

The singlet state in the Hubbard model with $U = \infty$

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We discuss, in connection with the problem of the ground state in the Hubbard model with $U = \infty$, the normal (nonmagnetic) N -state of a system over the entire range of electron concentrations $n \leq 1$. It is found that in a one-particle approximation, e.g., in the generalized Hartree–Fock approximation, the energy $\epsilon_0(n)$ of the N -state is lower than the energy $\epsilon_{\text{FM}}(n)$ of a saturated ferromagnetic state for all values of n . Using the random phase approximation we calculate the dynamical magnetic susceptibility and show that the N -state is stable for all values of n . A formally exact representation is derived for the mass operator of the one-particle electron Green's function, and its expression in the self-consistent Born approximation is obtained. We discuss the first Born approximation and show that when correlations are taken into account, the attenuation vanishes on the Fermi surface and the electron distribution function at $T = 0$ acquires a Migdal discontinuity, whose magnitude depends on n . The energy of the N -state in this approximation is still lower than $\epsilon_{\text{FM}}(n)$ for $n < 1$. We show that the spin correlation functions are isotropic, which is a characteristic feature of the singlet states of the system. We calculate the spin correlation function for the nearest neighbors in the zeroth approximation as a function of n . Finally, we conclude that the singlet state of the system in the thermodynamic limit is the ground state. © 1998 American Institute of Physics. [S1063-7761(98)01712-0]

1. INTRODUCTION. STATEMENT OF THE PROBLEM

In this paper we discuss the problem of the ground state and the electron distribution function in the Hubbard model¹ when the single-site repulsive potential is infinite, $U = \infty$.

The system Hamiltonian

$$H_\infty = \sum_{f\sigma\Delta} t(\Delta) X_f^{\sigma 0} X_{f+\Delta}^{0\sigma} - \lambda \sum_{f\sigma} X_f^{\sigma\sigma}, \quad (1)$$

specified on a d -dimensional lattice with N sites with a coordination number z and periodic boundary conditions, describes N_e electrons that tunnel to the nearest vacant sites (f stands for the lattice sites, Δ is the vector connecting the nearest neighbors, $t(\Delta)$ is the tunneling integral, and λ is the chemical potential). Since repulsion is assumed infinite, each site is either vacant or contains a single electron with spin projection σ (pairs are forbidden). This fact is reflected in the use of Hubbard operators with well-known commutation relations, which differ from those of fermions (see below).

At this point it is convenient to normalize the Hamiltonian to the halfwidth of the “bare” electron band zt :

$$h_\infty = H_\infty / zt, \quad t(\Delta) / zt = -1/z.$$

In the thermodynamic limit ($N \rightarrow \infty$, $N_e \rightarrow \infty$, $N_e/N = n = \text{const}$), all the properties of our system depend solely on

the topology of the lattice (the number d of the lattice dimensions and the number z of the nearest neighbors) and the electron concentration n ($0 \leq n \leq 1$).

Applying Fourier transformations to all the operators,

$$X_{k\sigma} = \frac{1}{\sqrt{N}} \sum_f e^{ikf} X_f^{0\sigma},$$

$$X^{\sigma\sigma'}(q) = \frac{1}{\sqrt{N}} \sum_f e^{iqf} X_f^{\sigma\sigma'}, \quad (2)$$

where the vectors k and q belong to the first Brillouin zone, we find that the Hamiltonian becomes

$$h_\infty = \sum_{k\sigma} (\omega_k - \mu) X_{k\sigma}^\dagger X_{k\sigma}, \quad (3)$$

where ω_k represents the dimensionless dispersion law in the nearest-neighbors approximation,

$$\omega_k = -\frac{1}{z} \sum_{\Delta} e^{ik\Delta} = -\gamma_k, \quad (4)$$

and $\mu = \lambda / zt$ is the dimensionless chemical potential.

The simplicity of the Hamiltonian (3) is an illusion, since the operators X obey the following commutation relations and completeness condition:

$$\{X_{k\sigma}, X_{p\sigma'}^\dagger\} = \frac{1}{N} \sum_f e^{i(k-p)f} (\delta_{\sigma\sigma'} X_f^{00} + X_f^{\sigma'\sigma}),$$

$$X_f^{00} + X_f^{\sigma\sigma} + X_f^{\bar{\sigma}\bar{\sigma}} = 1. \quad (5)$$

Using the commutation relations (5), we can write the equations of motion ($\hbar=1$) as follows:

$$i\dot{X}_{k\sigma} = [X_{k\sigma}, h_\infty] = \xi_k^0 X_{k\sigma} + R_{k\sigma}, \quad \xi_k^0 = \omega_k - \mu, \quad (6)$$

$$R_{k\sigma} = \frac{1}{\sqrt{N}} \sum_q \omega_{k-q} [X_{k-q}^{\bar{\sigma}\sigma} - X_{k-q}^{\sigma\bar{\sigma}}], \quad (7)$$

$$\bar{\sigma} = -\sigma.$$

The nonlinearity of Eq. (6) stems from the algebra of the operators X or the presence of "kinematic" correlations between electrons with opposite projections of spin.

What is important in the problem of strong electron correlations is the ground state of the system and the electron distribution function.

The energy of the system depends on the system's total spin S . In the case of a saturated ferromagnetic state ($S = N_e/2$), the solution of the problem is exact and trivial for any admissible number of electrons. In this case the system is an ideal Fermi gas of electrons with the projection of the spins in one direction (the state in the k -space is either vacant or occupied by a single electron). At $T=0$ the distribution function is a Fermi step function.

