\Gamma}|^2\begin{pmatrix} \omega(\gamma'-\gamma'') & \Big| & \gamma_1\cdots\gamma_\mu \\ & & \gamma_1\cdots\gamma_\mu\end{pmatrix}=1, \tag{14}$$

$$\sum_{\Gamma\neq(fGh)}B_{fG\Gamma}B_{hG\Gamma}\begin{pmatrix} \omega(\gamma'-\gamma'') & \Big| & \gamma_1\cdots\gamma_\mu \\ & & \gamma_1\cdots\gamma_\mu\end{pmatrix}=\frac{L-m-\mu}{L-m}. \tag{15}$$

The Eqs. (14) and (15) may be considered, either as giving the average over some sample of the quantity on the left, or as imposing conditions to be satisfied by the coefficients $B_{G\Gamma}$. Clearly, in order to put any of these two possibilities on a more secure basis, one has either to specify the sample to be averaged over or to show that Eqs. (14) and (15) can be solved. Since the author has not been able to satisfy completely any such requirement, the reasonableness of (14) and (15) is confirmed in two quite different ways.

Let us consider the consequences of (14) and (15). If (14) and (15) are inserted into (13), one finds with the

help of (12)

$$\rho_1(h\uparrow,f\uparrow)=w(h-f) \qquad \text{for } h=f,$$
$$=[(L-m-\mu)/(L-m)]w(h-f) \text{ for } h\neq f. \quad (16)$$

By taking the Fourier transform of (16), we find the occupation probability in reciprocal space:

$$n_{k\uparrow}=\sum_g e^{-ikg}\rho_1(g\uparrow,0\uparrow)=1-(\mu/L) \qquad \text{for } k\in(k),$$
$$=\mu m/L(L-m) \text{ for } k\notin(k). \quad (17)$$

This piecewise constant function with a discontinuity at the Fermi surface of the uncorrelated electron gas corresponding to the state Φ of (7) is plotted in Fig. 1.

Equation (17) has been written under the assumption that $m+\mu<L$. If one has $m+\mu>L$, however, the whole theory can be written in terms of holes rather than particles, and the formula (17) gives then an expression for the density of holes in reciprocal space where m and μ are the total numbers of spin-up and spin-down holes in the lattice.

Now, formula (17) is also obtained if we put $B_{G\Gamma}=\text{const}$ in (13) and then average the last determinant in (13) over all possible sets (κ). This means that we do not try to compensate for the enhanced exchange hole by letting $B_{G\Gamma}$ vary with the configurations G and Γ, but we average over all possible distributions (κ) or spin-down electrons in reciprocal space. Indeed, one finds without difficulty that

$$\sum_{(\kappa)}\left(\omega(\gamma'-\gamma'')\begin{vmatrix}\gamma_1\cdots\gamma_\mu\\ \gamma_1\cdots\gamma_\mu\end{vmatrix}\right)$$
$$=\left(L^{-1}\sum_\kappa e^{i\kappa(\gamma'-\gamma'')}\begin{vmatrix}\gamma_1\cdots\gamma_\mu\\ \gamma_1\cdots\gamma_\mu\end{vmatrix}\right)=1, \quad (18)$$

where we have to divide by $L!/(L-\mu)!\mu!$, the number of different sets (κ), in order to obtain the average. All terms in the summation over Γ in (13) are then the same; there are $(L-m)!/\mu!(L-m-\mu)!$ of them for $h=f$, and $(L-m-1)!/\mu!(L-m-\mu-1)!$ of them for $h\neq f$. The summation over Γ in (13) gives therefore $(\text{const})^2(L-m)!(L-\mu)!/L!(L-m-\mu)!$ for $h=f$, $(\text{const})^2(L-m-1)!(L-\mu)!/L!(L-m-\mu-1)!$ for $h\neq f$. After fixing the constant by normalizing $\rho_1(h\uparrow,h\uparrow)$ to m/L and after summing over all lattice sites $g_2,\cdots,g_m$, we find again (16). Thus, formula (17) is the correct average over all possible sets of wave vectors κ for the spin-down electrons.

The other way of confirming the reasonableness of (16) is based on a result which was mentioned in GI without proof. This result is derived in the Appendix and states the following. If all $B_{G\Gamma}$ are equal, the first part of (17), referring to k inside the Fermi surface, is true whatever the set (κ) for the spin-down electrons may be; but there is seemingly no such simple confirmation for the second part of (17), referring to k outside the Fermi surface. Obviously, the second part of (17) holds only for the average over all sets (κ), whereas the first part of (17) holds for each set (κ) separately.

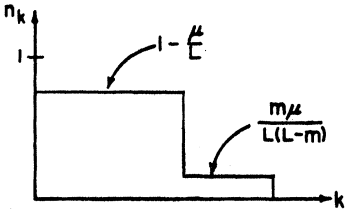

FIG. 1. Occupation probabilities in reciprocal space along a particular direction.

The author considers the result derived in the Appendix as very strong evidence for his claim that the spin-up electrons behave in a way which is largely independent of the way the spin-down electrons behave. In particular, the spin-down electrons might just as well be infinitely heavy as far as the spin-up electrons are concerned. The rest of this paper is then concerned with the physical consequences if this principle is stretched beyond the confirmation which has been presented.

