Phase diagram of ferromagnetic metal with nondegenerate band under conditions of strong Hubbard correlation

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It is shown that a regular representation for the self-energy part exists in the Hubbard model, in the form of a series in powers of the tunneling integral $t(\mathbf{f}-\mathbf{f}')$. The single-particle Green's function that appears in first order in $t(\mathbf{f}-\mathbf{f}')$ satisfies four exact relations for the spectral moments corresponding to the Kalashnikov–Fradkin canonical transformation, and is the best single-particle approximation of the problem for the class of solutions with two delta-functions. We investigate the homogeneous solutions in the Hubbard model for $U=\infty$ $(t>0)$. Of fundamental importance for the obtained Green's function is the presence of a term $\langle X_0^{\sigma 0} X_{\mathbf{h}}^{0\sigma}\rangle$ that represents the connection between the kinematic and spin degrees of freedom. Such a correlator determines the spin-dependent shift of the gravity center of the spin subbands and leads to a ferromagnetic ground state in the density region $0.7 \lesssim n \leqslant 1$ (n is the electron density in the lower Hubbard band). A phase diagram is constructed for the relative magnetization of a ferromagnetic metal. The contribution to the self-energy part is obtained in a self-consistent manner in second order in $t(\mathbf{f}-\mathbf{f}')$. The region of applicability of this theory is discussed.

1. INTRODUCTION

The investigation of the possible existence of ferromagnetism due to electron correlation in a narrow nondegenerate band dates back to Bloch's work.[1] The main quantitative and qualitative aspects of this question, however, are connected with the investigation of the magnetic properties of the Hubbard Hamiltonian:[2]

$$H=H_0+H_1=\sum_{\mathbf{f},\sigma}\frac{U}{2}n_{\mathbf{f}}^{\sigma}n_{\mathbf{f}}^{\bar{\sigma}}+\sum_{\mathbf{f},\mathbf{f}',\sigma}t(\mathbf{f}-\mathbf{f}')a_{\mathbf{f}\sigma}^{+}a_{\mathbf{f}'\sigma},\qquad \bar{\sigma}\equiv-\sigma. \tag{1}$$

The main argument in favor of the existence of a ferromagnetic solution in the framework of the Hamiltonian (1) is based on the accurate result obtained by Nagaoka.[3] He has shown that addition (removal) of a small number of electrons in a three-dimensional system described by the Hamiltonian (1) with $n=N_e/N=1$ (N_e is the number of electrons in the Hubbard band and N is the number of sites) stabilizes the ferromagnetic ground state. Whereas for divisible lattices (PC, BCC) the ferromagnetic state is invariant to simultaneous reversal of the signs of the occupation parameter $n_{\pm}=N_e-N$ and the matrix element $t_{\mathbf{ff}'}$ ($n_-<0, t>0 \to n_+>0, t<0$) no such symmetry was present in FCC and HCP. Note that the rigorous results of Ref. 3 were obtained for $n_{\pm}=\pm 1$ and $U=\infty$. A thermodynamic generalization to finite densities was made in the linear approximation on the basis of the hole density (i.e., $pt_{\mathbf{ff}'}$, $p=1-n$).

The problem of thermodynamic generalization $(0\leqslant n\leqslant 1)$ of the rigorous results of [3] is now very timely. This is connected first of all with the discussed possibility of nonphonon mechanisms in the HTSC problem. Thus, in Anderson's theory[4] the Nagaoka mechanism (kinematic exchange) limits substantially the probable onset of RVB states on lattices with PC and BCC symmetry. In the Schrieffer theory[5] the kinematic exchange plays a constructive role, ordering the electron spins in ferromagnetic fashion in a certain spin bag.

Notwithstanding the extensive use of the results of Ref. 3, the method of construction of the effective self-consistent field generated by the kinematic interaction is still unclear. We propose in the present paper an effective-field theory that takes into account the connection between the kinetic and spin degrees of freedom ($\langle X_0^{\sigma 0} X_{\mathbf{h}}^{0\sigma}\rangle$) in vacuum–vacuum hole translations over a lattice with arbitrary spin configurations. This connection is none other than the physical mechanism on which the theorems of Ref. 3 are based.

Before we proceed to an exposition of the main results, however, let us consider the Nagaoka results[3] as interpreted by Brinkman and Rice.[6] Their purpose was to investigate the kinematic effect of the presence of one hole $(t>0)$ in an $N\times N\times N$ system with different types of spin configurations. The example chosen was a PC lattice $(Z=6)$ and three types of spin configurations: R—random spin orientation; AF—antiferromagnetic (alternant) ordering; F—saturated ferromagnetic ordering. Using, just as in Ref. 3, expansion of the resolvent in a series in t/ω, they were able to establish a simple analytic connection between the spectral moments (M_l^{α}) of the density of states and the number of hole trajectories on the lattice:

$$M_l^{\alpha}=\frac{A_l^{\alpha}}{z^l},\qquad l\geqslant 2, \tag{2}$$

where z is the number of nearest neighbors, $A_l^{\alpha i}$ is the number of trajectories when the hole starts from a state i with spin configuration α_i and returns (without omissions) to the same $(i\alpha_i)$ state after l steps on the lattice (vacuum–vacuum transition). Solving the combinatorial calculation of A_l^{α}, they arrived at the following deductions (see Table I of Ref. 6).

1. Starting with the fourth spectral moment $(l=4)$ on the PC lattice (in this case the hole follows a cyclic passage through the slab), M_l^{α} acquires a specific dependence on the type of spin configuration in the lattice (kinematic exchange).

2. With increase of the number of steps, the difference in the number of trajectories between the F, R, and AF configu-

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rations increases rapidly, and always $M_l^F > M_l^R > M_l^{AF}$ ($l \geqslant 4$).

3. The series in l (or, equivalently, in $t_{ff'}$) always converges within each configuration.

4. The convergence is slowest in the F configuration, where the smallness parameter is the ratio $r_l/z^l < 1$ (r_l is the total number of trajectories made up of l steps).

The "decreased" value of the spectral moments for R and AF structures compared with the F configuration leads to a stronger correlation narrowing of the Hubbard subband in accordance with the loss in the kinetic energy of the hole. Thus, a hole in the R or AF configuration is a considerably more localized object than in the F configuration, and it is this which determines the ferromagnetic choice of the ground state.