An alternative of the ground state of the system is the singlet state ($S=0$ for an even number of electrons), which we also call a normal (N) strongly correlated state (the numbers of electrons with spin "up" and "down" are equal and there is no long-range magnetic order). The energy advantage of the N -state is due to the possibility of double occupancy of states in the k -space ($X_{k\alpha}^\dagger X_{k\beta}^\dagger |\psi_0\rangle \neq 0$), which lowers the chemical potential in comparison with that for the ferromagnetic state. Here, of course, pairs are forbidden in the direct space and $N_e \leq N$.

Correlations between electrons with opposite spin projections are strongest in the N -state. By "dispersing" the electrons according to their momenta such correlations, on the one hand, enhance the energy of the system and, on the other, may modify the Fermi step function at $T=0$. Here it is important to establish whether the Migdal discontinuity² in the distribution function is retained on the Fermi surface or whether it disappears, as it does in a marginal³ or Luttinger⁴ electron liquid.

The goal of this work is to calculate the distribution function of electrons in a system in the N -state at $T=0$ by the method of two-time retarded Green's functions.⁵ In contrast to the previous previous work of one of the authors (E.V.K),^{6,7} here we examine the approximation of the mass operator corresponding to the self-consistent Born approximation.

2. GREEN'S FUNCTIONS: GENERAL PROPERTIES

We consider the two-time retarded anticommutator Green's function

$$G_{k\sigma}(\tau) = -i\theta(\tau) \langle \{X_{k\sigma}(t), X_{k\sigma}^\dagger(t')\} \rangle, \quad \tau = t - t', \quad (8)$$

and its Fourier transform

$$\langle \langle X_{k\sigma} | X_{k\sigma}^\dagger \rangle \rangle_E \equiv G_{k\sigma}(E) = \int_{-\infty}^{\infty} d\tau e^{iE\tau} G_{k\sigma}(\tau), \quad (9)$$

where E is the spectral variable. It is convenient to write the Green's function as follows:

$$G_{k\sigma}(E) = c_\sigma F_{k\sigma}(E), \quad (10)$$

$$\langle \{X_{k\sigma}, X_{k\sigma}^\dagger\} \rangle = 1 - n_{\bar{\sigma}} \equiv c_\sigma, \quad n_{\bar{\sigma}} = \frac{1}{N} \sum_f \langle X_f^{\bar{\sigma}\bar{\sigma}} \rangle.$$

We introduce the spectral intensity

$$I_{k\sigma}(E) = -\frac{1}{\pi} \text{Im} F_{k\sigma}(E + i0). \quad (11)$$

Using this quantity and the spectral theorem, we can find the averages (here and in what follows we assume $T=0$):

$$\langle X_{k\sigma}^\dagger X_{k\sigma} \rangle = n_{k\sigma} = c_\sigma \int_{-\infty}^0 I_{k\sigma}(E) dE \equiv c_\sigma f_{k\sigma}. \quad (12)$$

The spectral intensity obeys the sum rule

$$\int_{-\infty}^{\infty} I_{k\sigma}(E) dE = 1. \quad (13)$$

The chemical potential can be found by solving the equation

$$n = \frac{1}{N} \sum_{k\sigma} n_{k\sigma} = \frac{1}{N} \sum_{k\sigma} c_\sigma \int_{-\infty}^0 I_{k\sigma}(E) dE, \quad (14)$$

where n is the given electron concentration. The system energy (per lattice site) is

$$\epsilon = \frac{1}{N} \sum_{k\sigma} \omega_k n_{k\sigma} = \frac{1}{N} \sum_{k\sigma} \omega_k c_\sigma \int_{-\infty}^0 I_{k\sigma}(E) dE. \quad (15)$$

Since all calculations are done in the thermodynamic limit, we can replace the sums by integrals:

$$\frac{1}{N} \sum_k A(\omega_k) = \int_{-1}^1 A(\omega) \rho(\omega) d\omega, \quad \int_{-1}^1 \rho(\omega) d\omega = 1,$$

where $\rho(\omega)$ is the density of states corresponding to the dispersion law ω_k (for alternant lattices $\rho(\omega) = \rho(-\omega)$, $-1 \leq \omega_k \leq 1$). After the chemical potential has been found, we can use formula (12) to find the one-particle distribution function.

A saturated ferromagnetic state in the Hubbard model can be described exactly. At $T=0$ the chemical potential and the system energy can be found by the formulas

$$n = \int_{-1}^{\mu} \rho(\omega) d\omega, \quad \epsilon_{\text{FM}}(n) = \int_{-1}^{\mu} \omega \rho(\omega) d\omega, \quad (16)$$

which makes it possible to determine the explicit dependence of the energy of the ferromagnetic state on the electron concentration n .