3. METHOD FOR ESTIMATING VARIOUS DENSITY FUNCTIONS IN THE PRESENCE OF CORRELATION

Formulas (14) and (15) express the idea that the coefficients can be chosen such as to give simple values to the density functions ρ_n, the choice being limited by the total number of configurations which contribute to a given ρ_n. It is believed that the properties of ρ_n obtained in this manner are typical for the correlated wave functions of interest in the narrow-band problem. The presence of the spin-down electron merely restricts the freedom of movement for the spin-up electrons without, however, destroying the phase relations among the latter.

In order to give the weighting factor η^ν in (8) a well-defined meaning, we assume that configurations with different values of ν have the same average weight apart from the factor η^ν. Then it is postulated that

$$\rho_n(h_1\uparrow,\cdots,h_n\uparrow,f_1\uparrow,\cdots,f_n\uparrow)=\text{const}\left(w(h-f)\begin{vmatrix}h_1\cdots h_n\\ f_1\cdots f_n\end{vmatrix}\right), \quad (19)$$
$$\rho_n(h_1\downarrow,\cdots,h_n\downarrow,f_1\downarrow,\cdots,f_n\downarrow)=\text{const}\left(\omega(h-f)\begin{vmatrix}h_1\cdots h_n\\ f_1\cdots f_n\end{vmatrix}\right),$$

where the constants depend on m, μ, η, and the number of different lattice sites appearing in (h) and (f). Explicit values for these constants are obtained by counting how many configurations Γ or G contribute toward computing the left-hand side of (19), and attaching the proper weight η^ν to each contributing configuration.

Example 1. $n=m$, $h_1=f_1,\cdots,h_m=f_m$. If there are ν doubly occupied sites, there is a total of $m!(L-m)!/\nu!(m-\nu)!(\mu-\nu)!(L-m-\mu+\nu)!$ configurations contributing to ρ_m. The constant appearing in (19) is given

apart from a normalization factor by

$$\sum_{\nu=0} \eta^{2\nu} m!(L-m)!/\nu!(m-\nu)!(\mu-\nu)!(L-m-\mu+\nu)!$$
$$= (L-m)!F(-m, -\mu; L-m-\mu+1; \eta^2)/\mu!(L-m-\mu)!. \quad (20)$$

If we had taken $n<m$, the constant appearing in (19) would still have been the same, since according to (6) we always have

$$\rho_n(h_1\uparrow,\cdots,h_n\uparrow; f_1\uparrow,\cdots,f_n\uparrow) = m!/n!(m-n)! \sum_{g_{n+1},\cdots,g_m} \rho_m(h_1\uparrow,\cdots,h_n\uparrow,g_{n+1}\uparrow,\cdots; f_1\uparrow,\cdots,f_n\uparrow,g_{n+1}\uparrow,\cdots). \quad (21)$$

In particular, we obtain the normalization from

$$\rho_0 = (\Psi|\Psi) = \sum_{g_1\cdots g_m} \rho_m(g_1\uparrow,\cdots,g_m\uparrow; g_1\uparrow,\cdots,g_m\uparrow) = \text{const} \sum_{g(1\cdots g_m)} \left(w(g'-g'') \begin{vmatrix} g_1\cdots g_m \\ g_1\cdots g_m \end{vmatrix} \right) = \text{const}, \quad (22)$$

where the constant is just given by (20). All quantities to be computed henceforth have, therefore, to be divided by (20).

Example 2. $n=m$, $h_1\neq f_1$, $h_2=f_2$, $\cdots$, $h_m=f_m$. There are a number of possibilities to be distinguished which lead to different contributions to the constant in (19). The sites h_1 and f_1 can both be doubly occupied; one but not the other can be doubly occupied; and, finally, none of them may be doubly occupied. One obtains therefore, a sum of expressions similar to (20):

$$(L-m)!/\mu!(L-m-\mu)! \times\{(L-m-\mu)F(1-m, -\mu; L-m-\mu; \eta^2)/(L-m) + 2\mu\eta F(1-m, 1-\mu; L-m-\mu+1; \eta^2)/(L-m) + \mu(\mu-1)\eta^2 F(1-m, 2-\mu; L-m-\mu+2; \eta^2)/(L-m-\mu+1)\}. \quad (23)$$

With the help of (12) and (21) we now get for ρ_1 the expression

$$\rho_1(h\uparrow,f\uparrow) = w(h-f) \quad \text{for} \quad h=f, \qquad = qw(h-f) \quad \text{for} \quad h\neq f, \quad (24)$$

where q is defined as the quotient (23)/(20), as a generalization of (16). Formula (24) again leads to a piecewise constant occupation probability in reciprocal space, as in Fig. 1, with $q+(1-q)m/L$ inside and $(1-q)m/L$ outside the Fermi surface. Since the hypergeometric function becomes 1 when its argument is zero, the result (16) is recovered for $\eta=0$. Also with the help of the Gauss formula[4]

$$F(a,b;c;1) = \Gamma(c)\Gamma(c-a-b)/\Gamma(c-a)\Gamma(c-b), \quad (25)$$

it is immediately checked that (23) = (20) for $\eta=1$. The evaluation of q for the values of η between 0 and 1 can be performed with the help of the formulas in the Appendix B. These formulas are asymptotically correct for very large L, m, and μ, which is our case of interest.

It goes without saying that a formula similar to (24) is obtained for $\rho_1(h\downarrow,f\downarrow)$. The only necessary modification is to exchange m and μ in (20) and (23).