2. BASIC EQUATIONS OF THE THEORY IN FIRST ORDER IN $t(\mathbf{f}-\mathbf{f}')$. EFFECTIVE FIELD OF KINEMATIC ORIGIN

A perturbation theory for the Hubbard Hamiltonian (1) from the atomic limit encounters a substantial difficulty because the ground state of the system is degenerate at $t(\mathbf{f}-\mathbf{f}')=0$. For $n=1$ (system 2^N-fold degenerate in spin) the degeneracy is lifted in second order in $t(\mathbf{f}-\mathbf{f}')$ and the ground state is either antiferromagnetic[7] or singlet[8] with $J \propto t^2/U$. If $n<1$ (the system is $2^N N!/N_e!N_p!$-fold degenerate in spin and in the hole locations N_p), however, the degeneracy is lifted in first order in $t(\mathbf{f}-\mathbf{f}')$. It is particularly important in this case to take correct account of all the effects that are linear in $t(\mathbf{f}-\mathbf{f}')$.

The main distinctive feature of the perturbation-theory formalism used by us is the method of finding an analytic equation for the self-energy part ($\mathbf{\Sigma}$) with the aid of the method of equations of motion for the retarded and advanced Green's functions.[9] Differentiation of the equations with respect to the right time (t') yields an expression for the Green's function in terms of a scattering matrix $\mathbf{T}$ made up of partial $\mathbf{T}_n$ matrices of the corresponding orders in the interaction potential, the role of which is played by the tunneling integral $t_{ff'}$:

$$\mathbf{G}=\mathbf{G}_0+\mathbf{G}_0\mathbf{T}\mathbf{G}_0, \quad \mathbf{T}=\epsilon\mathbf{T}_1+\epsilon^2\mathbf{T}_2+\ldots, \tag{3}$$

where $\mathbf{G}_0$ is in the general case the zeroth-approximation (atomic limit) matrix Green's function; ϵ is the formal parameter of the expansion in the interaction parameter. On the other hand, using the Dyson equation and an expansion of the self-energy part in powers of ϵ

$$\mathbf{G}=\mathbf{G}_0+\mathbf{G}_0\mathbf{\Sigma}\mathbf{G}, \quad \mathbf{\Sigma}=\epsilon\mathbf{\Sigma}_1+\epsilon^2\mathbf{\Sigma}_2+\ldots, \tag{4}$$

we obtain the connection between $\mathbf{T}$ and $\mathbf{\Sigma}$:

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

Consider the single-particle retarded Green's function[9]

$$G_{ff'}(\omega)=\sum_{\alpha\alpha'} G_{ff'}^{\alpha\alpha'}(\omega),$$

$$G_{ff'}^{\alpha\alpha'}(t,t')=\theta(t-t')\langle\{A_{f\alpha\sigma}(t); A_{f'\alpha'\sigma}^{+}(t')\}\rangle, \tag{6}$$

$$\theta(x)=\begin{cases}1, & x>0,\\ 0, & x<0,\end{cases}$$

where $A_{f\alpha\sigma}=n_{f\alpha}^{\bar\sigma}a_{f\sigma}$ are Hubbard operators with the following permutation properties:

$$\{A_{f\alpha\sigma}, A_{f'\alpha'\sigma}^{+}\}=\delta_{ff'}\delta_{\alpha\alpha'}n_{f\alpha}^{\bar\sigma}, \quad [A_{f\alpha\sigma}, H_0]=\varepsilon_\alpha A_{f\alpha\sigma},$$
$$n_{f+}^{\sigma}=n_f^{\sigma}, \quad n_{f-}^{\sigma}=1-n_f^{\sigma}, \quad \varepsilon_+=\varepsilon_0+U, \quad \varepsilon_-=\varepsilon_0, \quad \varepsilon_0=t_{ff}. \tag{7}$$

Differentiating the Green's function (6) with respect to the time t and next with respect to the time t' we obtain a system of closed equations (see Ref. 9), the solution of which can be written in the form (3):

$$\mathbf{G}=\mathbf{G}_0+\mathbf{G}_0[\mathbf{N}^{-1}(\mathbf{T}_1+\mathbf{T}_2)\mathbf{N}^{-1}]\mathbf{G}_0, \tag{8}$$

$$\{G_{ff'}^{0}(\omega)\}^{\alpha\alpha'}=\delta_{ff'}\delta_{\alpha\alpha'}\frac{\langle n_{f\alpha}^{\bar\sigma}\rangle}{\omega-\varepsilon_\alpha}, \tag{9}$$

$$\{N_{ff'}\}^{\alpha\alpha'}=\delta_{ff'}\delta_{\alpha\alpha'}\langle n_{f\alpha}^{\bar\sigma}\rangle, \tag{10}$$

$$\{\mathbf{T}_1\}_{ff'}^{\alpha\alpha'}=\langle\{Z_{f\alpha\sigma}, A_{f'\alpha'\sigma}^{+}\}\rangle, \quad \{\mathbf{T}_2\}_{ff'}^{\alpha\alpha'}=\langle\langle Z_{f\alpha\sigma}; Z_{f'\alpha'\sigma}^{+}\rangle\rangle_\omega. \tag{11}$$

The matrices $\mathbf{T}_1$ and $\mathbf{T}_2$ are proportional, respectively, at least to the first (ϵ) and second (ϵ^2) powers of the interaction potential ($t_{ff'}$), since $Z_{f\alpha\sigma}$ is an operator of the form

$$Z_{f\alpha\sigma}=[A_{f\alpha\sigma}, H_1]$$

$$=\sum_{f'} t(\mathbf{f}-\mathbf{f}')[a_{f'\sigma}^{+}a_{f\alpha}^{\bar\sigma}-\alpha(X_f^{\bar\sigma\sigma}a_{f'\bar\sigma}+\eta(\sigma)X_f^{\bar 0 2}a_{f'\bar\sigma}^{+})],$$

$$X_f^{\bar\sigma\sigma}=a_{f\bar\sigma}^{+}a_{f\sigma}, \quad X_f^{\bar 0 2}=\eta(\sigma)a_{f\bar\sigma}a_{f\sigma}, \quad \eta(\sigma)=\begin{cases}+1, & \sigma\equiv\uparrow,\\ -1, & \sigma\equiv\downarrow.\end{cases} \tag{12}$$

