16. S. N. Sokolov, Preprint IFVÉ OTF 74-135 [in Russian], Serpukhov (1974).
17. S. N. Sokolov, Preprint IFVÉ OTF 75-94 [in Russian], Serpukhov (1975).
18. S. N. Sokolov, Preprint IFVÉ OTF 76-50 [in Russian], Serpukhov (1976); Proc. Fourth Intern. Conf. on Nonlocal Field Theories, April 1976 [in Russian], Alushta, p. 77-86.
19. S. N. Sokolov, Dokl. Akad. Nauk SSSR, Ser. Mat.-Fiz., **233**, 575 (1977).
20. L. L. Foldy, Phys. Rev., **122**, 275 (1961).
21. S. N. Sokolov, Teor. Mat. Fiz., **23**, 355 (1975).
22. R. G. Newton, Scattering Theory of Waves and Particles, New York (1966).
23. R. F. Streater and A. S. Wightman, PCT, Spin and Statistics and All That, Benjamin, New York (1964).
24. F. Coester, Meson Theory of Nuclear Forces. Quanta, University of Chicago Press (1970, p.174-175; F. Coester, S. C. Pieper, and F. J. D. Serduke, Phys. Rev. C, **11**, 1 (1975); F. Coester and A. Ostbee, Phys. Rev. C, **11**, 1836 (1975).
25. S. N. Sokolov, Teor. Mat. Fiz., **32**, 354 (1977).

SELF-CONSISTENT THEORY OF ELECTRON CORRELATION IN THE HUBBARD MODEL

A. L. Kuzemskii

The Dyson equation for the two-time thermal Green's functions is used for a self-consistent calculation of the single-particle Green's functions in the Hubbard model. The method makes it possible to obtain a generalized interpolation solution of the Hubbard model valid for arbitrary relationship between the effective band width and the Coulomb repulsion parameter. Two variants of the theory make it possible to obtain two exact representations for the mass operator, which are used to obtain approximate solutions in the atomic and band limits.

1. The method of two-time thermal Green's functions [1, 2] is convenient and effective for investigating systems of many interacting particles. Recently, a helpful reformulation of this model has been given; it makes it possible to operate with the exact mass operator and perform the decouplings in the final stage. This approach is based on the introduction of irreducible Green's functions [2-6], which makes it possible, without recourse to a truncation of the hierarchy of equations for the Green's functions, to write down the Dyson equation and obtain an exact analytic representation for the mass operator. Approximate solutions are constructed as definite approximations for the mass operator.

The method of irreducible Green's functions has been used in a large number of investigations into the self-consistent theory of phonons, the Heisenberg model, the spin–phonon interaction, ferroelectricity, and more (see [2-6] and the literature quoted there). In the present paper, we consider the application of this approach to the Hubbard model, which is one of the ones most widely used to describe magnetic properties and the transition from the metallic to the nonmetallic state in transition metals and their chalcogenides [7, 8].

The Hamiltonian proposed by Hubbard [7],

$$H=\sum_{ij\sigma} t_{ij}a_{i\sigma}^{+}a_{j\sigma}+\frac{U}{2}\sum_{i\sigma} n_{i\sigma}n_{i-\sigma} \tag{1}$$

depends on two parameters: the effective band width $w=\left(N^{-1}\sum_{ij}|t_{ij}|^2\right)^{1/2}$ and the energy U of the intra-atomic Coulomb repulsion of the electrons. As their ratio changes, so does the band structure of the system. Thus, to describe transitions in the system, it is necessary to obtain an interpolation solution for the Hubbard Hamiltonian valid in a wide range of values of the parameter $z = w/U$ from the atomic limit ($z \to 0$) to the band limit ($z \gg 1$). The method of irreducible Green's functions makes it possible to construct such solutions

Joint Institute for Nuclear Research, Dubna. Translated from Teoreticheskaya i Matematicheskaya Fizika, Vol.36, No.2, pp.208-223, August, 1978. Original article submitted June 21, 1977.

 0040-5779/78/3602-0692$07.50

systematically.

2. Following [9, 10], we introduce the single-particle Green's functions

$$G_{k\sigma}(t)=\langle\langle a_{k\sigma}(t);a_{k\sigma}^{+}\rangle\rangle=-i\theta(t)\langle[a_{k\sigma}(t),a_{k\sigma}^{+}]\rangle=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}G_{k\sigma}(\omega)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega'}{\omega-\omega'}(e^{\beta\omega'}+1)J_{k\sigma}(\omega'),$$

where $\beta=(kT)^{-1}$, $J_{k\sigma}(\omega)$ is the spectral intensity. The equation for the Fourier transform $G_{k\sigma}(\omega)$ of the Green's function has the form

$$(\omega-\varepsilon_k)G_{k\sigma}(\omega)=1+\frac{U}{N}\sum_{pq}\langle\langle a_{k+p,\sigma}a_{p+q,-\sigma}^{+}a_{q,-\sigma}|a_{k\sigma}^{+}\rangle\rangle_{\omega}. \tag{2}$$

By definition, we introduce an irreducible Green's function that does not contain renormalizations of the average field,

$$\mathrm{ir}\langle\langle a_{k+p,\sigma}a_{p+q,-\sigma}a_{q,-\sigma}|a_{k\sigma}^{+}\rangle\rangle_{\omega}=\langle\langle a_{k+p,\sigma}a_{p+q,-\sigma}^{+}a_{q,-\sigma}|a_{k\sigma}^{+}\rangle\rangle_{\omega}-\delta_{p,0}\langle n_{q,-\sigma}\rangle G_{k\sigma}. \tag{3}$$