In order to be able to compute the expectation value of the energy we have to know $\rho_2(g\uparrow,g\downarrow; g\uparrow g\downarrow)$. More generally, we postulate formulas analogous to (19), namely,

$$\rho_{n+1}(h_1\uparrow,\cdots,h_n\uparrow,g\downarrow; f_1\uparrow,\cdots,f_n\uparrow,g\downarrow) = \text{const}\left(w(h-f) \begin{vmatrix} h_1\cdots h_n \\ f_1\cdots f_n \end{vmatrix} \right);$$
$$\rho_{n+1}(g\uparrow,h_1\downarrow,\cdots,h_n\downarrow; g\uparrow,f_1\downarrow,\cdots,f_n\downarrow) = \text{const}\left(\omega(h-f) \begin{vmatrix} h_1\cdots h_n \\ f_1\cdots f_n \end{vmatrix} \right), \quad (26)$$

with the constants again determined by counting the weighted configurations which contribute to the left-hand side. The validity of (26) is examined in Sec. 5. where we argue that Eq. (26) is better realized in three dimensions than in one dimension.

Example 3. $n=m$, $h_1=f_1\neq g$, $\cdots$, $h_m=f_m\neq g$. The constant multiplying (26) is found to be

$$(L-m-1)!F(-m, 1-\mu; L-m-\mu+1; \eta^2)/(\mu-1)!(L-m-\mu)!, \quad (27)$$

which has to be divided by (20) for normalization.

Example 4. $n=m$, $h_1=f_1=g$, $h_2=f_2\neq g$, $\cdots$, $h_m=f_m\neq g$ gives for the constant in (26) the value

$$(L-m)!\eta^2 F(1-m, 1-\mu; L-m-\mu+2; \eta^2)/(\mu-1)!(L-m-\mu+1)!, \quad (28)$$

to be divided again by (20) for normalizations. The consistency of this generalization is shown by checking that

$$\sum_g \rho_{m+1}(h_1\uparrow,\cdots,h_m\uparrow,g\downarrow; f_1\uparrow,\cdots,f_m\uparrow,g\downarrow) = \mu\rho_m(h_1\uparrow,\cdots,h_m\uparrow; f_1\uparrow,\cdots,f_m\uparrow). \quad (29)$$

As an application of the last formulas, we obtain

$$\rho_2(g\uparrow,g\downarrow; g\uparrow,g\downarrow) = \frac{m\mu}{L(L-m-\mu+1)} \times\eta^2 \frac{F(1-m, 1-\mu; L-m-\mu+2; \eta^2)}{F(-m, -\mu; L-m-\mu+1; \eta^2)}. \quad (30)$$

It is satisfying that this formula is symmetric in m and μ, although its derivation is not symmetric in spin-up and spin-down electrons.

[4] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, New York, 1927), p. 281.

Another formula of interest is obtained for $\rho_2(g\uparrow,\gamma\downarrow;\, g\uparrow,\gamma\downarrow)$, where $g\neq\gamma$. Its derivation is somewhat more tricky. We find that

$$(20)\rho_2(g\uparrow,\gamma\downarrow;\, g\uparrow,\gamma\downarrow)$$
$$=(27)\sum_{(g_2\cdots g_m)\neq\gamma}\left(w(g'-g'')\begin{vmatrix} gg_2\cdots g_m \\ gg_2\cdots g_m\end{vmatrix}\right)$$
$$+(28)\sum_{(g_3\cdots g_m)}\left(w(g'-g'')\begin{vmatrix} g\gamma g_3\cdots g_m \\ g\gamma g_3\cdots g_m\end{vmatrix}\right)$$
$$=(m\mu/L^2)(20)+w(g-\gamma)w(\gamma-g)[(27)-(28)]. \quad (31)$$

The difference (27)$-$(28) vanishes only for $\eta=1$. The second term represents an increase over the purely statistical value $m\mu/L^2$. Since the formula (31) is not symmetric in spin-up and spin-down electrons, it might be safer to claim its validity only in the case $w(g-\gamma)=\omega(g-\gamma)$, i.e., $m=\mu$.

Formula (31) shows explicitly that it is quite erroneous to assume statistical independence among spin-up and spin-down electrons at adjacent sites. Formula (31) might suggest the possible usefulness of a mixed density function, such as $\rho_1(g\uparrow;\,\gamma\downarrow)$ corresponding to an expectation value according to the definition (6), which one might assume to vanish at first. Such a mixed density function would describe a ground state in which configurations of different Z components for the total spin participate and have well-defined relative phases. Spin-flip excitations would be present in such a ground state, indicating a tendency toward antiferromagnetism, which is, of course, just described by formula (31).

The same phenomenon appears if we calculate the second-order density $\rho_2(h\uparrow,\gamma\downarrow;\, f\uparrow,\gamma\downarrow)$ with $\gamma\neq f\neq h\neq\gamma$ or with $\gamma=f\neq h$. The calculations are very tedious and the results very lengthy, unless the simplifications of Appendix B are used. The result can be written for $\gamma\neq f\neq h\neq\gamma$ as

$$\rho_2(h\uparrow,\gamma\downarrow,f\uparrow,\gamma\downarrow)=(\mu/L)\rho_1(h\uparrow,f\uparrow)+(m\mu-\nu L)$$
$$\times[w(h-\gamma)w(\gamma-f)-L^{-1}w(h-f)]/m(L-m), \quad (32)$$

and for $\gamma=f\neq h$ as

$$\rho_2(h\uparrow,\gamma\downarrow;\, f\uparrow,\gamma\downarrow)=(\mu/L)\rho_1(h\uparrow,f\uparrow)$$
$$+\left\{\frac{-\mu}{L}+\frac{[1-(\mu/L)]\nu}{\eta(m-\nu)}\right\}\frac{qw(h-f)}{[1+\nu/\eta(m-\nu)]}, \quad (33)$$

where the relation between ν and η as derived in Appendix B has to be inserted. The second terms in (32) and (33) would give a hint as to the values of the mixed density $\rho_1(h\uparrow,f\downarrow)$ for $h\neq f$ and $h=f$, if we were to express them as $\rho_1(h\uparrow;\,\gamma\downarrow)\rho_1(\gamma\downarrow;\, f\uparrow)$.

