Short-range effects in the Hubbard model

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The single-site coherent potential approximation is extended in the neutral Hubbard model. A one-particle Green's function is obtained which takes into account both local elastic scattering processes (which ensures the existence of the Hubbard III solution) and the nonlocal characteristics of the system which determine the intensity of the processes. In this case, the equation for the metallic order parameter is extended to finite temperatures. The nonlocal contribution, related mainly to the spin correlation function $\langle S_0 S_h \rangle$, is calculated in the appropriate self-consistent field approximation. A new dielectric phase region with respect to the parameter $\lambda = 2W/U$ is obtained on the phase diagram (W is the band half-width and U the Coulomb energy). The temperature-dependent region of the new phase is in the range $2/\sqrt{3} \leqslant \lambda \leqslant (1+\sqrt{2})^{1/2}$.

1. INTRODUCTION

The neutral Hubbard[1] model (number of electrons equal to number of lattice sites) is widely used in studying phase transitions in systems with strong Coulomb correlations:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 = \frac{U}{2}\sum_{f\sigma}(n_f^{\sigma} n_f^{-\sigma} - n_f^{-\sigma}) + \sum_{ff'\sigma} b(f-f')\, a_{f'\sigma}^{+} a_{f\sigma},$$

$$n_f^{\sigma} = a_{f\sigma}^{+} a_{f\sigma}. \qquad (1)$$

In Ref. 2 it was shown that for the SC and BCC lattices, the Hamiltonian (1) describes the metal-insulator phase transition (MIT), and the critical relation $\lambda_c = 2W/U = 2\sqrt{3}$ was found between the constants for the semielliptical density of states (Hubbard III [HIII] solution). In the work of Zaĭtsev,[3] based on a diagram technique, the result $\lambda_c = (z/3)^{1/2}$ (z is the number of nearest neighbors) was obtained for the SC and BCC lattices. Subsequently, it was shown that the decoupled Green's function procedure used in the derivation of the solution HIII is equivalent to the single-site coherent potential approximation (CPA).[4]

The shortcoming in such solutions is the absence of the temperature dependence of the self-energy part of the single-particle Green's function. As a result, the MIT line on the phase diagram (crosses in the figure) has no temperature slope.[5]

In this work, the single-particle Green's function is derived in a more general form than allowed by the CPA. Besides taking account of all single-site scattering processes (CPA) this Green's function contains nonlocal characteristics connected with the immediate environment of the site in the lattice. We note that there exist at least three reasons that such nonlocal characteristics are important. First, as was mentioned in Ref. 6, perturbation theory starting from the atomic limit experiences difficulties with the choice of ground state. The ground state is 2^N-fold degenerate. Starting from the point $b = 0$, we may find ourselves in the paramagnetic regime, when $U \gg |b| \gg T \gg b^2/U$, or in the antiferromagnetic regime, when $U \gg |b| \gg b^2/U \gg T$ (see Fig. 1). Thus, the Green's function, in a more general form than the solution HIII, must convey information about the degeneracy of the ground state (that is, "remember" from which region of the phase diagram the passage to the limiting point $b = 0$ is made). Such information is in the correlation functions of the form $\langle \mathbf{S}_0 \mathbf{S}_h \rangle$, contained in our Green's functions. Secondly, all the correlators of a nonlocal nature arising are temperature-dependent, which allows us to generalize the relationship between the metallic order parameter and the final temperature. In the results, this leads to: a) the slope of the MIT curve; b) the appearance of a new region of insulating phase. Third, in Ref. 7, the HIII solution was criticized because of the absence, in the metallic regime, of a temperature dependence in the quasiparticle decay—which contradicts the theory of the Fermi liquid. As will be

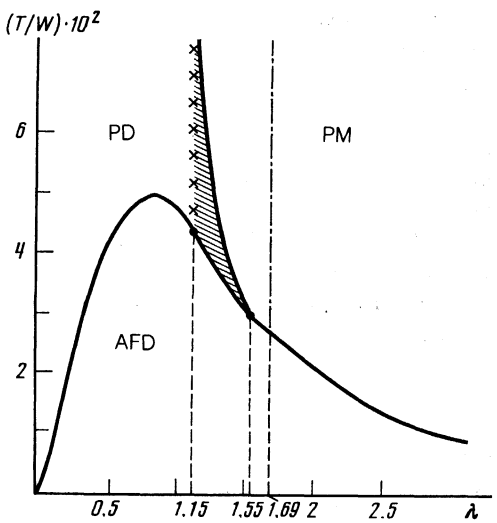

FIG. 1. Phase diagram for the neutral Hubbard model. PD denotes the paradielectric phase, PM the parametallic phase, and AFD the antiferrodielectric phase. The crosses are the HIII (CPA) solution. The dashed line is the asymptotic line dividing the phase with a local moment from the metallic zone (the significance of $\lambda^* = 1.69$ is derived in Ref. 8); the solid curve gives the qualitative form of the new solution, taking into account the effects of short-range order.