3. THE MASS OPERATOR OF THE GREEN'S FUNCTION AND ITS APPROXIMATION IN THE SELF-CONSISTENT BORN APPROXIMATION

In the exact equation (6) we can isolate the linear part, which corresponds to the generalized Hartree–Fock approximation. This is achieved by introducing the irreducible operator^{5–7}

$$\tilde{R}_{k\sigma} = R_{k\sigma} - \frac{\langle\{R_{k\sigma}, X_{k\sigma}^\dagger\}\rangle}{\langle\{X_{k\sigma}, X_{k\sigma}^\dagger\}\rangle} X_{k\sigma} \equiv R_{k\sigma} - \frac{a_{k\sigma}}{c_\sigma} X_{k\sigma}, \quad (17)$$

for which $\langle\{\tilde{R}_{k\sigma}, X_{k\sigma}^\dagger\}\rangle = 0$. Actually this means that the procedure allows for all ‘‘internal’’ pairings, which lead to linearization. Equation (6) takes the form

$$i\dot{X}_{k\sigma} = \xi_{k\sigma} X_{k\sigma} + \tilde{R}_{k\sigma}, \quad (18)$$

where

$$\xi_{k\sigma} = \xi_{k\sigma}^0 + \frac{1}{c_\sigma} \langle\{R_{k\sigma}, X_{k\sigma}^\dagger\}\rangle = \Delta_\sigma + \left(c_\sigma + \frac{\kappa_\sigma}{c_\sigma}\right) \omega_k - \mu, \quad (19)$$

$\Delta_\sigma = |\epsilon_{\bar{\sigma}}|/c_\sigma$, $\kappa_\sigma = \langle X_f^{\bar{\sigma}\sigma} X_{f+\Delta}^{\bar{\sigma}\sigma} + \nu_{f\bar{\sigma}} \nu_{f+\Delta\bar{\sigma}} \rangle$, and $\epsilon_{\bar{\sigma}}$ is the energy (per lattice site) of the subsystem of electrons with spin projections $\bar{\sigma}$, with $\nu_{f\bar{\sigma}} = X_f^{\bar{\sigma}\bar{\sigma}} - n_{\bar{\sigma}}$.

The Green’s function $G_{k\sigma}(E)$ (or $F_{k\sigma}(E)$) satisfies the Dyson equation. To set up the equation, we use the well-known method of first differentiating the Green’s functions with respect to the ‘‘first’’ time t and then with respect to the ‘‘second’’ time t' . Using the equation of motion in the generalized Hartree–Fock approximation, we arrive^{6,7} at

$$F_{k\sigma}(E) = \frac{1}{E - \xi_{k\sigma} - \Sigma_{k\sigma}(E) + i0}, \quad (20)$$

$$\Sigma_{k\sigma}(E) = \frac{1}{c_\sigma} \langle\langle \tilde{R}_{k\sigma} | \tilde{R}_{k\sigma}^\dagger \rangle\rangle_E^{(c)}.$$

The mass operator $\Sigma_{k\sigma}(E)$ (the self-energy part of the Green’s function) is the connected (index (c)) part of the higher-order Green’s function, which is not cut along the line of the graphical representation of the zeroth-order Green’s function $F_{k\sigma}^0(E) = (E - \xi_{k\sigma})^{-1}$. Assuming

$$\Sigma_{k\sigma}(E + i0) \equiv M_{k\sigma}(E) - i\Gamma_{k\sigma}(E), \quad (21)$$

we have

$$I_{k\sigma}(E) = -\frac{1}{\pi} \text{Im} F_{k\sigma}(E) = \frac{1}{\pi} \frac{\Gamma_{k\sigma}(E)}{[E - \xi_{k\sigma} - M_{k\sigma}(E)]^2 + \Gamma_{k\sigma}^2(E)}, \quad (22)$$

with $\Gamma_{k\sigma}(E) \geq 0$ (Ref. 5). Formally the representation (20) of the mass operator is exact. However, to perform calculations, we need the explicit form of the mass operator, which means we must use an approximation scheme of some sort.

The spectral representation of the higher-order retarded anticommutator Green’s function is

$$\langle\langle \tilde{R}_{k\sigma} | \tilde{R}_{k\sigma}^\dagger \rangle\rangle_E = \int_{-\infty}^{\infty} \frac{J_{k\sigma}(E')}{E - E' + i0} dE'. \quad (23)$$

If we now employ the spectral theorem, we can express the spectral density of this function in terms of time averages:

$$J_{k\sigma}(E) = \int_{-\infty}^{\infty} \frac{d\tau}{2\pi} e^{iE\tau} (\langle\tilde{R}_{k\sigma}^\dagger(0)\tilde{R}_{k\sigma}(\tau)\rangle + \langle\tilde{R}_{k\sigma}(\tau)\tilde{R}_{k\sigma}^\dagger(0)\rangle) \quad (24)$$

with $\Gamma_{k\sigma}(E) = \pi J_{k\sigma}(E)/c_\sigma$.

Using the definition (7) of the operator $R_{k\sigma}$, we calculate the averages in (24), writing them as a product of quasi-Bose and quasi-Fermi averages (i.e., carrying out ‘‘external’’ couplings). Each of these averages can be found by the spectral theorem⁵ in terms of the corresponding commutator and anticommutator Green’s functions. As a result we obtain

$$J_{k\sigma}(E) \approx \frac{1}{N} \sum_q \omega_{k-q}^2 \int_{-\infty}^{\infty} d\omega N(\omega) f(E - \omega) (1 + e^{\beta E}) \times [S^{\bar{\sigma}\sigma}(q, \omega) c_{\bar{\sigma}} I_{k-q, \bar{\sigma}}(E - \omega) + S^{\bar{\sigma}\bar{\sigma}}(q, \omega) c_\sigma I_{k-q, \sigma}(E - \omega)], \quad (25)$$

where

$$S^{\bar{\sigma}\sigma}(q, \omega) = -\frac{1}{\pi} \text{Im} \langle\langle X^{\bar{\sigma}\sigma}(q) | X^{\sigma\bar{\sigma}}(-q) \rangle\rangle_\omega, \quad (26)$$

$$S^{\bar{\sigma}\bar{\sigma}}(q, \omega) = -\frac{1}{\pi} \text{Im} \langle\langle X^{\bar{\sigma}\bar{\sigma}}(q) | X^{\bar{\sigma}\bar{\sigma}}(-q) \rangle\rangle_\omega, \quad (27)$$

and

$$F(E) = (e^{\beta E} + 1)^{-1}, \quad N(\omega) = (e^{\beta \omega} - 1)^{-1}.$$

A similar approximation was done by Plakida *et al.*⁸ (see also Ref. 9) for the t - J model. It corresponds to the self-consistent Born approximation.