It is now part of the main proposition of this paper to rule out, at least in a first approximation, the use of such a mixed first-order density function. The additional terms which appear in (31), (32), and (33) are interpreted instead in the simplest imaginable way as the direct consequence of the spin-down electrons which act like inert obstructions, distributed at random, to the movement of the spin-up electrons. In this view, it would seem rather artificial to write a relation like

$$\rho_2(h\uparrow,\gamma\downarrow;\, f\uparrow\gamma\downarrow)=\rho_1(h\uparrow,f\uparrow)\rho_1(\gamma\downarrow,\gamma\downarrow)$$
$$\pm\rho_1(\gamma\downarrow,f\uparrow)\rho_1(h\uparrow,\gamma\uparrow). \quad (34)$$

One might have thought of (34) as a possible representation of (30) through (33), but it turns out to be unfeasible.

4. CALCULATION OF THE ENERGY EXPECTATION VALUE

With the help of (24) and (30) we can compute the expectation value of the energy for the Hamiltonian

$$H=\sum_k(a_{k\uparrow}{}^\dagger a_{k\uparrow}+a_{k\downarrow}{}^\dagger a_{k\downarrow})\epsilon_k+C\sum_g a_{g\uparrow}{}^\dagger a_{g\downarrow}{}^\dagger a_{g\downarrow}a_{g\uparrow}. \quad (35)$$

This Hamiltonian was proposed in GI, and its physical significance has been discussed in HI and GII. It represents, in a certain sense, the opposite of the Hamiltonian which is usually investigated in the study of free electrons with Coulomb repulsion, and it is believed to be a good model for the situation in a d band.

If we eliminate the weighting factor η with the help of (B4), so as to express everything in terms of the number ν of doubly occupied sites, we obtain in the case of $m=\mu$ the formula (this case corresponds to the nonferromagnetic state and is indicated by the index N)

$$\langle H\rangle_N=2mq\bar{\epsilon}+\nu C, \quad (36)$$

where $\bar{\epsilon}=m^{-1}\sum_{(k)}\epsilon_k$ is the average energy of the electrons without correlation. If we normalize $\sum_k\epsilon_k=0$, we have $\bar{\epsilon}<0$. The factor $q<1$, which was defined in (24), gives the discontinuity of the occupation probability in reciprocal space at the Fermi surface. The number of doubly occupied lattice sites is then obtained by minimizing $\langle H\rangle_N$ with respect to ν.

The condition for ν becomes (with $\bar{\nu}=\nu/L$ and $\bar{m}=m/L$)

$$dq/d\bar{\nu}=-C/2\bar{m}\bar{\epsilon}. \quad (37)$$

If this relation is used to eliminate C from (36), the energy expectation value $\langle H\rangle_N$ becomes

$$\langle H\rangle_N=2m\bar{\epsilon}(q-\bar{\nu}dq/d\bar{\nu}). \quad (38)$$

The expectation value of the energy has been increased from its value $2m\bar{\epsilon}<0$ without interaction by the factor $(q-\bar{\nu}d\bar{h}/d\bar{\nu})<1$. With the help of the curves for $q(\bar{\nu})$ as obtained in Appendix B, we can now plot $q-\bar{\nu}dq/d\bar{\nu}$ as a function of $\bar{\nu}$. The slope at $\bar{\nu}=0$ is still infinite, indicating a very strong dependence of $\langle H\rangle$ on the number of doubly occupied sites, but the slope at $\bar{\nu}=\bar{m}^2$ is finite. The initial value for $\bar{\nu}=0$ is the same as for q, viz., $(1-2\bar{m})/(1-\bar{m})$, as shown in Fig. 2. For a given $\bar{\nu}$ and

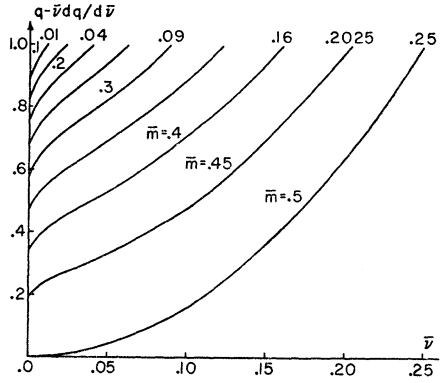

FIG. 2. Plot of $q-\bar{\nu}dq/d\bar{\nu}$, the reduction of the total energy from its value without interaction, versus $\bar{\nu}$, the density of doubly occupied sites, for various values of $\bar{m}=\bar{\mu}$, the density of spin-up and spin-down electrons. (The slopes at $\bar{\nu}=0$ are infinite.)

$\bar{m}$, the value of the interaction constant C may be obtained by using (37) and Fig. 3.