We call attention to the fact that the matrix element $\{\mathbf{G}^0(\omega)\}_{ff'}^{\alpha\alpha'}$ (9) has one simple pole, whereas $G_{ff'}^{0}(\omega)$ has two pole terms. It is natural to expect the spectral density of the complete single-particle function $G(\omega,\mathbf{k})$ to have at $W \ll U$ ($W=z|t|$ is the half width of the bare band) two peaks that converge in the metallic phase ($U \ll W$). This presupposes the use of the Dyson matrix equation for a matrix formulation of the self energy Σ. The Dyson equation, in the class of spatially homogeneous solution, takes in the $\mathbf{k}$ representation the form

$$G^{\alpha\alpha'}(\omega,\mathbf{k})=G_0^{\alpha\alpha'}(\omega)+G_0^{\alpha\alpha''}(\omega)\Sigma_1^{\alpha''\gamma}(\mathbf{k})G^{\gamma\alpha'}(\omega,\mathbf{k}), \tag{13}$$

where $\mathbf{\Sigma}_1^{\alpha''\gamma}(\mathbf{k})$ is the self-energy part calculated in an approximation linear in $t(\mathbf{f}-\mathbf{f}')$ (i.e., $\mathbf{\Sigma}_1=\mathbf{T}_1$). Solving the system of equations (13) and using next the representation (6) we find that the single-particle Green's function takes in the approximation linear in $t(\mathbf{f}-\mathbf{f}')$, in the limit as $U\to\infty$, the form[1)]

$$G_\sigma^{I}(\omega,\mathbf{k})=\frac{n_-^{\bar\sigma}}{\omega-n_-^{\sigma}\varepsilon(\mathbf{k})-\Omega_\sigma^{I}(\mathbf{k})/n_-^{\bar\sigma}}, \tag{14}$$

$$\Omega_\sigma^{I}(\mathbf{k})=K_\sigma(h)\varepsilon(\mathbf{k})-W\Delta_\sigma(h), \tag{15}$$

$$\Delta_\sigma(h)=\langle X_0^{\bar\sigma 0}X_h^{0\bar\sigma}\rangle, \tag{16}$$

$$K_\sigma(h)=\langle n_0^{\bar\sigma}n_h^{\sigma}\rangle-(n^{\bar\sigma})^2+\langle X_0^{\sigma\sigma}X_h^{\sigma\sigma}\rangle. \tag{17}$$

$$\varepsilon(\mathbf{k})=\sum_{\mathbf{h}} t(\mathbf{h})e^{i\mathbf{k}\mathbf{h}}, \quad X_f^{\bar\sigma 0}=A_{f,-,\bar\sigma}^{+}. \tag{18}$$

Note the main features of the Green's function (14).

1) If we neglect the nonlocal contribution to the mass operator [i.e., put $\Omega_\sigma^{\mathrm{I}}(\mathbf{k})=0$], then (14) goes over into a Green's function that corresponds to the single-node approximation of the coherent-potential method (CPM) (or the Hubbard-I approximation[2]). It is easy to verify[10] that there is no magnetic solution in this variant of the theory (i.e., $R=n^\sigma-n^{\bar\sigma}=0$ for all $n=n^\sigma+n^{\bar\sigma}$).[2)] We show in Appendix I that the local-effective-field approximation does not satisfy the fourth spectral moment of the theory, which is the decisive factor in the Nagaoka mechanism (kinematic exchange).

2) The Green's function with allowance for the nonlocal contribution $\Omega_\sigma^{\mathrm{I}}(\mathbf{k})$ satisfies all four exact spectral moments and is according to the Kalashnikov–Fradkin classification[13] the best single-particle approximation of the problem, where account is taken of all (local and nonlocal) effects that are linear in the tunneling integral $t(\mathbf{f}-\mathbf{f}')$. The proof of this fact is deferred to Appendix I.

3) The nonlocal contribution to the effective field is due to the kinematic nature of the vacuum transitions, which relates the kinetic (collective) degree of freedom with the spin configuration on the lattice (localized degree of freedom). As noted in the Introduction in connection with Ref. 6, it is just this relation which causes the ferromagnetic ordering in a system of strongly correlated electrons. It will be shown later on that allowance for the nonlocal contribution $\Omega_\sigma^{\mathrm{I}}(\mathbf{k})$ leads to a new energy balance between the ferro- and paraphases, which can be classified as due to two contributions: (a) the change of the chemical potential as a result of the shift of the gravity centers of the spin subbands [second term of (15)]; (b) the corrections to the chemical potential due to the change of the correlation width of the spin subband [first term in (15)]. Both terms are functions of the density n, the temperature T, and the relative magnetization R, and vanish as expected for $n=1$.

We obtain now a system of self-consistent equations for the single-particle spectrum (14). The Green's function (14) determines the equations for the occupation numbers $n^\sigma(n^{\bar\sigma})$

$$n^\sigma=(1-n^{\bar\sigma})\int d\varepsilon\rho(\varepsilon)f[(1-n^{\bar\sigma})\varepsilon+n^{\bar\sigma}\Omega_\sigma^{\mathrm{I}}(\varepsilon)] \tag{19}$$

and for the kinematic field $\psi^\sigma(\psi^{\bar\sigma})$

$$\psi^{\bar\sigma}=W\Delta^{\bar\sigma}(h)=(1-n^\sigma)\int d\varepsilon\rho(\varepsilon)\varepsilon f[(1-n^\sigma)\varepsilon+n^\sigma\Omega_{\bar\sigma}^{\mathrm{I}}(\varepsilon)]. \tag{20}$$

It is shown in Appendix II that in the approximation linear in $t(\mathbf{f}-\mathbf{f}')$ the binary correlation function $K_\sigma(\mathbf{h})$ is quadratic in the kinematic fields $\psi^\sigma(\psi^{\bar\sigma})$, so that

$$\Omega_\sigma^{\mathrm{I}}(\varepsilon)=\frac{1}{n^{\bar\sigma}(1-n^{\bar\sigma})}[\varphi^\sigma(\varepsilon)-\psi^\sigma],$$

$$\varphi^\sigma(\mathbf{k})=\sum_{\mathbf{h}\neq 0}t(\mathbf{h})e^{i\mathbf{k}\mathbf{h}}K^\sigma(\mathbf{h})$$

$$=-\frac{\varepsilon(\mathbf{k})}{1-n}\left[n_-^{\bar\sigma}\left(\frac{\psi^{\bar\sigma}}{W}\right)^2+\left(\frac{\psi^\sigma}{W}\right)\left(\frac{\psi^{\bar\sigma}}{W}\right)\right]. \tag{21}$$

Equations (19)–(21) determine the complete system of renormalizations of the single-particle spectrum and can be used to construct the phase diagram of the homogeneous state in the Hubbard model for $U=\infty$.

3. SOLUTION OF EQS. (19)–(21). ENERGIES OF FERROMAGNETIC AND PARAMAGNETIC PHASES. *R(n, T)* PHASE DIAGRAM

Analytic expressions for $R(n)$ and $T_C(n)$ can be obtained for the rectangular state density $\rho(\varepsilon)=\rho=1/2W$. Integrating in (19) and (20) at $T=0$ we get

$$n^\pm=\frac{1}{2\alpha^\pm}[\xi^\pm+(1-n^\mp)\alpha^\pm+\delta^\pm],$$

$$\alpha^\pm=1-\frac{1}{1-n}\left[(1-n^\mp)(\delta^\mp)^2+\frac{1-n^\pm}{1-n^\mp}\delta^+\delta^-\right], \tag{22}$$

$$\xi^\pm=\mu^\pm/W,\quad \delta^\pm=\psi^\pm/W(1-n^\pm),\quad \psi^\pm=-W\frac{(n\pm R)(1-n)}{(2-n\pm R)},$$

where $\mu_\pm$ is the chemical potential in the spin subbands (the plus and minus signs correspond to $\sigma\equiv\uparrow$ and $\sigma\equiv\downarrow$); $R=n^+-n^-$ and $n=n^++n^-$.