The irreducible Green's function in (2) is defined in such a way that it cannot be reduced to Green's functions of lower order with respect to the number of fermion operators by an arbitrary pairing of operators corresponding to one instant of time. Substituting (3) in (2), we obtain

$$G_{k\sigma}(\omega)=G_{k\sigma}^{\mathrm{HF}}(\omega)+G_{k\sigma}^{\mathrm{HF}}\frac{U}{N}\sum_{pq}^{ir}\langle\langle a_{k+p,\sigma}a_{p+q,-\sigma}^{+}a_{q,-\sigma}|a_{k\sigma}^{+}\rangle\rangle_{\omega}. \tag{4}$$

Here, we have introduced the notation

$$G_{k\sigma}^{\mathrm{HF}}(\omega)=(\omega-\varepsilon_{k\sigma}^{\mathrm{HF}})^{-1},\ \varepsilon_{k\sigma}^{\mathrm{HF}}=\varepsilon_k+\frac{U}{N}\sum_{q}\langle n_{q,-\sigma}\rangle.$$

To obtain the Dyson equation, we must express the Green's function $^{\mathrm{ir}}\langle\langle A|a_{k\sigma}^{+}\rangle\rangle$ on the right-hand side of (4) in terms of the total Green's function $G_{k\sigma}(\omega)$. For this, we differentiate this function with respect to the second time: $-i(d/dt)^{\mathrm{ir}}\langle\langle A;a_{k\sigma}^{+}(t)\rangle\rangle$. For the Fourier components, this is written in the form

$$(\omega-\varepsilon_k)^{\mathrm{ir}}\langle\langle A|a_{k\sigma}^{+}\rangle\rangle_{\omega}=^{\mathrm{ir}}\langle[A,a_{k\sigma}^{+}]_{+}\rangle+\frac{U}{N}\sum_{rs}\langle\langle A|a_{r,-\sigma}^{+}a_{r+s,-\sigma}a_{k+s,\sigma}^{+}\rangle\rangle_{\omega}. \tag{5}$$

The anticommutator in (5) is calculated on the basis of the definition of the irreducible part:

$$^{\mathrm{ir}}\langle[a_{k+p,\sigma}a_{p+q,-\sigma}^{+}a_{q,-\sigma},a_{k\sigma}^{+}]_{+}\rangle=\langle[a_{k+p,\sigma}a_{p+q,-\sigma}^{+}a_{q,-\sigma}-\langle a_{p+q,-\sigma}^{+}a_{q,-\sigma}\rangle a_{k+p,\sigma},a_{k\sigma}^{+}]_{+}\rangle\equiv 0. \tag{6}$$

Substituting (6) in Eq. (5) and introducing in it, as in (3), a Green's function irreducible with respect to the right-hand operators, we obtain

$$G_{k\sigma}(\omega)=G_{k\sigma}^{\mathrm{HF}}(\omega)+G_{k\sigma}^{\mathrm{HF}}(\omega)P_{k\sigma}(\omega)G_{k\sigma}^{\mathrm{HF}}(\omega), \tag{7}$$

where we have introduced the following notation for the radiation operator:

$$P_{k\sigma}(\omega)=\frac{U^2}{N^2}\sum_{pqrs}{}^{\mathrm{ir}}\langle\langle a_{k+p,\sigma}a_{p+q,-\sigma}^{+}a_{q,-\sigma}|a_{r,-\sigma}^{+}a_{r+s,-\sigma}a_{k+s,\sigma}^{+}\rangle\rangle_{\omega}^{\mathrm{ir}}=\frac{U^2}{N^2}\sum_{pqrs}G_{k\sigma}^{\mathrm{ir}}(p,q|r,s;\omega). \tag{8}$$

To separate the mass operator, it is necessary to separate the connected part of the irreducible Green's function in (8):

$$G_{k\sigma}^{\mathrm{ir}}(p,q|r,s;\omega)=L_{k\sigma}(p,q|r,s;\omega)+\frac{U^2}{N^2}\sum_{r_1s_1}\sum_{p_1q_1}L_{k\sigma}(p,q|r_1,s_1;\omega)G_{k\sigma}^{\mathrm{HF}}(\omega)G_{k\sigma}^{\mathrm{ir}}(p_1,q_1|r,s;\omega). \tag{9}$$

Here, $L_{k\sigma}(p,q|r,s;\omega)$ is the connected part of the Green's function $G_{k\sigma}{}^{\mathrm{ir}}(p,q|r,s;\omega)$, which in accordance with the definition (9) does not contain parts connected by one line $G_{k\sigma}^{\mathrm{HF}}(\omega)$. After simple transformations, we obtain from (7)

$$P_{k\sigma}(\omega)=M_{k\sigma}(\omega)+M_{k\sigma}(\omega)G_{k\sigma}{}^{\mathrm{HF}}(\omega)P_{k\sigma}(\omega), \tag{10}$$

where

$$M_{k\sigma}(\omega)=\frac{U^2}{N^2}\sum_{pqrs}L_{k\sigma}(p,q;r,s;\omega). \tag{11}$$

Finally, we obtain from (7) and (10)

$$G_{k\sigma}(\omega)=G_{k\sigma}^{HF}(\omega)+G_{k\sigma}^{HF}(\omega)M_{k\sigma}(\omega)G_{k\sigma}(\omega). \tag{12}$$