The question of the possibility of a ferromagnetic ground state can now be answered. A ferromagnetic state has the expectation value of H given by

$$\langle H\rangle_F = 2m\epsilon_F\,, \tag{39}$$

where ϵ_F is the average energy of the $2m$ electrons if they all have the same spin. The condition for a ferromagnetic ground state is therefore simply that ϵ_F be smaller than the average energy (38) of the electrons in the nonferromagnetic state, i.e.,

$$\epsilon_F < \bar{\epsilon}(q-\bar{\nu}dq/d\bar{\nu})\,, \tag{40}$$

where both ϵ_F and $\bar{\epsilon}$ are negative in our normalization.

The domain of existence for a ferromagnetic ground state can be obtained from (40), if we plot the ratio $\epsilon_F/\bar{\epsilon}$ as a function of $\bar{m}$ for a given band structure, viz., a given density-of-states curve, and if we draw into the same plot the function $(1-2\bar{m})/(1-\bar{m})$, i.e., the minimum value of $(q-\bar{\nu}dq/d\bar{\nu})$. Wherever $\epsilon_F/\bar{\epsilon}$ is larger than $(q-\bar{\nu}dq/d\bar{\nu})$, a ferromagnetic ground state exists for a sufficiently large value of C, e.g., for a constant density of states, we find in terms of the total bandwidth Δ that $\epsilon_F=-\Delta(1-2\bar{m})/2$ and $\bar{\epsilon}=\Delta(1-\bar{m})/2$. The condition for a ferromagnetic ground state is just not satisfied, because $|\epsilon_F|$ is too small relative to $|\bar{\epsilon}|$ for all $\bar{m}$.

It is easy to see the following: If the density of states is large at the band edges, the ratio $\epsilon_F/\bar{\epsilon}$ tends to be larger than $(1-2\bar{m})/(1-\bar{m})$, and ferromagnetism would appear to be possible if the intra-atomic Coulomb repulsion is strong enough. If the density of states curve is large at the center, its ratio $\epsilon_F/\bar{\epsilon}$ is smaller than $(1-2\bar{m})/(1-\bar{m})$, and a ferromagnetic ground state is excluded. The former case arises in a one-dimensional crystal, whereas the latter is typical of a three-dimensional crystal, although some structures in three dimensions, such as the fcc lattice, may present both aspects (cf. GI).

5. DISCUSSION

The remarks at the end of the preceding section show that the present approximate theory may lead to a ferromagnetic ground state in one dimension. Such a result is in disagreement with a theorem of Lieb and Mattis,[5] according to which the ground state in a one-dimensional system always has vanishing total spin momentum. Although the arguments of Lieb and Mattis are not completely suited to the Hamiltonian (35), their reasoning can be adapted to this simple model Hamiltonian (35). It is, therefore, worthwhile to examine at which point our procedure fails, at least, in one dimension, and what may be done to correct this situation. Also, some of the relevant statements may be true in more than one dimension, and it is of interest to point them out.

A sufficient condition for the coefficients $B_{G\Gamma}$ in (8) to generate a wave function of vanishing total spin momentum in any dimension is the following: The sets $(k_1,\cdots,k_m)$ and $(\kappa_1,\cdots,\kappa_\mu)$ are identical, and the values of $B_{G\Gamma}$ depend only on the set of occupied lattice sites regardless of how this set has been divided up into the subsets G and Γ. These conditions are a consequence of the state (7) having zero total spin if the sets $(k_1\cdots k_m)$ and $(\kappa_1\cdots\kappa_\mu)$ coincide, and of the fact that the total spin momentum operator only shifts the individual spins around the occupied lattice sites but does not shift the electrons themselves.

Even after the coefficients $B_{G\Gamma}$ have been restricted in this manner in order to obtain a state of vanishing total spin momentum, there are enough parameters available to make the requirements (19) and (26) seem reasonable, provided most of the lattice sites $(h_1,\cdots,h_n)$ and $(f_1,\cdots,f_n)$ coincide, as in the various examples of Sec. 3. In particular, the occupation probabilities in reciprocal space as given by (24) appear to be compatible with the requirement of vanshing total spin momentum.

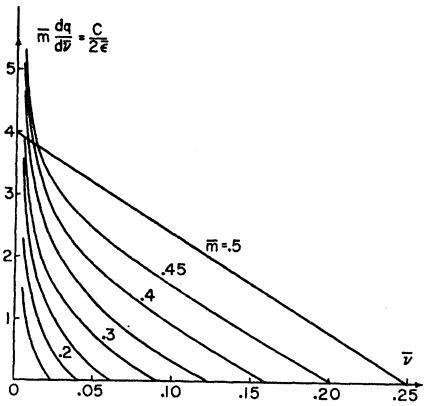

FIG. 3. Plot of $\bar{m}dq/d\bar{\nu}=C/2\bar{\epsilon}$, the ratio of the interaction strength C to twice the average energy per electron $\bar{\epsilon}$ in case of no interaction, versus $\bar{\nu}$, the density of doubly occupied sites. Given the ratio $C/2\bar{\epsilon}$, one can find $\bar{\nu}$ from this figure for a fixed value of $\bar{m}$. Figure 2 can then be used to find the reduction of the average energy per electron $\bar{\epsilon}$ due to the correlation.

[5] Elliott Lieb and Daniel Mattis, Phys. Rev. 125, 164 (1962).