In the N -state, all the main characteristics are independent of the spin projections ($c_\sigma = c = 1 - n/2$, $I_{p\sigma}(E) = I_p(E)$, etc.), and at $T = 0$ we have an expression for the imaginary part of the mass operator:

$$\Gamma_k(E) = \pi \frac{1}{N} \sum_q \omega_{k-q}^2 \int_{-\infty}^{\infty} d\omega [S(q, \omega) + \tilde{S}(q, \omega)] \times [\theta(E)\theta(\omega)\theta(E - \omega) - \theta(-E)\theta(-\omega)] \times \theta(|E| - |\omega|) I_{k-q}(E - \omega), \quad (28)$$

with the obvious redefinitions for $S(q, \omega)$ (Eq. (26)) and $\tilde{S}(q, \omega)$ (Eq. (27)). Thus, the imaginary part of the mass operator in the self-consistent Born approximation is represented by a convolution of the spectral intensities of quasi-Bose and quasi-Fermi excitations in the frequencies ω and momenta q . The real part of the mass operator is a Hilbert transform of $\Sigma_{k\sigma}(E)$, i.e.,

$$M_k(E) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\Gamma_k(E') dE'}{E - E'}. \quad (29)$$

If the functions (26) and (27), which describe the transverse and longitudinal components of spin density fluctua-

tions, have been calculated (at least approximately), the mass operator can be found self-consistently from (28) and (29), the representations (20) and (21), and the equation for the chemical potential

$$n = \frac{1}{N} \sum_{k\sigma} \langle X_{k\sigma}^\dagger X_{k\sigma} \rangle = (2-n) \frac{1}{N} \sum_k \int_{-\infty}^0 I_k(E) dE. \quad (30)$$

Note the difference between a true singlet state and a normal (paramagnetic) state. In addition to $\hat{S}^i|0\rangle$ vanishing in the singlet state, this state has a nontrivial, isotropic spin correlation function

$$\langle S_f^x S_{f+r}^x \rangle = \langle S_f^y S_{f+r}^y \rangle = \langle S_f^z S_{f+r}^z \rangle \equiv C(r), \quad (31)$$

$$\langle S_f^+ S_{f+r}^- \rangle = 2C(r),$$

which is independent of the direction of vector r . If there is no such correlation ($C(r)=0$), we have an ordinary paramagnetic state. Equations (31) are also true for the correlation functions $\langle S^i(q) S^i(-q) \rangle$ and the corresponding Green's functions.

4. THE ZEROth APPROXIMATION AND THE RANDOM PHASE APPROXIMATION

Let us start with the zeroth approximation, i.e., the N -state and $T=0$, where in describing the electron states we ignore the mass operator. In this case the spectral intensity is a delta function and the distribution function, a Fermi step function:

$$I_p^0(E) = \delta(E - \xi_p), \quad n_p^0 = c f_p^0 = c \theta(-\xi_p),$$

$$\xi_p \approx \Delta + c\omega_p - \mu. \quad (32)$$

Here $c=1-n/2$, $\Delta = |\epsilon_0|/2c$, $\epsilon_0(n)$ is the system energy (per site), and we have used an approximate expression for the one-particle spectrum (the correlation function κ is dropped from (19)). At this point it proves convenient to introduce the effective chemical potential $m = (\mu - \Delta)/c$. Then m and the system energy as functions of the electron concentration n are, respectively,

$$\frac{n}{2-n} = \int_{-1}^m \rho(\omega) d\omega \equiv g(m), \quad (33a)$$

$$\frac{\epsilon_0(n)}{2-n} = \int_{-1}^m \omega \rho(\omega) d\omega \equiv v(m). \quad (33b)$$

By excluding the upper limit m we can obtain the explicit dependence of ϵ_0 on n . Analysis shows^{6,7} that in the zeroth approximation $\epsilon_0(n) < \epsilon_{FM}(n)$ for all concentrations, i.e., the singlet (nonmagnetic) state is the energy-advantageous one. Moreover, Eq. (33a) allows correctly for the excluded-volume effect in the Hubbard model with $U=\infty$: the Fermi surface is inflated compared to the case of free electrons ($n-2g(m)$ for such electrons) and occupies the entire Brillouin zone as $n \rightarrow 1$ ($m \rightarrow 1$).