Equation (12) is the Dyson equation for the single-particle two-time thermal Green's function $G_{k\sigma}(\omega)$. It has the formal solution

$$G_{k\sigma}(\omega)=[\omega-\varepsilon_{k\sigma}^{HF}-M_{k\sigma}(\omega)]^{-1}. \tag{13}$$

The expression

$$M_{k\sigma}(\omega)=\frac{U^2}{N^2}\sum_{pqrs}\langle\langle a_{k+p,\sigma}a_{p+q,-\sigma}^{+}a_{q,-\sigma}|a_{r,-\sigma}^{+}a_{r+s,-\sigma}a_{k+s,\sigma}^{+}\rangle\rangle_{\omega}^{1r,c} \tag{14}$$

is an exact representation for the mass operator of the single-particle Green's function for the system of correlated electrons in the narrow energy bands (the superscript c in (14) denotes the connected part). The expression (14) can be written in the more convenient form

$$M_{k\sigma}(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega'}{\omega-\omega'}(e^{\beta\omega'}+1)\frac{U^2}{N^2}\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{i\omega t}\sum_{pqrs}\langle a_{r,-\sigma}^{+}a_{r+s,-\sigma}a_{k+p,\sigma}^{+}a_{k+p,\sigma}(t)a_{p+q,-\sigma}^{+}(t)a_{q,-\sigma}(t)\rangle^{1r,c}=$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega'}{\omega-\omega'}(e^{\beta\omega'}+1)U^2\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{i\omega' t}N^{-1}\sum_{i\neq j}e^{-ik(R_i-R_j)}\langle a_{j\sigma}^{+}n_{j-\sigma}n_{i-\sigma}(t)a_{i\sigma}(t)\rangle^{1r,c}. \tag{15}$$

The expression (15) for the mass operator $M_{k\sigma}$ of the single-particle Green's function of the Hubbard model is exact and valid for arbitrary z. It can be seen that the method of irreducible Green's functions is closely related to a definite method of projecting the higher Green's functions onto the original ones; as zeroth Green's function, one chooses a nonlocal Green's function renormalized with allowance for all renormalizations of the average field. The representation (15) is more convenient for obtaining approximate solutions in the band limit since it explicitly contains the factor U^2, but, in general, it can also be used to obtain approximate solutions in the case of strong correlation. To obtain approximate solutions, it is necessary to make definite assumptions about the approximate expression for the connected part of the correlation function on the right-hand side of (15).

3. By the introduction of irreducible parts, we have separated all the renormalizations of the average field, i.e., all the equal-time pairings. Different equal-time pairings in (15) will lead to different approximate solutions (see [2-6, 9]). We first make a simple binary decoupling:

$$\langle a_{r,-\sigma}^{+}a_{r+s,-\sigma}a_{k+s,\sigma}^{+}a_{k+p,\sigma}(t)a_{p+q,-\sigma}^{+}(t)a_{q,-\sigma}(t)\rangle^{1r,c}\approx\delta_{k+s,k+p}\delta_{r+s,p+q}\delta_{r,q}\langle a_{k+p,\sigma}^{+}a_{k+p,\sigma}(t)\rangle\langle a_{p+q,-\sigma}a_{p+q,-\sigma}^{+}(t)\rangle\langle a_{q,-\sigma}^{+}a_{q,-\sigma}(t)\rangle. \tag{16}$$

We then obtain

$$M_{k\sigma}^{p}(\omega)=\frac{U^2}{N^2}\sum_{p,q}\int\frac{d\omega_1\,d\omega_2\,d\omega_3}{\omega+\omega_1-\omega_2-\omega_3}\{n(\omega_1)[1-n(\omega_2)-n(\omega_3)]+n(\omega_2)n(\omega_3)\}\langle g_{p+q,-\sigma}(\omega_1)g_{k+p,\sigma}(\omega_2)g_{p,-\sigma}(\omega_3). \tag{17}$$

Here $g_{k\sigma}(\omega)=-(1/\pi)\operatorname{Im}G_{k\sigma}(\omega+i\varepsilon)$.

The binary decoupling was used in [9] to calculate the mass operator in the paramagnetic state. In the language of the diagram technique, the binary approximation corresponds to a simple vertex in the mass operator and can be used outside resonance regions of the collective excitations when the density of quasiparticles is sufficiently low. Equations (12) and (17) constitute a self-consistent system of equations for the single-particle Green's function in the framework of the binary approximation. Choosing a particular initial representation for the function $g_{k\sigma}(\omega)$ on the right-hand side of (17), we can calculate the Green's function $G_{k\sigma}$. In principle, substituting the result obtained once more in (17), we can find a more exact solution. In the band limit, a reasonable initial approximation that admits such an iteration is $g_{k\sigma}(\omega)=\delta(\omega-\varepsilon_k)$. At the same time we obtain from (17)

$$M_{k\sigma}^{p}(\omega)=\frac{U^2}{N^2}\sum_{pq}\frac{N_{kpq}^{\sigma}}{\omega_1-\Omega_{kpq}}, \tag{18}$$

$$N_{kpq}^{\sigma}=n_{p+q,-\sigma}[1-n_{k+p,\sigma}-n_{q,-\sigma}]+n_{k+p,\sigma}n_{q,-\sigma},\quad \Omega_{kpq}=-\varepsilon_{p+q}+\varepsilon_{k+p}+\varepsilon_q. \tag{19}$$

A mass operator of the form (18) for the Hubbard model was obtained earlier in [12] by Langer, who used the equation of motion for the second-order Green's function and an approximation of a density expansion type.