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apparent from the present work, in second order in b/U nonlocal averages play the role of intensities for quasiparticle scattering processes; this leads to a temperature-dependent coefficient in the imaginary part of the single-particle Green's function. We note, however, that at present the agreement with the results of the Fermi-liquid theory can be examined only outside the region of existence of a local magnetic moment, which is distributed in the metallic phase up to the value $\lambda^* > \lambda_c$ of the coupling constant (for a semielliptic density $\lambda^* = 16/3\pi$).[8]

2. GENERAL FORMALISM: SINGLE-PARTICLE GREEN'S FUNCTION WITH NONLOCAL CHARACTERISTICS TO FIRST ORDER IN b/U

The most important feature of the perturbation-theory formalism which we use, in comparison with the diagram formalism,[9] is the means of finding an analytic expression for the self-energy part Σ with the aid of the equation-of-motion method for the retarded temperature Green's function. Differentiation of such equations with respect to time (t')[10] allows one to derive an expression for the Green's function through the T-matrix, composed of the partial $\mathbf{T}_n$-matrices corresponding to orders of b/U:

$$\mathbf{G}=\mathbf{G}_0+\mathbf{G}_0\mathbf{T}\mathbf{G}_0, \quad \mathbf{T}=\varepsilon\mathbf{T}_1+\varepsilon^2\mathbf{T}_2+\dots, \tag{2}$$

where $\mathbf{G}_0$ is the Green's function in the zeroth-order approximation. On the other hand, using the Dyson equation and the expansion

$$\mathbf{G}=\mathbf{G}_0+\mathbf{G}_0\mathbf{\Sigma}\mathbf{G}, \quad \mathbf{\Sigma}=\varepsilon\mathbf{\Sigma}_1+\varepsilon^2\mathbf{\Sigma}_2+\dots, \tag{3}$$

it is easy to find the relationship of T to Σ:

$$\mathbf{T}=\mathbf{\Sigma}+\mathbf{\Sigma}\mathbf{G}_0\mathbf{T}=\varepsilon\mathbf{\Sigma}_1+\varepsilon^2(\mathbf{\Sigma}_2+\mathbf{\Sigma}_1\mathbf{G}_0\mathbf{\Sigma}_1)+O(\varepsilon^3)+\dots . \tag{4}$$

Comparing (2) and (4) for first (ε) and second (ε^2) orders, we conclude that

$$\mathbf{\Sigma}_1=\mathbf{T}_1, \quad \mathbf{\Sigma}_2=\mathbf{T}_2-\mathbf{T}_1\mathbf{G}_0\mathbf{T}_1. \tag{5}$$

This approach to finding the self-energy part allows us to avoid the laborious search for all the topologically inequivalent graphs in the diagram approach. For this reason, from now on the set of diagrams leading to the HIII solution will not be needed.

We will construct the perturbation theory from the atomic limit. Thus, $\mathscr{H}_0$ is the zero-order (unperturbed) part of the Hamiltonian (1), and $\mathscr{H}_1$ plays the role of the perturbation ($b_{ff'}$ is the interaction potential). We will examine the single-particle Green's function $\ll a_{j\sigma}(t); a^+_{j'\sigma}(t')\gg$ and its time Fourier transform

$$G_{ff'}(\omega)=\langle\langle a_{f\sigma}; a^+_{f'\sigma}\rangle\rangle_\omega=\sum_{\alpha\alpha'}G^{\alpha\alpha'}_{ff'}(\omega),$$
$$G^{\alpha\alpha'}_{ff'}(\omega)=\langle\langle A_{f\alpha\sigma}; A^+_{f'\alpha'\sigma}\rangle\rangle_\omega, \tag{6}$$

where the $A_{f\alpha\sigma}=n^{-\sigma}_{f\alpha}a_{j\sigma}$ are the Hubbard operators[2] with the following commutation properties:

$$\{A_{f\alpha\sigma}, A^+_{f'\alpha'\sigma}\}=\delta_{ff'}\delta_{\alpha\alpha'}n^{-\sigma}_{f\alpha}, \quad n^{-\sigma}_{f+}=n_f{}^{-\sigma}, \quad n^{-\sigma}_{f-}=1-n_f{}^{\sigma},$$
$$[A_{f\alpha\sigma}, \mathscr{H}_0]=\varepsilon_\alpha A_{f\alpha\sigma}, \quad \varepsilon_+=U/2, \quad \varepsilon_-=-U/2. \tag{7}$$

Using the equation-of-motion for the operator $A_{f\alpha\sigma}$ and the property of differentiability of the double-time Green's function with respect to time,[10] we obtain for $G^{\alpha\alpha'}_{ff'}(\omega)$

$$(\omega-\varepsilon_\alpha)G^{\alpha\alpha'}_{ff'}(\omega)=\delta_{ff'}\delta_{\alpha\alpha'}/2+\langle\langle Z_{f\alpha\sigma}; A^+_{f'\alpha'\sigma}\rangle\rangle_\omega,$$
$$\langle\langle Z_{f\alpha\sigma}; A^+_{f'\alpha'\sigma}\rangle\rangle_\omega(\omega-\varepsilon_{\alpha'})=\langle\{Z_{f\alpha\sigma}, A^+_{f'\alpha'\sigma}\}\rangle+\langle\langle Z_{f\alpha\sigma}; Z^+_{f'\alpha'\sigma}\rangle\rangle_\omega, \tag{8}$$