The spectral densities of the quasi-Bose states in the mass operator can be found in the random phase approximation. In the N -state, the commutator Green's functions of transverse and longitudinal spin fluctuations are⁷

$$\langle \langle S^+(q) | S^-(-q) \rangle \rangle_\omega = \langle \langle S^-(q) | S^+(-q) \rangle \rangle_\omega$$

$$= \frac{D_0(q, \omega)}{1 + P(q, \omega)} \equiv D(q, \omega), \quad (34a)$$

$$\langle \langle S^z(q) | S^z(-q) \rangle \rangle_\omega = \frac{1}{2} D(q, \omega), \quad (34b)$$

and

$$\langle \langle X^{\sigma\bar{\sigma}}(q) | X^{\sigma\bar{\sigma}}(-q) \rangle \rangle = \langle \langle X^{\sigma\sigma}(q) | X^{\sigma\sigma}(-q) \rangle \rangle_\omega$$

$$= \frac{D_0(q, \omega)}{1 - P^2(q, \omega)} \equiv \tilde{D}(q, \omega), \quad (35)$$

where

$$D_0(q, \omega) = -\chi_0^{+-}(q, \omega) = \frac{1}{N} \sum_p \frac{n_p^- - n_{p+q}}{\omega - c\omega_{pq}},$$

$$P(q, \omega) = \frac{1}{N} \sum_p \frac{n_{p+q}\omega_{p+q} - n_p\omega_p}{\omega - c\omega_{pq}}, \quad (36)$$

$$\langle X_{p\sigma}^\dagger X_{p\sigma} \rangle = \langle X_{p\bar{\sigma}}^\dagger X_{p\bar{\sigma}} \rangle = n_p, \quad \omega_{pq} = \omega_{p+q} - \omega_p.$$

Equation (34b) points to spin isotropy (see Eq. (31)), which is characteristic of a singlet state. In this state the correlator

$$\langle X^{\sigma\bar{\sigma}}(q) X^{\bar{\sigma}\sigma}(-q) \rangle + \langle X^{\bar{\sigma}\bar{\sigma}}(q) X^{\bar{\sigma}\bar{\sigma}}(-q) \rangle$$

$$= 3\langle S^z(q) S^z(-q) \rangle + \frac{1}{4}\langle \rho(q) \rho(-q) \rangle, \quad (37)$$

where $\rho(q)$ is the operator of electron number density fluctuations. In the random phase approximation we have

$$\langle \langle \rho(q) | \rho(-q) \rangle \rangle_\omega = \frac{D_0(q, \omega)}{1 - P(q, \omega)} \equiv \bar{D}(q, \omega), \quad (38)$$

so that in the singlet state the sum of the spectral intensities can be written as follows:

$$S(q, \omega) + \bar{S}(q, \omega) = \frac{3}{2}S(q, \omega) + \frac{1}{4}\bar{S}(q, \omega), \quad (39)$$

where $\bar{S}(q, \omega)$ is the imaginary part of the function (38).

If we use the Fermi step function $f_p^0 = \theta(-\xi_p) = \theta(m - \omega_p)$ to calculate the transverse susceptibility $\chi^{+-}(q, \omega) = -D(q, \omega)$, of the Hubbard electrons in the static case ($\omega=0$) for $q \rightarrow 0$ we obtain⁷

$$\lim_{q \rightarrow 0} \chi^{+-}(q, 0) = \frac{\rho(m)}{1 - g(m) + m\rho(m)} \equiv u(m)\rho(m), \quad (40)$$

where $u(m)$ is the paramagnetic gain factor. Equation (40) has no pole singularity, which is an indication that the N -state is stable against the development of ferromagnetism; this agrees with the results of Ref. 10.

Thus, the zeroth approximation and the random phase approximation are in full agreement (the absence of ferromagnetism in the Hubbard model with $U=\infty$ in the thermodynamic limit).

5. APPROXIMATIONS USED IN CALCULATING THE MASS OPERATOR AND THE DISTRIBUTION FUNCTION

Let us discuss the role of kinematic correlations in N -state of the system. Such correlations are described by the mass operator $\Sigma_k(E)$, and finding them self-consistently constitutes an extremely difficult problem, whose solution involves complicated numerical calculations. For this reason we introduce a number of simplifying assumptions, which, we believe, do not change the main conclusions and the essence of the problem.

1. The denominators of the functions $D(q, \omega)$, $\tilde{D}(q, \omega)$, and $\bar{D}(q, \omega)$ do not vanish, which is an indication that the model does not contain well-defined collective excitations (magnons or zero-point sound). This makes it possible to approximately replace the sum of spectral intensities (instead of using the random phase approximation) by

$$S(q, \omega) + \tilde{S}(q, \omega) \approx 2AS_0(q, \omega), \tag{41}$$

which is equivalent to considering the susceptibility of independent Hubbard electrons. In Eq. (41), A is a correction factor depending on the concentration (or on the chemical potential). With a distribution function of the general form $n_p = cf_p = cf(\omega_p)$ we have

$$\begin{aligned} -\frac{1}{\pi} \text{Im} D_0(q, \omega) &= S_0(q, \omega) \\ &= \frac{c}{N} \sum_p f(\omega_p) [1 - f(\omega_{p+q})] \\ &\quad \times [\delta(\omega - c\omega_{pq}) - \delta(\omega + c\omega_{pq})] \\ &\equiv S_0^{(+)}(q, \omega) - S_0^{(-)}(q, \omega). \end{aligned} \tag{42}$$

This function, known as the dynamic form factor,¹¹ is defined for both positive ($\omega > 0$) and negative ($\omega < 0$) frequencies, since $\omega_{pq} > 0$ (obviously, $S_0^{(-)}(q, -\omega) = S_0^{(+)}(q, \omega)$), and describes incoherent single-pair electron excitations with the spectrum ω_{pq} within the first Brillouin zone.