We now obtain an equation for the mean population numbers in the binary approximation. For this, following [13], we represent the spectral intensity of the Green's function in the form

$$g_{k\sigma}(\omega)=\frac{1}{\pi}\frac{\Gamma_{k\sigma}(\omega)}{(\omega-E_{k\sigma})^2+\Gamma_{k\sigma}^2}\approx(1-\alpha_{k\sigma})\delta(\omega-E_{k\sigma})+\frac{1}{\pi}\frac{\Gamma_{k\sigma}(\omega)}{(\omega-E_{k\sigma})^2} \tag{20}$$

where

$$\Gamma_{k\sigma}(\omega)=-\operatorname{Im}M_{k\sigma}^{p}(\omega+i\varepsilon)=\pi\frac{U^2}{N^2}\sum_{pq}N_{kpq}^{\sigma}\delta(\omega-\Omega_{kpq}),\quad E_{k\sigma}=\varepsilon_{k\sigma}^{HF}+\operatorname{Re}M_{k\sigma}^{p}(E_{k\sigma})=\varepsilon_{k\sigma}^{HF}+\delta\varepsilon,\quad \delta\varepsilon=\mathcal{P}\frac{U^2}{N^2}\sum_{pq}\frac{N_{kpq}^{\sigma}}{\omega-\Omega_{kpq}}.$$

The unknown factor $(1-\alpha_{k\sigma})$ of the delta function on the right-hand side of (20) is determined by the normalization conditions

$$\int_{-\infty}^{\infty}d\omega g_{k\sigma}(\omega)=1,$$

whence

$$\alpha_{k\sigma}=\frac{U^2}{N^2}\sum_{pq}\frac{N_{kpq}^{\sigma}}{(\Omega_{kpq}-E_{k\sigma})}. \tag{21}$$

With allowance for (21), we find an equation for the mean population numbers:

$$n_{\sigma}=\frac{1}{N}\sum_{k}n(E_{k\sigma})+\frac{U^2}{N^3}\sum_{kpq}\frac{N_{kpq}^{\sigma}}{(\Omega_{kpq}-E_{k\sigma})^2}[n(\Omega_{kpq})-n(E_{k\sigma})]. \tag{22}$$

Thus, the mean population numbers are determined in a self-consistent manner from Eq. (22). The first on the right-hand side of (22) describes the effects of renormalization of the energy of the particles in the average field (from which Stoner's magnetism criterion is obtained), and the second describes the effect of two-body collisions of quasiparticles in the second order in U. The density of quasiparticle states in this approximation is equal to

$$D_{\sigma}(\omega)=N^{-1}\sum_{k}g_{k\sigma}(\omega)=N^{-1}\sum_{k}\{(1-\alpha_{k\sigma})\delta(\omega-E_{k\sigma})+\alpha_{k\sigma}\delta(\omega-\Omega_{kpq})\}. \tag{23}$$

The average energy of the system in this approximation is determined by

$$\langle H\rangle=\frac{1}{2N}\sum_{k\sigma}\int_{-\infty}^{\infty}(\omega+\varepsilon_k)J_{k\sigma}(\omega)d\omega=\frac{1}{2N}\sum_{k\sigma}(E_{k\sigma}+\varepsilon_k)n(E_{k\sigma})+(\Delta E)_2,$$

where

$$(\Delta E)_2=-\frac{1}{2N}\frac{U^2}{N^2}\sum_{kpq\sigma}\frac{N_{kpq}^{\sigma}}{\Omega_{kpq}-E_{k\sigma}}[(E_{k\sigma}+\varepsilon_k)n(E_{k\sigma})-(\Omega_{kpq}+\varepsilon_k)n(\Omega_{kpq})]$$

is a quantity whose structure is similar to that of the second-order correction to the energy in the many-impurity Anderson model or the Hubbard model with s–d hybridization [14]. In the band limit, the second term on the right-hand side of (22) is small. We can therefore attempt to obtain a magnetism criterion in the given approximation. For this, following [15], we introduce the mean number of electrons $n=\frac{1}{2}(n_{\uparrow}+n_{\downarrow})$ and the magnetization $m=\frac{1}{2}(n_{\uparrow}-n_{\downarrow})$. Denoting $n_{\sigma}\equiv f(\varepsilon_f;\ \varepsilon_k+Un_{-\sigma})$ and considering the condition for the existence of solutions of the equation

$$m=\tfrac{1}{2}f(\varepsilon_f;\ \varepsilon_k+Un-Um)-\tfrac{1}{2}f(\varepsilon_f;\ \varepsilon_k+Un+Um),$$

we obtain a criterion for the occurrence of magnetism in our system. It has the form

$$N^{-1}\sum_{k}U_{eff}(k)g_{k\sigma}(\varepsilon_f)-\Delta(\varepsilon_f)>1. \tag{24}$$

Here,

$$U_{eff}(k)=U\left\{1+\frac{U^2}{2N^2}\sum_{pq}\frac{N_{kpq}^{\uparrow}-N_{kpq}^{\downarrow}}{[\Omega_{kpq}-(\varepsilon_k+Un)]^2}\right\},\quad \Delta=\frac{U^3}{N^3}\sum_{kpq}\frac{N_{kpq}^{\uparrow}-N_{kpq}^{\downarrow}}{[\Omega_{kpq}-(\varepsilon_k+Un)]^3}[n(\Omega_{kpq})-n(\varepsilon_k+Un)].$$