where $Z_{f\alpha\sigma}$ is an operator of the form

$$Z_{f\alpha\sigma}=[A_{f\alpha\sigma}, \mathscr{H}_1]$$
$$=\sum_{f'}b(f-f')[a_{f'\sigma}n^{-\sigma}_{f\alpha}-\alpha(X^{-\sigma\sigma}_f a_{f'-\sigma}+\eta(\sigma)X_f{}^{02}a^+_{f'-\sigma})], \tag{9}$$
$$X^{-\sigma\sigma}_f=a^+_{f-\sigma}a_{f\sigma}, \quad X_f{}^{02}=\eta(\sigma)a_{f-\sigma}a_{f\sigma}, \quad \eta(\sigma)=\begin{cases}+1, & \sigma\equiv\uparrow\\ -1, & \sigma\equiv\downarrow\end{cases}.$$

We will represent (8) in T-matrix form (2) and isolate on the right-hand side the terms

$$\{\mathbf{T}_1\}^{\alpha\alpha'}_{ff'}=\langle\{Z_{f\alpha\sigma}, A^+_{f'\alpha'\sigma}\}\rangle, \quad \{\mathbf{T}_2\}^{\alpha\alpha'}_{ff'}=\langle\langle Z_{f\alpha\sigma}; Z^+_{f'\alpha'\sigma}\rangle\rangle_\omega,$$

which are proportional, in agreement with the definition (9) of the operator $Z_{f\alpha\sigma}$, to the first (ε) and second (ε^2) powers of the interaction potential:

$$\{[(\omega\mathbf{I}-\mathbf{E})\mathbf{G}-\mathbf{N}](\omega\mathbf{I}-\mathbf{E})\}^{\alpha\alpha'}_{ff'}=\varepsilon\{\mathbf{T}_1\}^{\alpha\alpha'}_{ff'}+\varepsilon^2\{\mathbf{T}_2\}^{\alpha\alpha'}_{ff'}, \tag{10}$$

where

$$E^{\alpha\beta}_{ff'}=\delta_{\alpha\beta}\delta_{ff'}\varepsilon_\alpha, \quad N^{\alpha\beta}_{ff'}=\delta_{\alpha\beta}\delta_{ff'}/2.$$

Using the representations (3), (4), and (10), and satisfying (5) we obtain

$$\{\mathbf{\Sigma}_1\}^{\alpha\alpha'}_{ff'}=4\langle\{Z_{f\alpha\sigma}, A^+_{f'\alpha'\sigma}\}\rangle, \tag{11}$$
$$\{\mathbf{\Sigma}_2\}^{\alpha\alpha'}_{ff'}=4\langle\langle Z_{f\alpha\sigma}; Z^+_{f'\alpha'\sigma}\rangle\rangle-\{\mathbf{\Sigma}_1\mathbf{G}_0\mathbf{\Sigma}_1\}^{\alpha\alpha'}_{ff'}. \tag{12}$$

Here $G^0_{ff'}(\omega)=\delta_{ff'}\omega/(\omega^2-U^2/4)$ is the single-site Green's function. The components of the self-energy part of the Green's function to first order in the coupling constant for the paramagnetic neutral model can be reduced to the expression

$$\{\mathbf{\Sigma}_1\}^{\alpha\alpha'}_{ff'}=4b_{ff'}\begin{pmatrix} K(\mathbf{R}) & -K(\mathbf{R})+{}^1/_2\\ -K(\mathbf{R})+{}^1/_2 & K(\mathbf{R})\end{pmatrix},$$
$$K_\sigma(\mathbf{R})=K(\mathbf{R})=K(f-f')=\langle\mathbf{S}_f\mathbf{S}_{f'}\rangle-\langle X_f{}^{02}X_{f'}{}^{20}\rangle+{}^1/_4, \tag{13}$$

where $\mathbf{S}$ is the spin operator on site f, $\mathbf{R}=f-f'$. Below we will examine the usual case, when $B_{ff'}\neq 0$ only for nearest neighbors, that is, $\mathbf{R}=\mathbf{h}$.

For the class of spatially uniform solutions, equation (3) in the p-representation takes the form

$$G^{\alpha\alpha'}(\omega, p)=G_0{}^{\alpha\alpha}(\omega)+G_0{}^{\alpha\alpha}(\omega)\mathbf{\Sigma}_1{}^{\alpha\gamma}(p)G^{\gamma\alpha'}(\omega, p).$$

As a result, for $G(\omega,p)=\Sigma_{\alpha\alpha'}G^{\alpha\alpha'}(\omega,p)$ to first order in b/U we obtain

$$G^{\mathrm{I}}(\omega, p)=[\omega-\xi(p)]/D(\omega, p),$$
$$D(\omega, p)=[\omega-\xi(p)][\omega-\varepsilon(p)]-U^2/4. \tag{14}$$

Here $\varepsilon(p)=-W\gamma_p$ is the electronic dispersion relation in the periodic field of the lattice,

$$\gamma_p = z^{-1}\sum_h \exp(iph), \qquad \xi(p) = -4W(K-{}^1/_4)\gamma_p,$$

where $\xi(p)$ is the dispersion resulting from the existence of short-range order. For $K = 1/4$, which corresponds to the neglect of the nonlocal contribution, (14) agrees with the Green's functions of Ref. (1) (the Hubbard I (H I) solution). The critical value of λ follows: $\lambda_c = (K - 1/4)^{1/2}$. A self-consistent calculation, carried out in section 4, shows that $K \leqslant 1/4$. Thus, in this approximation, as in the solution H I, the insulating gap does not vanish.