The equation for the magnetization $R(n)$ follows from the condition that the chemical potentials be equal

$$\xi_+=\xi_-. \tag{23}$$

It is convenient to analyze (23) with consistent allowance for contributions (a) and (b) [see item 3 of Sec. 2). Allowance for only the contribution (a) (in this case $\alpha^\pm=1$) leads to the following results:

1) There is always a solution $R=0$ corresponding to a paramagnetic metal;

2) the second solution corresponds to the state with maximum number of parallel spins (saturated ferromagnetism):

$$R=n=n^\sigma. \tag{24}$$

Allowance for both contributions (a) and (b) leads (together with the trivial solution $R=0$) to the equation

$$Y^3-16Y(1-n)^2(5-n-n^2)+128(1-n)^3(2-n)=0,$$

$$Y=(2-n)^2-R^2. \tag{25}$$

One of the three real roots of (25) satisfies the condition $R\leqslant n$ and we have for it

$$R^2=(1+p)^2-8p(1+p-p^2/3)^{1/2}\cos\left(\frac{\pi-\varphi}{3}\right), \tag{26}$$

$$\varphi=\arccos[(1+p)(1+p-p^2/3)],\quad p=1-n.$$

The solution (26) describes an unsaturated ferromagnetism state with a critical point $n_c\approx 0.7$ of the concentration transition into the parametallic state.

Let us see which of the solutions has the lowest energy. The system energy can be expressed in terms of a single-particle Green's function[17]

$$E_0=\sum_{\mathbf{k},\sigma}\int\frac{1}{2}[\omega+\varepsilon(\mathbf{k})]f(\omega)\left(-\frac{1}{\pi}\mathrm{Im}\right)G_{\mathbf{k}}^\sigma(\omega+i\delta)d\omega. \tag{27}$$

Using the Green's function (14) and integrating with a rectangular density of states, we obtain the self-consistent values of the energy for the ferro- and paraphases:

$$E_0(R) = -\frac{W(1-n)}{2}\sum_{i=1}^{3} E_i(R), \tag{28a}$$

$$E_1(R) = n + \frac{4n(1-n)}{Y}, \tag{28b}$$

$$E_2(R) = -\frac{2(1-n)(n^2-R^2)[(2-n)n-R^2]}{Y^2}, \tag{28c}$$

$$E_3(R) = -\frac{16(1-n)(n^2-R^2)[n(2-n)^2+(3n-4)R^2]}{Y^3}, \tag{28d}$$

where E_1, E_2 and E_3 are the corresponding contributions to the energy from (16) and (17). Comparing $E_0(R)$ and $E_0(R=1)$ we can verify that

$$E_0(R) \leqslant E_0(R=0) \tag{29}$$

for all $R(n)$ from the solution (26).

Expanding the Fermi functions in (19) and (20) in powers of (T/W), we get expressions for $T_C(n)$. If only the contribution (a) is taken into account, the phase transition in temperature is of first order, with a discontinuity $\Delta R = R = n$. The Curie temperature is obtained in this case from the equality of the chemical potentials of the ferro- and paraphases:

$$\frac{T_c}{W} = \frac{1}{\pi}(6(1-n)n)^{1/2}. \tag{30}$$

If both contributions (a) and (b) are taken into account, the phase transition in temperature is not accompanied by a discontinuity of the ferromagnetic moment and is determined from the condition $R(n, T_C) = 0$. The equations for $R(n, T)$ can be obtained by iteration. Analysis shows that the solution $R = n$ is the better first iteration step. Indeed, calculating $\varphi^{\sigma}(\mathbf{k})$ with $R = n$ we find that $T_C(n)$ is given by

$$\frac{T_c}{W} \approx \frac{3}{\pi}(2-n)(1-n^2)\left(\frac{n-2/3}{2(2-n^2)}\right)^{1/2}. \tag{31}$$

It follows from (31) that the second critical point $n_c = 2/3$ is close to the concentration-transition point (≈ 0.7). Figure 1 shows for a ferromagnetic metal the phase diagram that follows from the results (24), (26), (30), and (31).

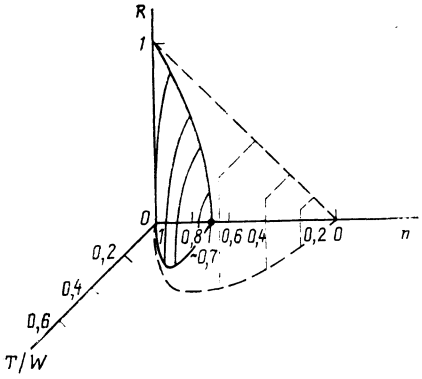

FIG. 1. Phase diagram $R(n, T)$ of a ferromagnetic metal for $U = \infty$ and $t > 0$ (rectangular density of state).

4. SECOND-ORDER PERTURBATION THEORY WITH RESPECT TO THE ENERGY OVERLAP INTEGRAL. CONVERGENCE OF THE THEORY

In second order in $t(\mathbf{f}-\mathbf{f}')$ the irreducible self-energy part of Σ_2 (5) is

$$\{\Sigma_2\}_{ff'}^{\alpha\beta} = \{\mathbf{N}^{-1}\mathbf{T}_2\mathbf{N}^{-1}\}_{ff'}^{\alpha\beta} - \{\Sigma_1\mathbf{G}_0\Sigma_1\}_{ff'}^{\alpha\beta},$$
$$\{\mathbf{N}^{-1}\mathbf{T}_2\mathbf{N}^{-1}\}_{ff'}^{\alpha\beta} = \frac{1}{n_\alpha^{\bar\sigma} n_\beta^{\bar\sigma}} \langle\langle Z_{f\alpha\sigma}; Z_{f'\beta\sigma}^{+}\rangle\rangle_{\omega}, \tag{32}$$
$$\{\Sigma_1\mathbf{G}_0\Sigma_1\}_{ff'}^{\alpha\beta} = \frac{(\omega-\varepsilon_\gamma)^{-1}}{n_\alpha^{\bar\sigma} n_\beta^{\bar\sigma} n_\gamma^{\bar\sigma}} \langle\{Z_{f\alpha\sigma}; A_{f'\gamma\sigma}^{+}\}\rangle\langle\{Z_{f'\gamma\sigma}; A_{f\beta\sigma}^{+}\}\rangle,$$

with summation over the intermediate index γ.