The correcting factor A can be found from the sum rule

$$\frac{1}{N} \sum_q \langle S_q^+ S_{-q}^- \rangle = \frac{1}{N} \sum_q \langle X_q^{\sigma\sigma} X_{-q}^{\sigma\sigma} \rangle = \frac{n}{2}. \tag{43}$$

Using (41) and the spectral theorem, at $T=0$ we have

$$\langle S_q^+ S_{-q}^- \rangle = \frac{Ac}{N} \sum_p f_p (1 - f_{p+q}). \tag{44}$$

If we take the Fermi step function $f_p^0 = \theta(m - \omega_p)$ as the zeroth distribution function with the effective chemical potential m and replace summation by integration with the electron state density $\rho(\omega)$, we find

$$\begin{aligned} \frac{n}{2} &= Ac \int_{-1}^1 d\omega \rho(\omega) \theta(m - \omega) \int_{-1}^1 d\omega' \rho(\omega') \theta(\omega' - m) \\ &= Acg(m)[1 - g(m)]. \end{aligned}$$

Since $c = 1 - n/2 = [1 + g(m)]^{-1}$ and $n/2 = g(m)[1 + g(m)]^{-1}$, we have

$$A(m) = [1 - g(m)]^{-1}. \tag{45}$$

After this approximation, the imaginary part of the mass operator can be written as follows ($S_0^+(q, \omega) \equiv S_0(q, \omega)$ for $\omega \geq 0$):

$$\Gamma_k(E) \approx \begin{cases} \Gamma_k^+ = \frac{2A\pi}{N} \sum_q \omega_{k-q}^2 \int_0^E d\omega S_0(q, \omega) I_{k-q}(E - \omega), & E > 0, \\ \Gamma_k^- = \frac{2A\pi}{N} \sum_q \omega_{k-q}^2 \int_0^{|E|} d\omega S_0(q, \omega) I_{k-q}(-|E| + \omega), & E < 0. \end{cases} \tag{46}$$

We see that the attenuation $\Gamma_k(E)$ vanishes as $E \rightarrow 0$. Note that the Fermi level corresponds to $E = 0$, so that there is no attenuation on the Fermi surface proper.

2. Instead of the dynamic form factor $AS_0(q, \omega) = S(q, \omega)$ we consider its value averaged over all the momenta:

$$S(q, \omega) \rightarrow \frac{A}{N} \sum_q S_0(q, \omega) \equiv S(\omega, m), \tag{47}$$

which is the number density of single-pair excitations with an energy ω and a chemical potential m . Using the Fermi step function, introducing a new variable, $\Omega = \omega/c$, and employing Eqs. (42) and (47), we get

$$S(\Omega, m) = A(m) \int_{m-\Omega}^m \rho(x) \rho(x + \Omega) dx, \quad 0 \leq \Omega \leq 2. \tag{48}$$

We see that $S(\Omega, m) \approx A(m)\rho^2(m)\Omega$ as $\Omega \rightarrow 0$. The shape of the function $S(\Omega, m)$ is depicted in Fig. 1 for an elliptical density of electron states, $\rho(x) = (2/\pi)\sqrt{1-x^2}$. Analysis of (48) shows that the behavior and numerical values of $S(\Omega, m)$ do not change significantly with other densities of states for two- and three-dimensional alternant lattices.

The essence of the approximation (47) is as follows. The general expressions (25) and (28) describe processes of the following type: an electron with an ‘‘energy’’ E and momentum k passes to the state $E - \omega$, $k - q$, exciting in the process an electron-hole pair with momentum q and energy $\omega = \omega_{pq}$. When the approximation (47) is used, we ignore the detailed description of states in the momenta and specify the transition of the electron from the constant-energy surface E to the constant-energy surface $E - \omega$; such transitions take place with different momenta q , which is reflected in (47). Since the description of states is done on a constant-energy

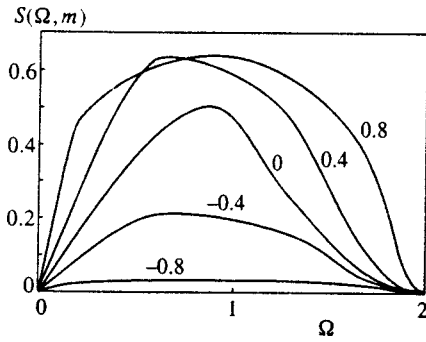


FIG. 1. The density of single-pair excitations for different values of the chemical potential m (Ω is the excitation energy). Here an elliptical density of electron states is used.

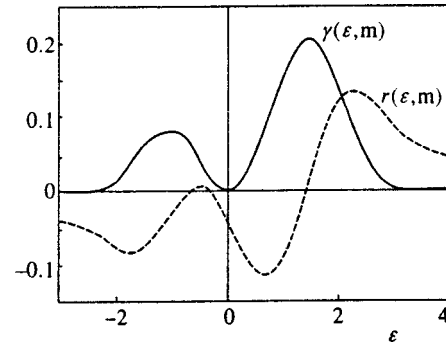


FIG. 2. The real ($r(\epsilon, m)$) and imaginary ($\gamma(\epsilon, m)$) parts of the mass operator in the first Born approximation as functions of the spectral variable ϵ at $m = -0.4$.

surfaces, the dependence of the attenuation and the entire mass operator on the quasimomentum k is lost, i.e., $\Sigma_k(E) \rightarrow \Sigma(E) \equiv M(E) - i\Gamma(E)$. Now, setting E at $c\varepsilon$, we obtain