It is important to note that all the effects connected with the temperature corrections result only from the consideration of nonlocal terms, and therefore in this case problems of improving the accuracy do not arise.

3. SECOND-ORDER PERTURBATION THEORY: THE EQUATION FOR THE METALLIC ORDER PARAMETER

The mechanism responsible for the MIT is connected with the consideration of elastic scattering processes in the static and dynamic state fluctuations which arise in second-order perturbation theory in the coupling constant. The situation in this case is highly analogous to scattering by heavy (bound) impurities. As shown in Ref. 11, consideration of such processes gives the nonvanishing imaginary part of the mass operator in all regions of p-space and, most importantly, on the Fermi surface. We recall that inelastic processes for $T = 0$ are proportional to $(p - p_F)^2$ and, consequently, do not have the required effect. On the other hand, the Hubbard model does not, intrinsically, contain separate subsystems with heavy impurities and light carriers, but as a result of the collectivation of atomic excitations each quasi-particle has two degrees of freedom: collective and localized. The "scattering" of these degrees of freedom on each other leads to elastic scattering (because flipping a spin in the paraphase requires no energy) and to Fermi surface extinction. Thus, the analogy between scattering processes in the Hubbard model and the problem of scattering on bound impurities would be complete if we only considered static spin fluctuations which are included in Green's functions of the type $\ll X_f^{-\sigma 2}(d); X_f^{2-\sigma}(t') \gg$ and $\ll X_f^{0\sigma}(t); X_f^{\sigma 0}(t') \gg$. Consideration of the collective degree of freedom for an initially fixed electron leads to the existence of processes of scattering on dynamic spin fluctuations, for which Green's functions of the type $\ll X_f^{-\sigma\sigma} a_{f'-\sigma}(t); \; a^+_{f'-\sigma} X_f^{\delta-\delta}(t') \gg$ and $\ll X_f^{0\sigma}(t); X_f^{\sigma-\sigma} a^+_{f'-\sigma}(t') \gg$. The analogy in alloys is scattering on ionized impurities.

Processes of scattering from static and dynamic state fluctuations are contained in the diagonal approximation for the self-energy part in second order in b/U: $\{\Sigma_2\}^{\alpha\alpha'}_{ff'} \approx \{\Sigma_2\}^{\alpha\alpha'}_{ff}$. This approximation includes all single-site scattering processes (the CPA) and two-center correlations. Outside its limits there are only the three-center correlations, which are important in the correct description of the zone boundary ($\lambda \to \infty$).

Let us turn to the calculation of $\ll Z_{f\alpha\sigma}; Z^+_{f\alpha'\sigma} \gg_\omega$. In the definition (9) $Z_{f\alpha\sigma}$ is represented by three operators $Z_{f\alpha\sigma} = Z^{(1)}_{f\alpha\sigma} + Z^{(2)}_{f\alpha\sigma} + Z^{(3)}_{f\alpha\sigma}$) which we will express in terms of the Hubbard operators:

$$Z^{(1)}_{f\alpha\sigma} = \sum_{f'} b_{ff'} n^{-\sigma}_{f\alpha} \sum_\tau A_{f\tau\sigma},$$

$$Z^{(2)}_{f\alpha\sigma} = -\alpha \sum_{f'} b_{ff'} X_f^{-\sigma\sigma} \sum_\tau A_{f'\tau-\sigma},$$

$$Z^{(3)}_{f\alpha\sigma} = -\alpha \sum_{f'} b_{ff'} \eta(\sigma) X_f^{02} \sum_\tau A^+_{f'\tau-\sigma}.$$

The matrix element $\ll Z_{f\alpha\sigma}(t); Z^+_{f\alpha'\sigma}(t') \gg$ contains nine terms, for the determination of which, in second order, we use the equation of motion

$$\omega \ll Z^{(i)}_{f\alpha\sigma}; Z^{(i)+}_{f\alpha'\sigma} \gg_\omega = \langle \{Z^{(i)}_{f\alpha\sigma}, Z^{(i)+}_{f\alpha'\sigma}\} \rangle + \ll [Z^{(i)}_{f\alpha\sigma} \mathcal{H}_0]; Z^{(i)+}_{f\alpha'\sigma} \gg_\omega + O(\varepsilon^3).$$

Each term of the matrix element takes into account a specific process in the system, with an intensity which contains the appropriate correlator, reflecting the existence of short-range order. The value of each term is given in the Appendix, where the expression for the irreducible self-energy part $\{\Sigma_2\}^{\alpha\alpha'}_{ff'}$ is also derived. Then, for the Fourier transform of the Green's function and the irreducible self-consistent ($G_0 \to G$) self-energy part $\Omega(\omega)$ ($\{\Sigma_2\}^{\alpha\alpha'}_{ff'} = \alpha\alpha' 4\Omega(\omega)$) we have

$$G(\omega, p) = \frac{\omega - 4\Omega(\omega) + \varepsilon(p)(1-4K)}{\omega^2 - U^2/4 - 4\omega\Omega(\omega) - 4\varepsilon(p)[K\omega - \Omega(\omega)] - \varepsilon^2(p)(1-4K)} \tag{15}$$

$$\Omega(\omega) = 2(1-4K^2)\int_0^W \rho(\varepsilon)\varepsilon^2 d\varepsilon \int_{-W}^{W} \rho(\varepsilon') G(\omega, \varepsilon') d\varepsilon', \tag{16}$$

where in (16) we have gone from a summation over p to an integration over the density of states $\rho(\varepsilon)$ corresponding to the dispersion relation $\varepsilon(p)$.