In general, one can assume that (24) is a generalization of Stoner's criterion for the occurrence of ferromagnetism in the Hubbard model. The relation (24) takes a form closest to this criterion when one can assume $U_{eff}(k)\approx U_{eff}(0)$. Then from (24) we obtain

$$U_{\text{eff}}D_\sigma(\varepsilon_f)-\Delta(\varepsilon_f)>1. \tag{25}$$

It can be seen from this result that the occurrence of magnetism in the system is determined by the electron density of states. The occurrence of the renormalized quantity U_{eff} and the parameter Δ is natural when a more accurate allowance is made for the correlation than in the Hartree–Fock approximation, which leads to Stoner's criterion. It is well known that in the Hartree–Fock approximation the tendency of the system to form a magnetically ordered state is strongly overestimated. As we have already said above, in the band limit the representation (17) for the mass operator can be used for iterative calculation of the higher (in the interaction parameter U) orders of the mass operator, for which it is necessary to substitute (23) in (17). Thus, the proposed self-consistent procedure makes it possible to construct a perturbation theory for the mass operator. Because the resulting expressions are cumbersome, we do not give them here but refer to [11], in which the use of a two-pole representation for the spectral density (two delta functions) as initial approximation is also considered.

4. In the region of resonance of the single-particle and collective excitations the binary approximation breaks down. In particular, to describe a magnetically ordered state it is particularly important to take into account the contribution of the spin-flip processes to the mass operator. The method developed here permits this in a simple and perspicuous manner. For this, we perform in (15) the following different-time decouplings:

$$\langle a_{j\sigma}^{+}n_{j-\sigma}n_{i-\sigma}(t)a_{i\sigma}(t)\rangle^{\text{tr,c}}\approx\langle n_{j-\sigma}n_{i-\sigma}(t)\rangle\langle a_{j\sigma}^{+}a_{i\sigma}(t)\rangle+\langle a_{j\sigma}^{+}a_{j-\sigma}a_{i-\sigma}^{+}(t)a_{i\sigma}(t)\rangle\langle a_{j-\sigma}^{+}a_{i-\sigma}(t)\rangle+$$
$$\langle a_{j\sigma}^{+}a_{j-\sigma}^{+}a_{i-\sigma}(t)a_{i\sigma}(t)\rangle\langle a_{j-\sigma}a_{i-\sigma}^{+}(t)\rangle. \tag{26}$$

Then the mass operator (15) is written in the form

$$M_{k\sigma}(\omega)\approx M_{k\sigma}^{\text{el}}(\omega)+M_{k\sigma}^{\text{s}}(\omega)+M_{k\sigma}^{\text{d}}(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega'}{\omega-\omega'}(e^{\beta\omega'}+1)U^2N^{-1}\sum_{i\neq j}e^{-ik(R_i-R_j)}\times$$
$$\left\{\int_{-\infty}^{\infty}dEn_{\text{F}}\left(-\frac{1}{\pi}\operatorname{Im}\langle\langle a_{i\sigma}|a_{j\sigma}^{+}\rangle\rangle_{E+i\varepsilon}\right)n_{\text{B}}(\omega'-E)\left(-\frac{1}{\pi}\operatorname{Im}\langle\langle n_{i-\sigma}|n_{j-\sigma}\rangle\rangle_{\omega'-E+i\varepsilon}\right)+\right.$$
$$\left.\int_{-\infty}^{\infty}dEn_{\text{F}}(E)\left(-\frac{1}{\pi}\operatorname{Im}\langle\langle a_{i-\sigma}|a_{j-\sigma}^{+}\rangle\rangle_{E+i\varepsilon}\right)n_{\text{B}}(\omega'-E)\ -\frac{1}{\pi}\operatorname{Im}\langle\langle a_{i-\sigma}a_{i\sigma}|a_{j\sigma}^{+}a_{j-\sigma}^{+}\rangle\rangle_{\omega'-E+i\varepsilon}\right)\right\}. \tag{27}$$

Here $M_{k\sigma}^{\text{el}}(\omega)$, $M_{k\sigma}^{\text{s}}(\omega)$, $M_{k\sigma}^{\text{d}}(\omega)$ are the contributions to the mass operator that take into account the collective motions of the electron density, the spin density, and the pair density, respectively;

$$n_{\text{F}}^{\text{B}}=[\exp(\omega/\theta)\mp1]^{-1}.$$

We consider, for example, the calculation of the contribution $M_{k\sigma}^{\text{el}}(\omega)$ in the simplest approximation

$$M_{k\sigma}^{\text{el}}(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega'}{\omega-\omega'}(e^{\beta\omega'}+1)U^2N^{-1}\sum_{i\neq j}e^{-ik(R_i-R_j)}\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{i\omega' t}\{\langle a_{j\sigma}^{+}a_{i\sigma}(t)\rangle(n_{-\sigma}^{2}+K_{ij}(t))\},$$
$$K_{ij}(t)=\langle(n_{j-\sigma}-n_{-\sigma})(n_{i-\sigma}(t)-n_{-\sigma})\rangle. \tag{28}$$