In one dimension, the coefficients $A_{G\Gamma}$ have an additional important property. If the common set $(k_1,\cdots,k_m)=(\kappa_1,\cdots,\kappa_\mu)$ consists of all wave vectors inside some segment in reciprocal space which is centered at the origin, each determinant in (8) is positive if $0\leq g_1<g_2<\cdots<g_m<L$, $0\leq\gamma,\ <\gamma_2<\cdots<\gamma_\mu<L$, and $k_1<k_2<\cdots<k_m$. Therefore, the amplitude $A_{G\Gamma}$ is positive. We can prove this statement exactly as the statements made earlier in this section by simply remarking that the amplitudes $A_{G\Gamma}$ arise from the known ground state in the case of no interaction. According to Lieb and Mattis, the correlated state Ψ seems to be a good candidate for the ground state with interaction.

It is quite clear what causes the trouble in our approach for the one-dimensional case. The difficulty comes from the long tail of the occupation probability in reciprocal space outside the Fermi surface. That tail goes clear out to the zone boundary according to (24), which is particularly serious in one dimension where the density of states in the simple cases is large at the band edges rather than in the center. If we could modify (24) so as to make the occupation probability vanish at the zone boundary, a lot could be gained in one dimension. This could be achieved by a more careful choice of the coefficients B which appear in (13).

The sum over all configurations Γ of spin-down electrons in (13) depends on the set of points $(f,g_2,\cdots,g_m,h)$, i.e., the configuration of spin up electrons with the initial site h and the final site f. For the discussion, we can simplify this dependence by regarding the second line in (13) as a product, the first factor being a function of the set $(g_2,\cdots,g_m)$ of spin-up electrons which remain at their sites, and the second factor being a function of the initial site h and the final site f of the spin-up electron being transferred. It turns out that the first dependence does not influence the constancy of the occupation probability in reciprocal space outside the Fermi surface, if there is no dependence on f and h. We are, therefore, led to consider the sum over Γ in (13), primarily as it depends on f and h, and to disregard its dependence on $(g_2,\cdots,g_m)$. This dependence on f and h comes over and above the main dependence of the second line in (13) on whether or not $f=h$. Such an additional dependence, e.g., on whether or not f and h are nearest neighbors seems particularly indicated in one dimension, where any pair of sites is not surrounded by many third sites close by. This dependence on the exact relative positions of f and h should be much stronger in one dimension than in three.

The result in one dimension can only be improved if one is willing to go through more involved calculations which consist in evaluating sums over Γ, like the second line in (13), at least approximately for certain more specific assumptions about the coefficients B. It may be, however, that such improvements are not badly needed in three dimensions, where the averaging in any small neighborhood is likely to give better results than in one dimension.

ACKNOWLEDGMENT

The author would like to thank Professor David Paul for interesting discussions and helpful suggestions.

APPENDIX A

In the case $B=1$, $\eta=0$, we can write the correlated wave function as

$$\Psi=\prod_g(1-n_{g\uparrow}n_{g\downarrow})\Phi, \tag{A1}$$

where Φ is the independent electron wave function (7). In order to obtain the first-order density function, we have to evaluate $(\Psi|a_{h\uparrow}a_{f\uparrow}^\dagger|\Psi)$, which becomes, for $f\neq h$, simply equal to

$$(\Phi|a_{h\uparrow}\prod_g(1-n_{g\uparrow}n_{g\downarrow})a_{f\uparrow}^\dagger|\Phi)$$
$$=(1/L)\sum_{kl>k_F}e^{-ikf+ilh}(\Phi_{l\uparrow}|\prod_g(1-n_{g\uparrow}n_{g\downarrow})|\Phi_{k\uparrow}). \tag{A2}$$

The index $l\uparrow$ or $k\uparrow$ on Φ indicates the addition of an electron of wave vector l or k and spin-up to the state Φ. The product over all lattice sites g is now expanded, and we examine a particular term $(\Phi_{l\uparrow}|n_{g1\uparrow}n_{g1\downarrow}\cdots n_{g\nu\uparrow}n_{g\nu\downarrow}|\Phi_{k\uparrow})$. If we expand the wave functions $\Phi_{l\uparrow}$ and $\Phi_{k\uparrow}$ into configurations, this expectation value can be expressed as a sum over products of determinants, one term for each arrangement of the remaining $m+1-\nu$ spin-up electrons at the sites $g_{\nu+1}\cdots g_{m+1}$ and the $\mu-\nu$ spin-down electrons at the sites $\gamma_{\nu+1}\cdots\gamma_\mu$. The evaluation of this sum

$$\sum_{(g_{\nu+1}\cdots g_{m+1})}\left(L^{-1/2}e^{-ikg}\begin{vmatrix}lk_1\cdots k_m\\ g_1\cdots g_{m+1}\end{vmatrix}\right)\left(L^{-1/2}e^{ikg}\begin{vmatrix}kk_1\cdots k_m\\ g_1\cdots g_{m+1}\end{vmatrix}\right)$$
$$\times\sum_{(\gamma_{\nu+1}\cdots\gamma_\mu)}\left(L^{-1/2}e^{-i\kappa\gamma}\begin{vmatrix}\kappa_1\cdots\kappa_\mu\\ g_1\cdots g_\nu\gamma_{\nu+1}\cdots\gamma_\mu\end{vmatrix}\right)\left(L^{-1/2}e^{i\kappa\gamma}\begin{vmatrix}\kappa_1\cdots\kappa_\mu\\ g_1\cdots g_\nu\gamma_{\nu+1}\cdots\gamma_\mu\end{vmatrix}\right) \tag{A3}$$