For $K = 1/4$ Eq. (16), after integration over the semielliptic density of states $\rho_0(\varepsilon) = 2[1 - \varepsilon/W)^2]^{1/2}/\pi W$ used in Ref. 2, and the substitution $F(\omega) = \omega - U^2/4[\omega - 4\Omega(\omega)]$ leads to the basic equation of Ref. 2 [see there formula (70)]. In this case (15) also coincides with the Green's function of solution HIII [formulas (58), (59)]. Thus, our proposed method of finding the self-energy part through perturbation theory in b/U completely reproduces the CPA[4] result and the solution HIII[2] in the limiting case where nonlocal effects are neglected.

Below, we shall follow the concept of the metallic order parameter introduced in Ref. 3 and independently in the theory of localization of Ref. 12. The fixation of the MIT line is connected with the appearance of a purely imaginary root in Eq. (16) for $\omega = 0$. Equation (16) is the equation for the metallic order parameter, but in the present work, due to the presence of the correlator K, it depends intrinsically on tem-

perature. On the MIT line $\Omega(0)\to 0$; therefore, expanding $G(\omega,\varepsilon)$ in (16) to first order in $\Omega(0)$, we obtain

$$1=16(1-4K^2)\int_0^W \varepsilon^2\rho(\varepsilon)\,d\varepsilon\left[J+(1-4K)\frac{\partial J}{\partial(1-4K)}\right], \tag{17}$$

$$J=\int_0^W \rho(\varepsilon)\frac{d\varepsilon}{U^2/4+\varepsilon^2(1-4K)}.$$

For comparison in the limiting case with the result HIII we restrict the integration in (17) to the semi-elliptic density of states cited previously. Then, for the critical value of the coupling constant we have the expression

$$\lambda_c^2=\left(\frac{4W^2}{U^2}\right)_c=\frac{1}{1-4K^2}\left\{\frac{1-4K}{1-4K^2}+\left[\left(\frac{1-4K}{1-4K^2}\right)^2+1\right]^{1/2}\right\}, \tag{18}$$

$$\partial\lambda_c/\partial K<0, \quad K\leqslant 1/4. \tag{19}$$

As we expect, for $K=1/4$ we obtain from (18) the HIII solution, $\lambda_c=2/\sqrt{3}$.

We will make one comment on the replacement of the quantity $\Sigma_h|b(h)|^2=z|b|^2$ in (A3) by the quantity which results from integration over the model (semielliptic) density of states, that is,

$$z|b|^2=\int_{-W}^{W}\rho(\varepsilon)\varepsilon^2\,d\varepsilon\leqslant\int_{-W}^{W}\rho_0(\varepsilon)\varepsilon^2\,d\varepsilon=\frac{W^2}{4}.$$

It is easy to show that the use of the value $|b|^2z$ in (16) leads in formula (18) to the replacement $1-4K^2\to 4(1-4K^2)/z$. In this case for $K=1/4$ we have $\lambda_c=(z/3)^{1/2}$, which agrees with the result of Ref. 3. As will be seen subsequently, the result for λ_c with $K=1/4$ is the asymptotic limit for $t=T/U\to\infty$. Therefore in our theory the value of λ_c as $T\to\infty$ has the meaning of a reference point for a new insulating phase and is unimportant in the basic result of the work. We will base our work on the solution HIII, as it flows logically from Eq. (16) with the use of the semi-elliptic density of states. The appearance of a z-dependence in λ_c is related to the integration of Eq. (16) with densities of states corresponding to SC and BCC lattices.

4. SELF-CONSISTENT CALCULATION OF THE CORRELATION FUNCTION K

Since the correlation function K enters into the coefficient determining the intensity of the scattering processes [see formula (16)], which on the MIT line are calculated from the linear expansion in $\Omega(0)$, it is sufficient to calculate the function $K(\lambda, T, \Omega(0))$ to first order in b/U (that is, for $\Omega(\omega)=0$). For this purpose we introduce the set of operators P_j $(j=1, 2, 3, 4)$, the specific operator structure of which will be set forth below. On the basis of the equation of motion for the operators $a_{p\sigma}$, $A^{(ir)}_{p+\sigma}=A_{p+\sigma}-a_{p\sigma}/2$:

$$\begin{aligned} i\dot a_{p\sigma}&=\varepsilon_p a_{p\sigma}+UA^{(ir)}_{p+\sigma},\\ i\dot A^{(ir)}_{p+\sigma}&=1/4Ua_{p\sigma}+\xi_pA^{(ir)}_{p+\sigma},\end{aligned} \tag{20}$$