We shall be guided from now on by the following rule: From among all the spatial sums in the correlation functions, which result from the calculation of $\{\Sigma_2\}_{ff'}^{\alpha\beta}$, we retain only the correlators of two nearest neighbors, since their expected value is maximal. This follows directly from the very idea of the existence of an expansion in $t(\mathbf{f}-\mathbf{f}')$. Indeed, the expected value of the correlators for two nearest sites is at least linear in $t(\mathbf{f}-\mathbf{f}')$, at least quadratic in $t(\mathbf{f}-\mathbf{f}')$ for three non-equivalent sites, etc. As already noted, for $n < 1$ the degeneracy of the system is lifted in first order in $t(\mathbf{f}-\mathbf{f}')$. It is therefore necessary and sufficient to calculate the ensuing correlation functions to first order in the coupling constant, whence the aforementioned rule. This is attained in practice by calculating $\{\Sigma_2\}_{ff'}^{\alpha\beta}$ in an approximation diagonal in the site indices, namely

$$\{\Sigma_2\}_{ff'}^{\alpha\beta} \approx \{\Sigma_2\}_{ff}^{\alpha\beta}. \tag{33}$$

As a result the self-energy part $\Sigma^{\alpha\gamma}(\omega, \mathbf{k})$ can be expressed in the form

$$\Sigma_\sigma^{\alpha\gamma}(\omega, \mathbf{k}) = \varepsilon(\mathbf{k}) + \frac{\alpha\gamma}{n_\alpha^{\bar\sigma} n_\gamma^{\bar\sigma}}\Omega_\sigma(\omega, \mathbf{k}), \tag{34}$$

$$\Omega_\sigma(\omega, \mathbf{k}) = \Omega_\sigma^{\mathrm{I}}(\mathbf{k}) + \Omega_\sigma^{\mathrm{II}}(\omega), \tag{35}$$

where $\Omega_\sigma^{\mathrm{I}}(\mathbf{k})$ is the result (15) obtained in first order in $t(\mathbf{f}-\mathbf{f}')$ and $\Omega_\sigma^{\mathrm{II}}(\omega)$ is the contribution from the second order:

$$\Omega_\sigma^{\mathrm{II}}(\omega) = \frac{1}{N}\sum_{\mathbf{k},\gamma}\left\{\varepsilon^2(\mathbf{k})\frac{(n_\gamma^{\bar\sigma})^2 - [(n_\gamma^{\bar\sigma})^2 + K_\sigma]^2}{(n_\gamma^{\sigma})^2} - \frac{(W\Delta_\sigma)^2}{(n_\gamma^{\bar\sigma})^2}\right\} G_\sigma^{0\gamma}(\omega). \tag{36}$$

where $G_\sigma^{0\gamma}(\omega)$ is the atomic function (9). It follows from (36) that the quasiparticle Green's function calculated in second order in $t(\mathbf{f}-\mathbf{f}')$ is connected, through the self-energy part $\{\Sigma_2(\omega)\}_{ff}$ with the unperturbed ($t_{ff'} = 0$) local functions $G_{ff}^{0\gamma}(\omega)$.[9] The thermodynamic self-consistency condition in the lattice model requires the substitution[3)]

$$G_\sigma^{0\gamma}(\omega) \to \frac{1}{N}\sum_{\mathbf{k}} G_\sigma^{\gamma}(\omega, \mathbf{k}), \tag{37}$$

which transforms (36) into an equation for the self-constent values of Re $\Omega_\sigma^{\mathrm{II}}(\omega)$ and Im $\Omega_\sigma^{\mathrm{II}}(\omega)$.

All the calculations that follow will be for $U = \infty$ and a rectangular denstity of states. As a result we obtain

$$\frac{2}{\pi}\left[\operatorname{Im}\frac{\Omega_\sigma^{II}(\omega)}{W}\right]_{max}=\left[\operatorname{Re}\frac{\Omega_\sigma^{II}(\omega)}{W}\right]_{max}$$
$$=\frac{1}{3}\frac{(n_-^{\bar\sigma})^2-3\Delta_\sigma^2-[(n_-^{\bar\sigma})^2+K_\sigma]^2}{(n_-^{\bar\sigma})^2+K_\sigma}. \qquad (38)$$

To analyze the corrections in second order in $t(\mathbf{f}-\mathbf{f}')$ we write for the Green's function calculated in second order

$$G_\sigma(\omega,\mathbf{k})=\frac{G_\sigma^0(\omega)}{1-G_\sigma^0(\omega)\Sigma_\sigma(\omega,\mathbf{k})},$$
$$\Sigma_\sigma(\omega,\mathbf{k})=(n_-^{\bar\sigma})^{-2}[\Sigma_1(\mathbf{k})+\Sigma_2(\omega)],$$
$$\Sigma_1(\mathbf{k})=\varepsilon(\mathbf{k})(n_-^{\bar\sigma})^2+\Omega_\sigma^{I}(\mathbf{k}),\quad \Sigma_2(\omega)\equiv\Omega_\sigma^{II}(\omega). \qquad (39)$$

With the aid of (26) and (22) [see also (46) below] we can obtain expressions for $\Sigma_1(\mathbf{k})$ and $[\Sigma_2(\omega)]_{max}$ in the low-density region:

$$\frac{\Sigma_1(\mathbf{k})}{W}\approx\begin{cases}\left[1-\frac{2}{\sqrt{3}}(1-n^{1/2})\right]\gamma(\mathbf{k})+\frac{1}{\sqrt{3}}(1-n)^{1/2}, & n\to 1,\\ (1-n)\gamma(\mathbf{k})+\frac{n}{2}, & n\to 0\quad (R=0),\end{cases} \qquad (40)$$

$$\left[\frac{\Sigma_2(\omega)}{W}\right]_{max}\approx\begin{cases}\frac{1+n}{\sqrt{3}}(1-n)^{1/2}, & n\to 1,\\ \frac{n}{2}\left(1-\frac{n}{4}\right), & n\to 0\quad (R=0),\end{cases} \qquad (41)$$

where $\gamma(\mathbf{k})=z^{-1}\Sigma_{\mathbf{h}}\exp i\mathbf{kh}$.

From (40) and (41) we conclude that a strong inequality

$$\left|\frac{[\Sigma_2(\omega)]_{max}}{\Sigma_1\left(\mathbf{k}=\begin{pmatrix}0\\ \mathbf{Q}\end{pmatrix}\right)}\right|_{\substack{n\to 0\\ n\to 1}}\ll 1, \qquad (42)$$

obtains at the center ($\mathbf{k}=0$) and on the edge [$\mathbf{k}=\mathbf{Q}=(\pi/a)(1,1,1)$] of the Brillouin zone as $n\to 0$ and $n\to 1$ and guarantees convergence of the series in this range of parameters.