If we restrict ourselves to the static approximation for $K_{ij}(t)$, i.e., we set $K_{ij}(t)\approx K_{ij}(0)$ (see [5]), then from (28) we obtain

$$M_{k\sigma}^{\text{el}}(\omega)=\frac{U^2}{N}\sum_{q}\int_{-\infty}^{\infty}\frac{dE}{\omega-E}(e^{\beta E}+1)\left\{-\frac{1}{\pi}\operatorname{Im}G_{q\sigma}(E+i\varepsilon)\right\}(n_{-\sigma}^{2}+K_{k-q})n_{\text{F}}(E). \tag{29}$$

Equations (29) and (12) are a self-consistent system of equations for the single-particle Green's function $G_{k\sigma}$ in the given approximation. Taking as initial value $g_{q\sigma}(\omega)=\delta(\omega-\varepsilon_q)$, we obtain from (29)

$$M_{k\sigma}^{\text{el}}(\omega)=\frac{U^2}{N}\sum_{q}(\omega-\varepsilon_{k-q})^{-1}\{n_{-\sigma}^{2}+K_q\}. \tag{30}$$

Simple estimates of $M_{k\sigma}^{\text{s}}$ and $M_{k\sigma}^{\text{d}}$ can be obtained similarly. A more accurate calculation of the mass operator (27) and the collective Green's functions and an application to definite physical systems will be presented in a separate paper.

5. In the present section, we consider the scheme for calculating a second exact representation for the mass operator. This representation is also valid for arbitrary z but is more convenient for obtaining approximate representations in the strong-correlation limit since it explicitly contains the factor $|t_{ij}|^2$. As zeroth Green's function, we again choose the nonlocal Green's function renormalized with allowance for all renormalizations of the average field. In a number of papers [16, 17] a perturbation theory has been constructed in the atomic limit on the basis of the local zeroth Green's function of the atomic limit: $G=(\omega-Un_{-\sigma})/(\omega-U)\omega$. As was noted in [18, 19], this leads to inaccurate results since even in the atomic limit the solution is definitely nonlocal, i.e., one must from the very start take into account nondiagonal elements of the solution. If one attempts to dispense with the method of Green's function, it is necessary to construct a systematic perturbation theory in the atomic limit, which is a very nontrivial problem because of the high multiplicity of degeneracy of the energy levels of the unperturbed Hamiltonian. At the same time, it is necessary to solve the problem of volume divergences and construct a special variant of the very cumbersome diagram technique [19]. We mention here that in [19] a method was formulated for constructing an effective Hamiltonian in the Hubbard model by a unitary transformation and it was shown that the simplest – Heisenberg – interaction is the main exchange interaction in the Hubbard model. In the present paper, this group of questions is not discussed, and we merely calculate the excitation spectrum of quasiparticle states of systems within the framework of the method of irreducible Green's functions, which gives a self-consistent scheme of systematic construction of generalized interpolation solutions of the Hubbard Hamiltonian valid in a wide range of z.

The construction of the mass operator is based on the introduction of irreducible parts for the Green's function $G_{ij\sigma}(t)=\langle\langle a_{i\sigma}(t);\ a_{j\sigma}^{+}\rangle\rangle$, which is written in the form

$$G_{ij\sigma}(\omega)=\langle\langle a_{i\sigma}|a_{j\sigma}^{+}\rangle\rangle_{\omega}=\sum_{\alpha\beta}\langle\langle d_{i\alpha\sigma}|d_{j\beta\sigma}^{+}\rangle\rangle_{\omega}=\sum_{\alpha\beta}G_{ij\sigma}^{\alpha\beta}(\omega),\quad d_{i\alpha\sigma}\equiv n_{i-\sigma}^{\alpha}a_{i\sigma}(\alpha=\pm),\ n_{i\sigma}^{+}=n_{i\sigma};\ n_{i\sigma}^{-}=(1-n_{i\sigma}),\tag{31}$$

where $G_{i,\sigma}^{\alpha\beta}$ is the matrix Green's function

$$\overline{G}_{ij\sigma}(\omega)=\langle\langle\begin{pmatrix}d_{i+\sigma}\\ d_{i-\sigma}\end{pmatrix}|(d_{j+\sigma}^{+}d_{j-\sigma}^{+})\rangle\rangle_{\omega}=\begin{bmatrix}\langle\langle d_{i+\sigma}|d_{j+\sigma}^{+}\rangle\rangle & \langle\langle d_{i+\sigma}|d_{j-\sigma}^{+}\rangle\rangle\\ \langle\langle d_{i-\sigma}|d_{j+\sigma}^{+}\rangle\rangle & \langle\langle d_{i-\sigma}|d_{j-\sigma}^{+}\rangle\rangle\end{bmatrix},\tag{32}$$

the equation of motion for its components having the form

$$(\omega-E_{\alpha})G_{ij\sigma}^{\alpha\beta}(\omega)=\delta_{ij}\delta_{\alpha\beta}n_{-\sigma}^{\alpha}+\sum_{l\neq i}t_{il}\langle\langle n_{i-\sigma}^{\alpha}a_{l\sigma}+\alpha a_{i\sigma}b_{il,-\sigma}|d_{j\beta\sigma}^{+}\rangle\rangle_{\omega}.\tag{33}$$