is a simple exercise in determinant manipulation. After the summation over k and l, one obtains

$$(\Phi|a_{h\uparrow}n_{g1\uparrow}n_{g1\downarrow}\cdots n_{g\nu\downarrow}a_{f\uparrow}^\dagger|\Phi)=\begin{vmatrix}\chi(h-f) & -\chi(h-g_1) & -\chi(h-h_2)\cdots\\ \chi(g_1-f) & w(g_1-g_1) & w(g_1-g_2)\cdots\\ \chi(g_2-f) & w(g_2-g_1) & w(g_2-g_2)\cdots\\ \vdots & \vdots & \vdots\end{vmatrix}\begin{vmatrix}\omega(g_1-g_1) & \omega(g_1-g_2)\cdots\\ \omega(g_2-g_1) & \omega(g_1-g_2)\cdots\\ \vdots & \vdots\end{vmatrix}, \tag{A4}$$

where

$$\chi(h-f)=\delta_{hf}-w(h-f)=L^{-1}\sum_{k>k_F}\exp(ikh-ikf).$$

The formula (A4) is correct even for $h=f$. But in that case it is not always useful, because

$$(\Psi|a_{f\uparrow}a_{f\uparrow}^{\dagger}|\Psi)=(\Phi|a_{f\uparrow}\prod_{g\neq f}(1-n_{g\uparrow}n_{g\downarrow})a_{f\uparrow}^{\dagger}|\Phi), \tag{A5}$$

so that only sets $(g_1\cdots g_\nu)$ occur in the summation which do not contain the site f. There is no such restriction on the sets $(g_1\cdots g_\nu)$ if $f\neq h$. Therefore, we obtain a term in addition to the sum over the expressions (A4), but this term is restricted to $f=h$. In this manner, one finds that

$$(\Psi|a_{f\uparrow}^{\dagger}a_{h\uparrow}|\Psi)-\delta_{fh}(\Psi|\Psi)=-\chi(h-f)+\sum_{\nu=1}\frac{(-1)^\nu}{\nu!}\sum_{g_1\cdots g_\nu}\begin{vmatrix}-\chi(h-f) & \chi(h-g_1)\cdots\\ \chi(g_1-f) & w(g_1-g_1)\cdots\\ \vdots & \vdots\end{vmatrix}\begin{vmatrix}\omega(g_1-g_1) & \omega(g_1-g_2)\cdots\\ \omega(g_2-g_1) & \omega(g_2-g_2)\cdots\\ \vdots & \vdots\end{vmatrix}$$

$$+\delta_{hf}\sum_{\nu=0}\frac{(-1)^\nu}{\nu!}\sum_{g_1\cdots g_\nu}\begin{vmatrix}\chi(h-f) & w(h-g_1)\cdots\\ \chi(g_1-f) & w(g_1-g_1)\cdots\\ \vdots & \vdots\end{vmatrix}\begin{vmatrix}\omega(h-f) & \omega(h-g_1)\cdots\\ \omega(g_1-f) & \omega(g_1-g_1)\cdots\\ \vdots & \vdots\end{vmatrix}. \tag{A6}$$

This expression can be further simplified, first, by separating out of the first sum everything that is multiplied with the $-\chi(h-f)$ in the left-hand upper corner of the determinant, and remembering that

$$(\Psi|\Psi)=1+\sum_{\nu=1}\frac{(-1)^\nu}{\nu!}\sum_{g_1\cdots g_\nu}\begin{vmatrix}w(g_1-g_1) & w(g_1-g_2)\cdots\\ w(g_2-g_1) & w(g_2-g_2)\cdots\\ \vdots & \vdots\end{vmatrix}\begin{vmatrix}\omega(g_1-g_1) & \omega(g_1-g_2)\cdots\\ \omega(g_2-g_2) & \omega(g_2-g_2)\cdots\\ \vdots & \vdots\end{vmatrix}; \tag{A7}$$

second, by inserting the definition of χ into the second sum and then, instead of putting $h=f$, by writing $L^{-1}\sum(f=h)$; third, by carrying out the summation over h as far as possible with the help of the simple relation

$$\sum_g\omega(h-g)\omega(g-f)=\omega(h-f). \tag{A8}$$

This gives the final expression

$$(\Psi|a_{f\uparrow}^{\dagger}a_{h\uparrow}|\psi)=[w(h-f)-\delta_{hf}\mu/L](\Psi|\Psi)$$

$$+\sum_{\nu=1}\frac{(-1)^\nu}{\nu!}\sum_{g_1\cdots g_\nu}\begin{vmatrix}0 & \chi(h-g_1) & \chi(h-g_2)\cdots\\ \chi(g_1-f) & w(g_1-g_1) & w(g_1-g_2)\cdots\\ \chi(g_2-f) & w(g_2-g_1) & w(g_2-g_2)\cdots\\ \vdots & \vdots & \vdots\end{vmatrix}\begin{vmatrix}\omega(g_1-g_1) & \omega(g_1-g_2)\cdots\\ \omega(g_2-g_1) & \omega(g_1-g_1)\cdots\\ \vdots & \vdots\end{vmatrix}, \tag{A9}$$

where we have used the fact that $\omega(g-g)=\mu/L$.