For the values of the quasimomentum $\mathbf{k}=\mathbf{Q}/2$ ($\gamma(\mathbf{Q}/2)=0$) we have in the region of interest to us

$$\lim_{\substack{n\to 0\\ n\to 1}}[\Sigma_2(\omega)]_{max}=\lim_{\substack{n\to 0\\ n\to 1}}[\Sigma_1(\mathbf{k}=\mathbf{Q}/2)]=0. \qquad (43)$$

This means that for integration over the total Brillouin zone the contribution from the regions with quasimomentum values $\mathbf{k}=\mathbf{Q}/2$ will be small as $n\to 1$ or $n\to 0$. As $n\to 1$ this behavior of $\{\Sigma_2(\omega)\}_{max}$ is a reflection of the fact that the ground state in our theory is ferromagnetic ($0.7\lesssim n\leqslant 1$) and in the Nagaoka limit ($n\to 1$, $R\to n$) scattering by local spin fluctuations is completely suppressed.

It is important to note that as $n\to 1$ the results of the linear approximation in $t(\mathbf{f}-\mathbf{f}')$ become exact (in the aforementioned restriction to the class of homogeneous solutions). This fact requires no assumption concerning the model density of states and is general. Indeed, using information on the ground state at $n=1$ (the ground state is ferromagnetic with a maximum spin $R=n^\sigma=1, n^{\bar\sigma}=0$) we have

$$\Delta_\sigma=0,$$
$$K_\sigma=\langle S_0S_{\mathbf{h}}\rangle-{}^3/_4=0. \qquad (44)$$

Substituting (44) in the most general equation (36) for $\Omega_\sigma^{II}(\omega)$ at $U=\infty$ we verify that

$$\Omega_\sigma^{II}(\omega,n=1)=0. \qquad (45)$$

For $n\to 1$ the theory becomes thus exact and its result agrees with the theorems of Nagaoka.[3]

Figure 2 shows the calculated $[\Sigma_2(\omega)]_{max}$ and $\Sigma_1(\mathbf{k})$ for $\mathbf{k}=0$ (or $\mathbf{k}=\mathbf{Q}$) at arbitrary densities. In density region $1\geqslant n\gtrsim 0.77$–0.75 the inequality (42) is valid and this region corresponds fully to a ferromagnetic metallic state ($1\geqslant n\gtrsim 0.7$). The convergence of the perturbation-theory series in $t(\mathbf{f}-\mathbf{f}')$ is thus ensured in the ferromagnetic phase all the way to concentrations close to $n_c\approx 0.7$. In this region there are two small parameters, the number $p=1-n$ of the holes and the number n^0 of the flipped spins.

In the region 0.77–$0.75>n>0.48$–0.45 the inequality (42) no longer holds. This region includes the concentration phase-transition point, and the intervals $\Delta n_f\approx 0.07$ to the left of n_c and $\Delta n_p\approx 0.25$ to the right of n_c, which pertained in the first-order theory to the ferro- and paraphase, respectively. A characteristic attribute of this region is the absence of a small parameter, since $n^{\bar\sigma}=n^\sigma\approx p$, which leads apparently to strong critical-fluctuations that cannot be described in the framework of the self-consistent-field theory.

The inequality (42) becomes valid again in the region 0.48–$0.45>n\geqslant 0$. This density region is located entirely in the paraphase, where the small parameter is the number of electrons $n^{\bar\sigma}=n^\sigma\ll 1$.

The energy overlap-integral perturbation-theory series represented by Eq. (4) converges thus in the density region $n>n_c+\Delta n_f$ corresponding to a ferromagnetic metal, and in the region $n<n_c-\Delta n_p$ corresponding to a paramagnetic metal; in the region $n_c+\Delta n_f>n>n_c-\Delta n_p$ the results of the theory must be interpreted as interpolations.

5. CONCLUSION

We note certain features of our results and compare them with the known solutions.

As already noted (see the Introduction), an attempt was made in Ref. 3 to generalize the results for a single hole to include the thermodynamic region. Account was taken

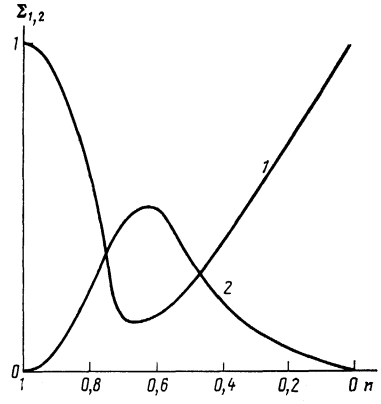

FIG. 2. Contribution to self-energy part in first order $[|\Sigma_1(\mathbf{k}=(^0_Q))|]$ (curve 1) and in second order $[\Sigma_2(\omega)]_{max}$ (curve 2) in $t(\mathbf{f}-\mathbf{f}')$ vs the electron density n.

there, however, only of effects proportional to $t(\mathbf{f}-\mathbf{f}')$, which are in turn linear in the hole density, i.e., $pt(\mathbf{f}-\mathbf{f}')$. This result by Nagaoka is the first term of the expansion of our theory in terms of p. In fact, as $p\to 0$ we obtain from (26)

$$\varphi=p^{1/3}+O(p), \quad R=(1-p)-\frac{2}{\sqrt{3}}p^{3/2}-O(p^2). \tag{46}$$

In an approximation linear in the hole density our theory reduces thus to Nagaoka's result: $R=n$ (saturated ferromagnetism).

Callaway (see, e.g., Ref. 19) has developed in a number of papers a program for exact diagonalization of the Hubbard Hamiltonian for small clusters (e.g., $2\times 2\times 2$, Ref. 19). It was shown that the Nagaoka state ($R=n$) is unstable with a decrease of the number of electrons, starting with $N_e=6$ (two holes). It follows from this numerical calculation that the ferromagnetic moment does not decrease linearly with decrease of the number of electrons, in agreement with our theory.