Introducing the matrix notation

$$\overline{E}=\begin{bmatrix}(\omega-E_{+}) & 0\\ 0 & (\omega-E_{-})\end{bmatrix}\ \text{and}\ \overline{\Phi}=\begin{bmatrix}n_{-\sigma}^{+} & 0\\ 0 & n_{-\sigma}^{-}\end{bmatrix},\tag{34}$$

we rewrite Eq. (33) in the form

$$\{\overline{E}\overline{G}_{ij\sigma}(\omega)-\overline{\Phi}\delta_{ij}\}_{\alpha\beta}=\sum_{l\neq i}t_{il}\langle\langle n_{i-\sigma}^{\alpha}a_{l\sigma}+\alpha a_{i\sigma}b_{il,-\sigma}|d_{j\beta\sigma}^{+}\rangle\rangle_{\omega}.\tag{35}$$

By definition, we now introduce the matrix irreducible Green's function $\overline{D}_{il}^{\,\mathrm{ir}}(\omega)$:

$$\overline{D}_{il}^{\,\mathrm{ir}}(\omega)=\begin{bmatrix}\langle\langle n_{i-\sigma}^{+}a_{l\sigma}+a_{i\sigma}b_{il,-\sigma}|d_{j+\sigma}^{+}\rangle\rangle & \langle\langle n_{i-\sigma}^{+}a_{l\sigma}+a_{i\sigma}b_{il,-\sigma}|d_{j-\sigma}^{+}\rangle\rangle\\ \langle\langle n_{i-\sigma}^{-}a_{l\sigma}-a_{i\sigma}b_{il,-\sigma}|d_{j+\sigma}^{+}\rangle\rangle & \langle\langle n_{i-\sigma}^{-}a_{l\sigma}-a_{i\sigma}b_{il,-\sigma}|d_{j-\sigma}^{+}\rangle\rangle\end{bmatrix}-\sum_{\alpha'}\left\{\begin{bmatrix}A_{il}^{+\alpha'}\\ A_{il}^{-\alpha'}\end{bmatrix}\times[G_{ij\sigma}^{\alpha'}G_{ij\sigma}^{\alpha'}]-\begin{bmatrix}B_{li}^{+\alpha'}\\ B_{li}^{-\alpha'}\end{bmatrix}\times[G_{lj\sigma}^{\alpha'}G_{lj\sigma}^{\alpha'}]\right\}.\tag{36}$$

The coefficients $\overline{A}_{il}$ and $\overline{B}_{li}$ are determined from the condition

$$\langle[\{\overline{D}_{il}^{\,\mathrm{ir}}\}_{\alpha\beta},\ d_{j\beta\sigma}]_{+}\rangle\equiv 0.\tag{37}$$

Calculating the corresponding commutators in (37) and equating the terms proportional to δ_{ij} and δ_{jl}, respectively, we obtain ($i\neq l$)

$$\{\overline{A}_{il}\}_{\alpha\beta}=\alpha(\langle d_{i\beta-\sigma}a_{l-\sigma}\rangle+\langle d_{i-\beta-\sigma}a_{l-\sigma}^{+}\rangle)(n_{-\sigma}^{\beta})^{-1},\quad\{\overline{B}_{li}\}_{\alpha\beta}=\{\langle n_{l-\sigma}^{\beta}n_{i-\sigma}^{\alpha}\rangle+\alpha\beta(\langle a_{i\sigma}a_{i-\sigma}^{+}a_{l-\sigma}a_{l\sigma}^{+}\rangle-\langle a_{i\sigma}a_{i-\sigma}a_{l-\sigma}^{+}a_{l\sigma}^{+}\rangle)\}(n_{-\sigma}^{\beta})^{-1}.\tag{38}$$

The part of the higher Green's function that we have expressed in terms of the original Green's functions can be conveniently expressed by means of the zeroth-order Green's function containing all renormalizations of the average field:

$$\{\bar{E}\bar{G}_{0ij}-\Phi\delta_{ij}\}_{\alpha\beta}=\sum_{l\alpha'}t_{il}\left\{\begin{bmatrix}A_{il}^{+\alpha'}\\A_{il}^{-\alpha'}\end{bmatrix}\times[G_{0ij}^{\alpha'+}G_{0ij}^{\alpha'-}]-\begin{bmatrix}B_{li}^{+\alpha'}\\B_{li}^{-\alpha'}\end{bmatrix}\times[G_{0lj}^{\alpha'+}G_{0lj}^{\alpha'-}]\right\}. \tag{39}$$

By means of the Fourier transformation $\bar{G}_{0ij}=N^{-1}\sum_q\bar{G}_{0q}\exp[iq(R_i-R_j)]$ we can find the explicit form of the matrix $\bar{G}_{0q}$:

$$\begin{bmatrix}G_{0q}^{+\,+}(\omega) & G_{0q}^{+-}(\omega)\\ G_{0q}^{-+}(\omega) & G_{0q}^{--}(\omega)\end{bmatrix}=\begin{bmatrix}n_{-\sigma}^{+}b & n_{-\sigma}^{-}d\\ n_{-\sigma}^{+}c & n_{-\sigma}^{-}a\end{bmatrix}(ab-cd)^{-1}. \tag{40}$$

The coefficients a, b, c, d are equal to

$$\left.\begin{matrix}a\\b\end{matrix}\right\}=\left(\omega-E_{\pm}-N^{-1}\sum_{\tau}\varepsilon_{\tau}(A^{\pm\pm}(-\tau)-B^{\pm\pm}(\tau-q))\right),\ \left.\begin{matrix}c\\d\end{matrix}\right\}=N^{-1}\sum_{\tau}\varepsilon_{\tau}(A^{\mp\pm}(-\tau)-B^{\mp\pm}(\tau-q)). \tag{41}$$