$\Gamma(\varepsilon)$

$$\approx \begin{cases} 2\pi \int_0^\varepsilon d\Omega S(\Omega, m) \frac{1}{N} \sum_p \omega_p^2 I_p(\varepsilon - \Omega), & \varepsilon > 0, \\ 2\pi \int_0^{|\varepsilon|} d\Omega S(\Omega, m) \frac{1}{N} \sum_p \omega_p^2 I_p(-|\varepsilon| + \Omega), & \varepsilon < 0, \end{cases} \quad (49)$$

and

$$M(\varepsilon) = \text{Re } \Sigma(\varepsilon) \approx \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\Gamma(E') dE'}{\varepsilon - E'}. \quad (50)$$

3. Let us study the first Born approximation (the first iteration step in the self-consistent solution):

$$I_p(\varepsilon - \Omega) \rightarrow I_p^0(\varepsilon - \Omega) = \delta(\varepsilon - \Omega - (\omega_p - m)).$$

The sum in (49) is

$$\begin{aligned} \frac{1}{N} \sum_p \omega_p^2 I_p^0(\varepsilon - \Omega) &\approx \frac{1}{zN} \sum_p I_p^0(\varepsilon - \Omega) \\ &= \frac{1}{z} \int_{-1}^1 dx \rho(x) \delta[\varepsilon - \Omega + m - x] \\ &= \frac{1}{z} \rho(\varepsilon - \Omega + m), \end{aligned}$$

where

$$\frac{1}{z} = \frac{1}{N} \sum_p \omega_p^2 = \int_{-1}^1 \omega^2 \rho(\omega) d\omega \quad (51)$$

is the average value of the square of the bare spectrum over the entire Brillouin zone. In this case the attenuation is

$$\gamma(\varepsilon, m) = \Gamma^{(1)}(\varepsilon)$$

$$\approx \begin{cases} \frac{2\pi}{z} \int_0^\varepsilon d\Omega S(\Omega, m) \rho(\varepsilon - \Omega + m), & 0 \leq \varepsilon \leq 3 - m, \\ \frac{2\pi}{z} \int_0^{|\varepsilon|} d\Omega S(\Omega, m) \rho(-|\varepsilon| + \Omega + m), & -(3 + m) \leq \varepsilon \leq 0, \end{cases} \quad (52)$$

with $-1 \leq m \leq 1$.

As usual, on the Fermi surface $\gamma(\varepsilon) \rightarrow 0$ as $\varepsilon \rightarrow 0$. Near the Fermi surface ($\varepsilon \rightarrow 0$, so that $\Omega \rightarrow 0$) we have

$$S(\Omega, m) \approx A(m) \rho^2(m) \Omega, \quad \rho(\varepsilon - \Omega + m) \approx \rho(m),$$

and

$$\gamma(\varepsilon, m) \approx \frac{\pi}{z} A(m) \rho^3(m) \varepsilon^2. \quad (53)$$

It should be recalled that in our calculations we deal with dimensionless units; actually, $1/z$ has the dimensions of energy squared and γ , of energy. The functional dependence of (53) on ε agrees with Landau's theory of a Fermi liquid¹² (indeed, if we put $\varepsilon = \varepsilon_p - \varepsilon_F = (p^2 - p_F^2)/2m \approx v_F(p - p_F)$, we find that $\gamma \propto (p - p_F)^2$) and with the results of quasiparticle lifetime calculations in the generalized random phase approximation (see Ref. 11). The results of calculations of $\gamma(\varepsilon, m)$ and of $r(\varepsilon, m)$, the real part of the mass operator (the Hilbert transform of $\gamma(\varepsilon, m)$), are depicted in Fig. 2.

Within these approximations, the spectral intensity can be written as follows:

$$\begin{aligned} I_p(\varepsilon) &= I(\varepsilon, \omega_p, m) \\ &= \frac{1}{\pi} \frac{\gamma(\varepsilon, m)}{[\varepsilon - (\omega_p - m) - r(\varepsilon, m)]^2 + \gamma^2(\varepsilon, m)}. \end{aligned} \quad (54)$$

It has been proved, both numerically and analytically, that the spectral intensity obeys the sum rule

$$\int_{-\infty}^{\infty} d\varepsilon I(\varepsilon, \omega_p, m) = 1$$

for arbitrary ω_p and m . The distribution function

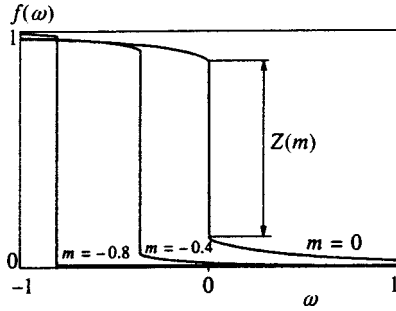


FIG. 3. Typical shape of the distribution function in the Hubbard model with $U = \infty$ at $T = 0$.

$$n_k = c f_k = c f(\omega_k, m), \quad f(\omega_k, m) = \int_{-\infty}^0 I(\varepsilon, \omega_k, m) d\varepsilon, \quad (55)$$

has a discontinuity at $\omega_k = m$ (Fig. 3). Equation (30) for the chemical potential with the distribution function (55) reduces to

$$\frac{n}{n-2} = \int_{-1}^1 \rho(\omega) f(\omega, m) d\omega. \quad (56)$$

From (56) we see that to a high degree of accuracy the chemical potential calculated in the first Born approximation does not differ from m . Figure 4 depicts the dependence of the discontinuity $Z(n)$ on the electron concentration n . The energies of the saturated ferromagnetic state, $\varepsilon_{FM}(n)$, and of the N -state in the zeroth approximation, $\varepsilon_0(n)$, and in the first Born approximation, $\varepsilon_1(n)$, are depicted in Fig. 5. We see that although the kinematic correlations of the electrons in the N -state raise the energy of the system in comparison to the zeroth approximation, the N -state is still the most advantageous one energetically.