To illustrate the physical mechanisms represented by Eqs. (19)–(21), we can calculate the quantities indicative of the placement of the spin quasibands relative to one another. What is instructive in this respect is the distance, in energy scale, between the Fermi level and the bottom of the spin quasiband:

$$\gamma_\sigma=\mu-W_\sigma=W\alpha_\sigma[n+\eta(\sigma)R], \quad \alpha_\sigma=1-\frac{\varphi_\sigma(\mathbf{k}=0)}{W(1-n^{\bar\sigma})^2}. \tag{47}$$

From (47) and (24) one can see why allowance for only the shift of the energy centroids of the spin quasibands [the contribution (a)] does not lead to a transition into a paramagnetic state at $n\neq 0$. In this case the quasiband with spin $\bar\sigma$ is "pushed out" upwards above the Fermi level ($\gamma_{\bar\sigma}=0$) and remains empty all the way to densities $n=0$. Therefore the decrease of the magnetization R is due only to depletion of the quasiband with spin σ (the width of this band is $\gamma_\sigma=2Wn$) with decrease of $n=n^\sigma$. It is understandable therefore that a contribution of type (a) corresponds to the approximation of Ref. 3, where the "excluded volume effect," which takes place generally speaking for all finite hole densities, is completely ignored for holes.

The situation is quite different when account is taken of both contributions (a) and (b). Recall that the contribution (b) is quadratic in the effective kinematic fields ψ^σ and $\psi^{\bar\sigma}$ and renormalizes the correlation width of the spin subband. In this case, when the density decreases from $n=1$ there appear in the system electrons with opposite spins and therefore $\gamma_{\bar\sigma}\neq 0$. As n decreases, the arrangement of the spin quasiband is modified as follows: the width of the quasiband with spin σ decreases, but the width of the quasiband with spin $\bar\sigma$ increases; the distance between the centroids of the spin quasibands decreases. It becomes therefore obvious that a transition to the state of a paramagnetic metal takes place at finite electron density in the quasiband.

Since the effective kinematic field, which is the analog of the exchange interaction, depends not only on the density but also on the temperature, the decrease of the magnetic moment with temperature is not due to excitation of collective degrees of freedom (spin waves), but is the analog of Stoner single-particle thermal excitations.

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APPENDIX I

Kalashnikov and Fradkin[13] have formulated a principle for the choice of the best single-particle approximation: an approximation of the spectral density (or of the corresponding Green's function) will be more accurate the larger the number of relations (correlation moments) is satisfies rigorously.

Let us define, in accordance with Ref. 13, the single particle density $\Lambda^\sigma_{\mathbf{ff}'}(t-t')$ and its corresponding correlation spectral moments $M^{(n+1)}_{\mathbf{k}\sigma}$ as follows:

$$\Lambda^\sigma_{\mathbf{ff}'}(t-t')=\langle\{a_{\mathbf{f}}^+(t);a_{\mathbf{f}'}(t')\}\rangle, \tag{AI.1}$$

$$M^{(n+1)}_{\mathbf{k}\sigma}=\frac{1}{2\pi}\int d\omega\Lambda^\sigma_{\mathbf{k}}(\omega)\omega^n. \tag{AI.2}$$

We represent the connection between $\Lambda^\sigma_{\mathbf{k}}(t-t')$ and $M^{(n+1)}_{\mathbf{k}\sigma}$ by the series

$$\Lambda^\sigma_{\mathbf{k}}(t-t')=\sum_{n=0}^{\infty}M^{(n+1)}_{\mathbf{k}\sigma}\frac{(-i)^n(t-t')^n}{n!}. \tag{AI.3}$$

Using (AI.3) we find

$$M^{(n+1)}_{\mathbf{k}\sigma}=\frac{1}{N}\sum_{\mathbf{f},\mathbf{f}'}e^{i\mathbf{k}(\mathbf{f}-\mathbf{f}')}\left\langle\left\{\left(i\frac{\partial}{\partial t}\right)^r a_{\mathbf{f}}^+(t);\left(-i\frac{\partial}{\partial t'}\right)^{n-r}a_{\mathbf{f}'}(t')\right\}\right\rangle,$$
$$n=0,1,2,\ldots;\quad r\leqslant n. \tag{AI.4}$$

To transform the system of exact relations (AI.4) into a system of closed equations we must assume a class of functions that can be chosen to approximate $\Lambda^\sigma_{\mathbf{ff}'}(\omega)$. To solve the problem of the one-particle approximation with an undamped spectrum it suffices to approximate $\Lambda^\sigma_{\mathbf{k}}(\omega)$ on a class of delta-functions.

Let us prove that in first-order perturbation theory in $t(\mathbf{f}-\mathbf{f}')$ the Green's function conserves the first four moments and is therefore the best single-particle approximaton on a class of solutions with two delta-functions. The spectral density corresponding to a two-pole single-particle approximation with undamped spectrum is of the form

$$\Lambda^\sigma_{\mathbf{k}}(\omega)=2\pi\alpha_+^\sigma(\mathbf{k})\delta(\omega-\omega_+^\sigma(\mathbf{k}))+2\pi\alpha_-^\sigma(\mathbf{k})\delta(\omega-\omega_-^\sigma(\mathbf{k})). \tag{AI.5}$$

To find the spectrum $\omega^\sigma_{+,-}(\mathbf{k})$ of the single-particle excitations and of the corresponding amplitudes $\alpha^\sigma_+(\mathbf{k})$ and $\alpha^\sigma_-(\mathbf{k})$ we use the first four exact equations of (AI.4):[4)]

$$\begin{aligned}
&\alpha_+^\sigma(\mathbf{k})+\alpha_-^\sigma(\mathbf{k})=1,\\
&\alpha_+^\sigma(\mathbf{k})\omega_+^\sigma(\mathbf{k})+\alpha_-^\sigma(\mathbf{k})\omega_-^\sigma(\mathbf{k})=\varepsilon(\mathbf{k})+Un^{\bar\sigma},\\
&\alpha_+^\sigma(\mathbf{k})(\omega_+^\sigma(\mathbf{k}))^2+\alpha_-^\sigma(\mathbf{k})(\omega_-^\sigma(\mathbf{k}))^2\\
&\quad=\varepsilon^2(\mathbf{k})+2U\varepsilon(\mathbf{k})n^\sigma+U^2n^{\bar\sigma},\\
&\alpha_+^\sigma(\mathbf{k})(\omega_+^\sigma(\mathbf{k}))^3+\alpha_-^\sigma(\mathbf{k})(\omega_-^\sigma(\mathbf{k}))^3\\
&\quad=\varepsilon^3(\mathbf{k})+3U\varepsilon^2(\mathbf{k})n^{\bar\sigma}+2U^2\varepsilon(\mathbf{k})n^{\bar\sigma}+U^3n^{\bar\sigma}\\
&\qquad+U^2(n^{\bar\sigma})^2\varepsilon(\mathbf{k})+U^2\Omega_\sigma^{\mathrm{I}}(\mathbf{k}),
\end{aligned} \tag{AI.6}$$

where $\Omega_\sigma^I(\mathbf{k})$ is the nonlocal-correlation function (15), but in the definitions of $\Delta_\sigma(\mathbf{h})$ and $K_\sigma(\mathbf{h})$ account is taken of spatial correlations with "twofold" excitations (since $U \neq \infty$):

$$K_\sigma(\mathbf{h}) = \langle n_0^{\bar\sigma} n_{\mathbf{h}}^{\bar\sigma}\rangle - (n^{\bar\sigma})^2 + \langle X_0^{\sigma\sigma} X_{\mathbf{h}}^{\sigma\bar\sigma}\rangle - \langle X_0^{02} X_{\mathbf{h}}^{20}\rangle,$$

$$\Delta_\sigma(\mathbf{h}) = \langle a_{0\bar\sigma}^{+} a_{\mathbf{h}\bar\sigma} n_0^{\sigma}\rangle - \langle a_{\mathbf{h}\bar\sigma}^{+} a_{0\bar\sigma}(1-n_0^{\sigma})\rangle. \qquad \text{(AI.7)}$$