we obtain

$$\ll a_{p\sigma};P_j\gg_\omega=\langle\{a_{p\sigma},P_j\}\rangle G^I(\omega,p)+4\langle\{A^{(ir)}_{p+\sigma},P_j\}\rangle\ll A^{(ir)}_{p+\sigma};a_{p\sigma}^+\gg_\omega, \tag{21}$$

where $\ll A^{(ir)}_{p+\sigma};a^+_{p\sigma}\gg_\omega$ is calculated in the same way as $G^I(\omega,p)$ [Eq. (14)] in first order in b/U, and has the form

$$\ll A^{(ir)}_{p+\sigma};a_{p\sigma}^+\gg_\omega=U/4D(\omega,p). \tag{22}$$

Using the spectral theorem,[13] we obtain from (21), (14), and (22) the basic relationship for the subsequent derivation of the correlator:

$$\begin{aligned}&\langle P_ja_{p\sigma}\rangle=\langle\{a_{p\sigma},P_j\}\rangle l_{p\sigma}+\langle\{A^{(ir)}_{p+\sigma},P_j\}\rangle m_{p\sigma},\\ &l_{p\sigma}=l_p=[(\omega_p^+-\xi_p)f(\omega_p^+)\\ &\qquad-(\omega_p^--\xi_p)f(\omega_p^-)]/(\omega_p^+-\omega_p^-)-1/2,\\ &m_{p\sigma}=m_p=U\frac{f(\omega_p^+)-f(\omega_p^-)}{\omega_p^+-\omega_p^-},\quad f(\omega)=\left[\exp\left(\frac{\omega}{T}\right)+1\right]^{-1},\\ &\omega_p^\pm=\frac{\xi(p)+\varepsilon(p)}{2}\pm\left\{\left[\frac{\xi(p)-\varepsilon(p)}{2}\right]^2+\frac{U^2}{4}\right\}^{1/2}.\end{aligned} \tag{23}$$

We introduce the operator $(j=1)$

$$P_1=\frac{1}{N^{1/2}}\sum_f e^{-ipf}n^\sigma_{f+h}a_{f\sigma}^+, \quad h\neq 0, \tag{24}$$

having the property

$$\frac{1}{N}\sum_p\langle P_1a_{p\sigma}\rangle=\frac{1}{N}\sum_f\langle n^\sigma_{f+h}n_f^\sigma\rangle=\langle n_h^\sigma n_0^\sigma\rangle=\langle n_0^\sigma n_h^\sigma\rangle. \tag{25}$$

Summing (23) for $j=1$ and calculating the expectation value from the anticommutators, we obtain

$$\langle S_0^zS_h^z\rangle=\langle n_0^\sigma n_h^\sigma\rangle-1/4=-l^2(h)+(\langle n_h^\sigma n_0^{-\sigma}\rangle-1/4)m(0), \tag{26}$$

$$l(h)=\frac{1}{N}\sum_p e^{-iph}l_p, \qquad m(0)=\frac{1}{N}\sum_p m_p.$$

In (26) it is taken into consideration that $m(h)=N^{-1}\Sigma_p\exp(-iph)m_p=0$. To derive the correlator $\langle n_h^\sigma n_0^{-\sigma}\rangle$ we introduce the second $(j=2)$ operator

$$P_2=\frac{1}{N^{1/2}}\sum_f e^{-ipf}n^\sigma_{f+h}a^+_{f-\sigma}, \qquad \frac{1}{N}\sum_p\langle P_2a_{p-\sigma}\rangle=\langle n_h^\sigma n_0^{-\sigma}\rangle. \tag{27}$$

From (23) for $j=2$ it follows that

$$\langle n_h^\sigma n_0^{-\sigma}\rangle-1/4=\langle S_0^zS_h^z\rangle m(0). \tag{28}$$

Substituting (28) in (26), we find for the correlator $\langle S^z_0S^z_h\rangle$ the final form

$$\langle S_0^zS_h^z\rangle=-l^2(h)/[1-m^2(0)]. \tag{29}$$

In an analogous way we introduce the operators P_3 and P_4:

$$P_3=\frac{1}{N^{1/2}}\sum_f e^{-ipf}X^{\sigma-\sigma}_{f+h}a^+_{f-\sigma}, \qquad \frac{1}{N}\sum_p\langle P_3a_{p\sigma}\rangle=\langle S_h^+S_0^-\rangle,$$

$$P_4=\frac{1}{N^{1/2}}\sum_f e^{-ipf}X^{20}_{f+h}a_{f-\sigma}, \qquad \frac{1}{N}\sum_p\langle P_4a_{p\sigma}\rangle=\langle X_h^{20}X_0^{02}\rangle,$$

This permits us to calculate to first order in the coupling constant the correlators

$$\langle S_0^+ S_h^- \rangle = -l^2(h)/[1+m(0)],$$
$$\langle X_0^{02} X_h^{20} \rangle = l^2(h)/[1-m(0)]. \quad (30)$$

Consequently the correlator K can be put into the form

$$K = \frac{1}{4} - \frac{3}{1-m^2(0)} \frac{1}{N^2} \sum_{p_1 p_2} \gamma(p_1+p_2) l_{p_1} l_{p_2},$$
$$\gamma(p_1+p_2) = \frac{1}{z} \sum_h e^{i(p_1+p_2)h}. \quad (31)$$

Integration of (31) with the semielliptic density of states in the case $t \gg 1$ leads to the following result:

$$K \approx {}^1/_4 [1 - {}^3/_4 \lambda^2/(16t^2-1)]. \quad (32)$$

From (32) it follows that $K = 1/4$ for $t \to \infty$, which reflects the fact that our solution asymptotically coincides with the solution HIII.