Now, we can write the occupation probability in reciprocal space as

$$(\psi|n_{k\uparrow}|\Psi)=(1/L)\sum_{fh}e^{ik(f-h)}(\Psi|a_{f\uparrow}^{\dagger}a_{h\uparrow}|\Psi) \tag{A10}$$

and insert (A9). The first term on the right-hand side of (A9) is trivial, since the summation over f and h applied to $w(h-f)$ gives 1 for k inside and 0 for k outside the Fermi surface of the free spin-up electrons, whereas applied to δ_{hf} this summation gives 1 for all k. On the other hand, if k is outside the Fermi surface of the free spin-up electrons, the first row in the first determinant is modified to $(0,L^{-1/2}e^{ikg_1},\cdots,L^{-1/2}e^{-ikg_\nu})$ and the first column to $(0,L^{-1/2}e^{ikg_1},\cdots,L^{-1/2}e^{ikg_\nu})$ by the summation over h and f, whereas both the first row and the first column vanish, if k is inside the Fermi surface. Therefore, the occupation probability $n_{k\uparrow}$ for k inside the Fermi surface follows entirely from the first term on the right-hand side of (A9), and it is given by the value established in (17), q.e.d.

APPENDIX B

All the hypergeometric series of interest are of the form

$$F=(\alpha-m,\beta-\mu;L-m-\mu+\delta;\eta^2)=\sum_{\nu=0}^{\infty}\frac{(\alpha-m)\cdots(\alpha-m+\nu-1)(\beta-\mu)\cdots(\beta-\mu+\nu-1)}{(L-m-\mu+\delta)\cdots(L-m-\mu+\delta+\nu-1)\nu!}\eta^{2\nu}. \tag{B1}$$

Since m and μ are of the order of the number L of lattice sites, it is sufficient to evaluate the series by considering only the largest terms. The biggest terms occur for the values of ν, where

$$[(\alpha-m+\nu)(\beta-\mu+\nu)/(\nu+1)(L-m-\mu+\delta+\nu)]\eta^2\cong 1. \tag{B2}$$

With the help of Stirling's formula, it follows in the standard manner that the sum is essentially equal to its largest term. We can then approximate $F(\alpha-m,\beta-\mu;L-m-\mu+\delta;\eta^2)$ by

$$\frac{\Gamma(m-\alpha+1)\Gamma(\mu-\beta-1)\Gamma(L-m-\mu+\delta)\eta^{2\nu}}{\Gamma(m-\alpha-\nu+1)\Gamma(\mu-\beta-\nu+1)\Gamma(L-m-\mu+\delta+\nu)\nu!}, \tag{B3}$$

provided α, β, and δ are of order 1, and ν is obtained from the condition

$$[(m-\nu)(\mu-\nu)/\nu(L-m-\mu+\nu)]\eta^2=1. \tag{B4}$$

The result for the hypergeometric function is correct within a factor $[1+0(L^{-1})]$, provided one considers always ratios of two hypergeometric functions. Since ν is independent of α, β, and δ, the quotient of two hypergeometric functions becomes a quotient of Γ functions, which is a rational function, if α, β, and δ are integers.

As a first simple example we evaluate (30), and find immediately that

$$\rho(g\uparrow,g\downarrow;g\uparrow;g\downarrow)=\nu, \tag{B5}$$

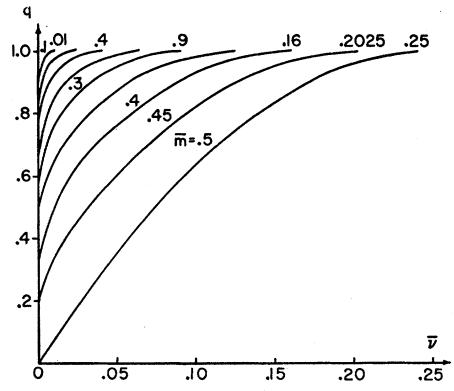

FIG. 4. Plot of q, the occupation probability inside the Fermi surface, versus $\bar{\nu}$, the density of doubly occupied sites.

with ν given by (B4). The quantity η^2 plays, therefore, the same role as the Boltzmann factor in the law of mass action. Indeed, $m-\nu$,and $\mu-\nu$ are the average numbers of dissociated spin-up and spin-down particles, whereas ν is the average number of "bound" spin pairs and $L-m-\mu+\nu$ is the average number of empty lattice sites. The method presented in this paper can be compared to the "quasichemical" method in the theory of mixtures.[6] As η varies from 0 to 1, ν varies from 0 to $m\mu/L$, which is the number of crowded sites without correlation.

In order to obtain the expectation value of the energy (36), we calculate with the help of (B3) the quotient

$$q=\frac{(m-\nu)(L-m-\mu+\nu)}{m(L-m)}\left(1+\frac{(\mu-\nu)\eta}{L-m-\mu+\nu}\right)^2. \tag{B6}$$

In the important special case $m=\mu$, we have

$$\eta=[\nu(L-2m+\nu)]^{1/2}/(m-\nu). \tag{B7}$$

This leads to the expression

$$q=(m-\nu)[(L-2m-\nu)^{1/2}+(\nu)^{1/2}]^2/m(L-m). \tag{B8}$$

The left-hand side is plotted as function of $\bar{\nu}=\nu/L$ for various values of $\bar{m}=m/L<\frac{1}{2}$ in Fig. 4. Note the infinite slope at $\bar{\nu}=0$ and the vanishing slope at $\bar{\nu}=\bar{m}^2$. A reduction in $\bar{\nu}$ can, therefore, be achieved without losing much of the kinetic and crystal potential energy.

[6] E. A. Guggenheim, *Mixtures* (Oxford University Press, New York, 1952), p. 38.