The solution of the system (AI.6) is unique and can be obtained.[14] It is necessary next to use the property of Green's propagator functions:[15]

$$-i\Lambda_{\mathbf{k}}^{\sigma}(\omega) = G_{\mathbf{k}}^{\sigma}(\omega+i0) - G_{\mathbf{k}}^{\sigma}(\omega-i0). \qquad \text{(AI.8)}$$

As a result we get

$$G_\sigma^I(\omega, \mathbf{k}) = \{[\tilde G_\sigma^I(\omega, \mathbf{k})]^{-1} - \varepsilon(\mathbf{k})\}^{-1}, \qquad \text{(AI.9)}$$

$$\tilde G_\sigma^I(\omega, \mathbf{k}) = \frac{\omega - n_-^{\bar\sigma} U - \Omega_\sigma^I(\mathbf{k})/n_+^{\bar\sigma} n_-^{\bar\sigma}}{[\omega - \Omega_\sigma^I(\mathbf{k})/n_-^{\bar\sigma}][\omega - U - \Omega_\sigma^I(\mathbf{k})/n_+^{\bar\sigma}] - [\Omega_\sigma^I(\mathbf{k})]^2/n_+^{\bar\sigma} n_-^{\bar\sigma}}. \qquad \text{(AI.10)}$$

As $U \to \infty$ the Green's function $G_\sigma^I(\omega,\mathbf{k})$ goes over into (14), thus proving our statement. The single-node CPM (Hubbard-I) approximation does not satisfy the fourth moment of the theory precisely in view of the presence of the last term ($\Omega_\sigma^I(\mathbf{k})$). As already noted, the nonlocal contribution $\Omega_\sigma^I(\mathbf{k})$ is not the "Nagaoka scale" of the problem, when the connection between the spatial and the spin degrees of freedom begins to play a decisive role.

It is necessary in this connection to approach with due caution theories in which a Hubbard-I approximation appears in first order in the tunneling integral $t(\mathbf{f}-\mathbf{f}')$.[16]

APPENDIX II.

In the calculation of binary correlation functions $K^\sigma(\mathbf{h})$ in the approximation linear in $t(\mathbf{f}-\mathbf{f}')$, successive account is taken of the corresponding correlations between the single-particle excitations (kinematic fields), and there is no contribution from the collective modes.[16] We shall use the method of Ref. 9 and calculate the sought correlation functions in a variant with a single-particle kinematic interaction.[5)] According to Ref. 9, a Green's function of the form

$$\langle\langle X_{\mathbf{k}}^{0\sigma} P_j(\mathbf{k},\mathbf{h})\rangle\rangle_\omega = \frac{\langle\{X_{\mathbf{k}}^{0\sigma}, P_j\}\rangle}{n_-^{\bar\sigma}} G_\sigma^I(\omega,\mathbf{k}) \qquad \text{(AII.1)}$$

makes it possible to calculate the sought binary correlation functions in $K_\sigma(\mathbf{h})$ under the condition that the generating operators $P_j(\mathbf{k},\mathbf{h})$ be determined from the relations

$$\frac{1}{N}\sum_{\mathbf{k}} \langle P_1(\mathbf{k},\mathbf{h}) X_{\mathbf{k}}^{0\bar\sigma}\rangle = \langle n_0^{\bar\sigma} n_{\mathbf{h}}^{\bar\sigma}\rangle, \quad \frac{1}{N}\sum_{\mathbf{k}} \langle P_2(\mathbf{k},\mathbf{h}) X_{\mathbf{k}}^{0\bar\sigma}\rangle = \langle n_0^{\bar\sigma} n_{\mathbf{h}}^{\sigma}\rangle,$$

$$\frac{1}{N}\sum_{\mathbf{k}} \langle P_3(\mathbf{k},\mathbf{h}) X_{\mathbf{k}}^{0\sigma}\rangle = \langle X_0^{\bar\sigma\sigma} X_{\mathbf{h}}^{\sigma\bar\sigma}\rangle. \qquad \text{(AII.2)}$$

From (AII.2) we obtain the generating operators $P_j(\mathbf{k},\mathbf{h})$.[16] Using next (AII.1) and the spectral theorem,[15] we obtain

$$\langle n_0^{\bar\sigma} n_{\mathbf{h}}^{\bar\sigma}\rangle = [(n^{\bar\sigma})^2 - \langle n_0^{\bar\sigma} n_{\mathbf{h}}^{\sigma}\rangle n^{\bar\sigma} - (\Delta^\sigma(\mathbf{h}))^2]/n_-^{\bar\sigma},$$

$$\langle n_0^{\bar\sigma} n_{\mathbf{h}}^{\sigma}\rangle = [n^{\bar\sigma} n^{\sigma} - \langle n_0^{\bar\sigma} n_{\mathbf{h}}^{\bar\sigma}\rangle n^{\sigma}]/n_-^{\bar\sigma},$$

$$\langle X_0^{\bar\sigma\sigma} X_{\mathbf{h}}^{\sigma\bar\sigma}\rangle = -\frac{\Delta^{\bar\sigma}(\mathbf{h})\Delta^{\sigma}(\mathbf{h})}{1-n}. \qquad \text{(AII.3)}$$

Expression (21) follows from Eqs. (AII.3).

[1)] The passage to the limit ($U \to \infty$) was made after calculating the function $G_\sigma^I(\omega,\mathbf{k})$ for finite U. The same sequence of operations will be used hereafter.

[2)] Note that the situation is not remedied by the Hubbard-III approximation,[11] where there are likewise no magnetic solutions.[12]

[3)] By analogy with Refs. 3 and 11 (see also Ref. 18).

[4)] For simplicity, Eqs. (AI.6) were written for $\varepsilon_0 = 0$ but this, naturally, does not make them less general.

[5)] It follows from analysis[16] that this variant of constructing an effective self-consistent field is the only one acceptable when it comes to obtaining a complete closed system of equations that renormalize a single-particle spectrum.

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