5. RESULTS; COMPARISON WITH PREVIOUS THEORIES

The basic result of our work is the determination of the sign of the derived function $\lambda_c = \Phi[K(\lambda,t)]$. Having (32) available, and using (19), we find

$$\frac{d\lambda_c}{dt} = \frac{(\partial\lambda_c/\partial K)(\partial K/\partial t)_{\lambda_c}}{1-(\partial\lambda_c/\partial K)(\partial K/\partial\lambda_c)_t} < 0. \quad (33)$$

Let us estimate the region in λ where the new insulating phase exists. The first possibility of such an estimate is tied to the derivation of a self-consistent point for $T = 0$. In this case (31) is expressed in terms of complete elliptic integrals which are represented in the form of a series in $p^2/(1+p^2)$, where $p^2 = \lambda^2(2K-1)^2$. Consequently we have, for the desired correlator at $T = 0$, $K = -0.35 + 0.055\lambda^2$. Solution of this equation together with (18) gives the following result: $K = -0.1357$, $\lambda_c = 1.9736$. Obviously, such an estimate is exaggerated, as the negative sign for K testifies to the strong antiferromagnetic instability at $T = 0$. The value for λ_c itself is outside the region where a local moment ($\lambda_c > \lambda^*$) exists, which from the physical point of view is incorrect.

The manifestation of an antiferromagnetic instability in the system makes it possible to carry out a more accurate calculation. In fact, by definition the correlator $K(T,\lambda) \geqslant 0$; the value $K(h) = 0$ is attained in the limit of the antiferromagnetic Néel structure, when $K(R) = [1+(-1)^R]/4$ (R is the number of the coordination sphere, $R = h = 1$). The vanishing of the correlator (31) fixes the point of instability of the paramagnetic phase. In the figure this is the point where the lines for a phase transition of the 3, 5, type[3] and for a transition of the 2 type intersect (the triple point). Inserting the value $K(T_N,\lambda_c) = 0$ in (18), we obtain $\lambda_c = (1+\sqrt{2})^{1/2} \approx 1.55$. Thus, the additional region of existence of the insulating phase (by comparison with the solution HIII) is between the limits

$$2/\sqrt{3} \leqslant \lambda \leqslant (1+\sqrt{2})^{1/2}, \quad T \geqslant T_N(\lambda) \quad (34)$$

and is located wholly within the region where localized moments exist (we recall that $\lambda^* = 1.69$).

So, taking account of the nonlocal environment leads, first of all, to a broadening of the region of existence of the insulating phase by comparison to the solution HIII. Secondly, in the new region of the insulating phase ($1.15 \leqslant \lambda \leqslant 1.55$) there exists a temperature MIT. This region is shaded in the figure.

In References 8, 14, and 15 an approach to a description of the MIT from the zone limit is developed on the basis of a functional integral method. The authors of this work, having shown that a region exists in which a local moment in the metallic phase develops, obtain results different from HIII. In Ref. 8 the value $\lambda_c = 3/2$ is found, which agrees with the interval (34). The result of Ref. 14, represented in the analytic form $\lambda_c \approx 3/2 - 4t$, agrees with (33) in the sign of the slope of the MIT line. In Ref. 15 the result of a numerical calculation gives a small positive slope for the MIT line; this contradicts not only our relation (33) but the result of Ref. 14.

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APPENDIX

To second order in ε we have for the nine matrix elements

$$\langle\langle Z^1_{f\alpha\sigma}; Z^{1+}_{f\alpha'\sigma} \rangle\rangle_\omega = \delta_{\alpha\alpha'} \sum_{f'} |b_{ff'}|^2 \sum_\tau \frac{\langle n_{f\alpha-\sigma} n_{f'\tau-\sigma} \rangle}{\omega - \varepsilon_\tau},$$

$$\langle\langle Z^2_{f\alpha\sigma}; Z^{2+}_{f\alpha'\sigma} \rangle\rangle_\omega = \alpha\alpha' \sum_\tau \frac{1}{\omega-\varepsilon_\tau} \Big\{ \sum_{f'} |b_{ff'}|^2 \langle n_{f'\tau\sigma} X_f^{\sigma\sigma} \rangle$$
$$+ \sum_{f'f''} b_{ff'} b^*_{ff''} \langle A_{f'\tau-\sigma} a^+_{f''-\sigma} (X_f^{-\sigma-\sigma} - X_f^{\sigma\sigma}) \rangle \Big\},$$

$$\langle\langle Z^3_{f\alpha\sigma}; Z^{3+}_{f\alpha'\sigma} \rangle\rangle_\omega = \alpha\alpha' \sum_\tau \frac{1}{\omega+\varepsilon_\tau} \Big\{ \sum_{f'} |b_{ff'}|^2 \langle n_{f'\tau\sigma} X_f^{22} \rangle$$
$$+ \sum_{f'f''} b_{ff'} b^*_{ff''} \langle A^+_{f'\tau-\sigma} a_{f''-\sigma} (X_f^{00} - X_f^{22}) \rangle \Big\},$$