Let us discuss the spin structure of this state. Spin isotropy, which is a characteristic feature of the singlet state (34b), is retained if we use the approximation (41). The spin correlation function for the nearest neighbors (in the first coordination sphere) is

$$C_1 = \frac{1}{2N} \sum_q \gamma_q \langle S_q^+ S_{-q}^- \rangle. \quad (57)$$

In the approximation (41) we have

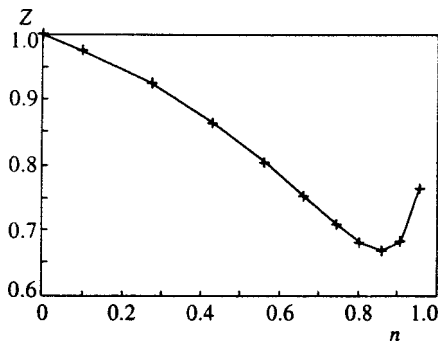


FIG. 4. Dependence of the discontinuity on the Fermi surface on the electron concentration n .

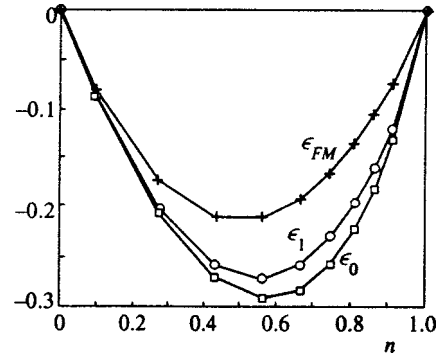


FIG. 5. The energies of the saturated ferromagnetic state, $\varepsilon_{FM}(n)$, the normal state in the zeroth approximation, $\varepsilon_0(n)$, and the normal state in the first Born approximation, $\varepsilon_1(n)$.

$$C_1 = \frac{cA}{2N} \sum_q \gamma_q \frac{1}{N} \sum_p f_p^0 (1 - f_{p+q}^0) = \frac{cA}{2N} \sum_p \theta(m - \omega_p) \frac{1}{N} \sum_k \gamma_{k-p} \theta(\omega_k - m). \quad (58)$$

For the square and cubic lattices there is the well-known symmetry effect of “splitting” of γ_{k-p} , i.e.,

$$C_1 = \frac{cA}{2N} \sum_p [\theta(m - \omega_p) \gamma_p] \frac{1}{N} \sum_k \gamma_k \theta(\omega_k - m) = \frac{cA}{2} \left(\int_{-1}^m \rho(\omega) \omega d\omega \right) \left(\int_m^1 \rho(\omega') \omega' d\omega' \right) = -\frac{1}{2} \frac{v^2(m)}{1 - g^2(m)}. \quad (59)$$

Using (33), we finally get

$$C_1 = -\frac{1}{8} \frac{\varepsilon_0^2(n)}{1 - n}. \quad (60)$$

If, e.g., we take the “rectangular” density of states $\rho(\omega) = 1/2$ we have $\varepsilon_0(n) = -n(1-n)(1-n/2)^{-1}$, so that

$$C_1(n) = -\frac{1}{8} \frac{n^2(1-n)}{(1-n/2)^2}.$$

In the present model the correlations are due solely to electrons hopping to neighboring vacant sites and, naturally, $C_1(n) \rightarrow 0$ as $n \rightarrow 1$.

Thus, our N -state is a singlet state with a nontrivial isotropic spin correlation function.

6. CONCLUSION

Our analytical and numerical analysis of the Hubbard model for the limit of infinite repulsion at a single site ($U = \infty$) has shown that qualitatively the properties of the electron system are the same as those of a normal metal with electron–electron coupling. What is important here is that the kinematic electron correlations do not disrupt the Fermi surface, but leave a “signature” in the form of a Migdal discontinuity in the distribution function. Although this re-

sult has been obtained in the first Born approximation, we believe that it is not altered by further iterations, since the attenuation (the imaginary part of the mass operator) always vanishes on the Fermi surface, i.e., for a zero value of the spectral variables E .

Our numerical calculations have shown that the normal (nonmagnetic) singlet state is the ground state. The main reason for this is that the chemical potential is lower than that of the saturated ferromagnetic state, which is indicated already by the zeroth approximation. Our study was done in the thermodynamic limit, with the result that the subtle quantum mechanical effect described by the Nagaoka theorem,¹³ which concerns the ground ferromagnetic state in the presence of one hole, does not appear in this limit. In this connection we would like to mention To'th's paper,¹⁴ where it was stated that in the presence of two holes the ferromagnetic state is not the ground state.

In the model with $U = \infty$ we considered only the N -state as the main contender for the ground state of the system. Here the state with the electron concentration $n = 1$ is the "punctured" point with zero energy and high degree of degeneracy. At finite but large values of Coulomb repulsion ($U \gg t$), the degeneracy is lifted by the antiferromagnetic exchange interactions $J \approx t^2/U$, and long-range antiferromagnetic order emerges at low hole concentrations.⁹ However, as the concentration grows, long-range antiferromagnetic order disappears and the system passes into its normal (metallic) state of the type described above.

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