$$\langle\langle Z^1_{f\alpha\sigma}; Z^{2+}_{f\alpha'\sigma} \rangle\rangle_\omega = \alpha' \sum_\tau \frac{1}{\omega-\varepsilon_\tau} \Big\{ \gamma \sum_{f'} |b_{ff'}|^2 \langle X_{f'}^{-\sigma\sigma} X_f^{\sigma-\sigma} n_{f\alpha-\sigma} \rangle$$
$$+ \alpha \sum_{f'f''} b_{ff'} b^*_{ff''} \langle A_{f'\tau\sigma} a^+_{f''-\sigma} X_f^{\sigma-\sigma} \rangle \Big\},$$
$$\langle\langle Z^1_{f\alpha\sigma}; Z^{3+}_{f\alpha'\sigma} \rangle\rangle_\omega = -\alpha' \sum_\tau \frac{1}{\omega-\varepsilon_\tau} \Big\{ \gamma \sum_{f'} |b_{ff'}|^2 \langle X_{f'}^{02} X_f^{20} n_{f\alpha-\sigma} \rangle \quad (A.1)$$
$$+ \eta(\sigma) \alpha \sum_{f'f''} b_{ff'} b^*_{ff''} \langle A_{f'\tau\sigma} a_{f''-\sigma} X^{20} \rangle \Big\},$$

$$\langle\langle Z^2_{f\alpha\sigma}; Z^{1+}_{f\alpha'\sigma} \rangle\rangle_\omega = \alpha \sum_\tau \frac{1}{\omega-\varepsilon_\tau} \Big\{ \gamma \sum_{f'} |b_{ff'}|^2 \langle X_{f'}^{\sigma-\sigma} n_{f\alpha'-\sigma} X_f^{-\sigma\sigma} \rangle$$
$$+ \alpha' \sum_{f'f''} b_{ff'} b^*_{ff''} \langle A_{f'\tau-\sigma} a^+_{f''\sigma} X_f^{-\sigma\sigma} \rangle \Big\},$$

$$\langle\langle Z^{3}_{f\alpha\sigma}; Z^{1+}_{f\alpha'\sigma}\rangle\rangle_\omega = \alpha\sum_\gamma \frac{1}{\omega+\varepsilon_\gamma}\Big\{\gamma\sum_{f'}|b_{ff'}|^2\langle X^{20}_{f'}\, n_{f\alpha'-\sigma}X_f^{02}\rangle$$

$$-\eta(\sigma)\alpha'\sum_{f'f''} b_{ff'}b^{*}_{ff''}\langle A^{+}_{f'\gamma-\sigma}a^{+}_{f'',\sigma}X_f^{02}\rangle\Big\},$$

$$\langle\langle Z^{3}_{f\alpha\sigma}; Z^{2+}_{f\alpha'\sigma}\rangle\rangle_\omega = \langle\langle Z^{2}_{f\alpha\sigma}; Z^{3+}_{f\alpha'\sigma}\rangle\rangle_\omega = 0,$$

where $\gamma = +, -$ and the following operators are introduced:

$$X_f^{22} = n_f^\sigma n_f^{-\sigma}, \quad X_f^{-\sigma-\sigma} = n_f^\sigma(1-n_f^\sigma), \quad X_f^{00} = (1-n_f^\sigma)(1-n_f^{-\sigma}).$$

We note that in (A.1), in the summation over f', f'' only the terms for $f' = f''$ are retained, since for $f' \neq f''$ the summed correlators are of "superfluous" degree in ε. The remaining transforms are analogous to those we carried out in the calculation of Σ_1, so that in matrix notation $\alpha\alpha'$ we obtain

$$\langle\langle Z_{f\alpha\sigma}; Z^{+}_{f\alpha'\sigma}\rangle\rangle_\omega = \sum_{f'}|b_{ff'}|^2\begin{pmatrix} \frac{1/2}{\omega-U/2}+\frac{1-2K(ff')}{\omega+U/2} & -[1-2K(ff')]G^0_{f'f'}(\omega) \\ -[1-2K(ff')]G^0_{f'f'}(\omega) & \frac{1-2K(ff')}{\omega-U/2}+\frac{1/2}{\omega+U/2}\end{pmatrix}. \tag{A.2}$$

Just as in the diagram method, the calculation of $\Sigma_1\mathbf{G}^0\Sigma_1$ from (A.2) takes into account only the contribution of the irreducible second order blocks. The expression for $\Sigma_1\mathbf{G}^0\Sigma_1$ is found by multiplying the matrix $\mathbf{G}_0$ and (13). As a result, from the definition of the irreducible part of the mass operator (12) it follows that

$$\{\Sigma_2\}_{ff}^{\alpha\alpha'} = \alpha\alpha'\cdot 4\Omega(\omega)$$

$$= \alpha\alpha'\cdot 4\sum_{f'}[1-4K^2(f,f')]\,|b_{ff'}|^2 G^0_{f'f'}(\omega). \tag{A.3}$$

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