Substituting (40) in (36), we obtain

$$\bar{G}_{q\sigma}(\omega)=\bar{G}_{0q}(\omega)+\bar{G}_{0q}(\omega)\bar{\Phi}^{-1}D_{1q}(\omega),\quad D_{1q}^{\alpha\beta}=\left\{\left\langle\!\left\langle\sum_{l}t_{il}D_{il,\alpha}^{1r}\middle|d_{j\beta\sigma}^{+}\right\rangle\!\right\rangle_{\omega}\right\}_{q}. \tag{42}$$

Thus, to obtain the Dyson equation we must calculate the matrix $\bar{D}_{1q}(\omega)$. For this, we differentiate this matrix Green's function with respect to the second time:

$$-i\frac{d}{dt}\left\langle\!\left\langle\sum_{l}t_{il}D_{il,\alpha}^{1r};\ d_{j\beta\sigma}^{+}(t)\right\rangle\!\right\rangle. \tag{43}$$

Separating now in Eq. (43) the Green's function irreducible with respect to the right-hand operators in the same way as in (36), we obtain the Dyson equation

$$\bar{G}_{q\rho}(\omega)=\bar{G}_{0q}(\omega)+\bar{G}_{0q}(\omega)\bar{M}_{q\sigma}(\omega)\bar{G}_{q}(\omega). \tag{44}$$

The mass operator has the form

$$\bar{M}_{q\sigma}(\omega)=\bar{P}_{q}^{c}(\omega)=\bar{\Phi}^{-1}\left\{\sum_{lm}t_{il}t_{mj}\langle\!\langle\bar{D}_{il}^{1r}|D_{mj}^{1r}\rangle\!\rangle_{\omega}^{c}\right\}_{q}\bar{\Phi}^{-1}. \tag{45}$$

The formal solution of the Dyson equation (44) has the form

$$\bar{G}_{q\sigma}(\omega)=\{\bar{G}_{0q}^{-1}(\omega)-\bar{M}_{q\sigma}(\omega)\}^{-1}=\frac{1}{\det(\bar{G}_{0q}^{-1}-\bar{M}_{q\sigma})}\begin{vmatrix}\left(\frac{b}{n_{-\sigma}^{-}}-M_{q\sigma}^{--}\right) & \left(\frac{d}{n_{-\sigma}^{+}}+M_{q\sigma}^{+-}\right)\\ \left(\frac{c}{n_{-\sigma}^{-}}+M_{q\sigma}^{-+}\right) & \left(\frac{a}{n_{-\sigma}^{+}}-M_{q\sigma}^{++}\right)\end{vmatrix}. \tag{46}$$

Thus, the problem of finding the Green's function $\bar{G}_{q\sigma}$ has been reduced to calculating the matrix elements $\bar{G}_{0q}^{-1}$ and $\bar{M}_{q\sigma}$.

6. We consider the zeroth-order Green's function (40). In accordance with (31), the total zeroth-order Green's function $G_{0\sigma}(q,\omega)$ is equal to

$$G_{0\sigma}(q,\omega)=(ab-cd)^{-1}(n_{-\sigma}^{-}a+n_{-\sigma}^{+}b+n_{-\sigma}^{-}d+n_{-\sigma}^{+}c)=$$

$$\frac{\omega-(n_{-\sigma}^{+}E_{-}+n_{-\sigma}^{-}E_{+})-\lambda(q)}{(\omega-E_{+}-n_{-\sigma}^{-}\lambda_{1}(q))(\omega-E_{-}-n_{-\sigma}^{+}\lambda_{2}(q))-n_{-\sigma}^{-}n_{-\sigma}^{+}\lambda_{3}(q)\lambda_{4}(q)}, \tag{47}$$

where

$$\lambda_{1\atop 2}(q)=\frac{1}{n_{-\sigma}^{\mp}}\sum_{\tau}\varepsilon_{\tau}(A^{\pm\pm}(\tau)-B^{\pm\pm}(\tau-q)),\quad \lambda_{3\atop 4}(q)=\frac{1}{n_{-\sigma}^{\mp}}\sum_{\tau}\varepsilon_{\tau}(A^{\pm\mp}(-\tau)-B^{\pm\mp}(\tau-q)),$$

$$\lambda(q)=(n_{-\sigma}^{-})^{2}(\lambda_{1}+\lambda_{3})+(n_{-\sigma}^{+})^{2}(\lambda_{2}+\lambda_{4}). \tag{48}$$

The Green's function of "zeroth" order (47) has a two-pole structure close to the Hubbard III solution [20] and Roth's solution [21, 22], but takes into account more accurately the nondiagonal matrix elements since it contains all renormalizations of the average field. In particular, the Hubbard III solution gives the local mass operator.

The equation for the poles of the Green's function (47) has the form

$$\left\{\left(\omega-E_{+}-N^{-1}\sum_{\tau}\varepsilon_{\tau}(A^{++}(-\tau)-B^{++}(\tau-q))\right)\left(\omega-E_{-}-N^{-1}\sum_{\tau}\varepsilon_{\tau}(A^{--}(-\tau)-B^{--}(\tau-q))\right)-\right.$$

$$\left.N^{-1}\sum_{\tau}\varepsilon_{\tau}(A^{-+}(-\tau)-B^{+-}(\tau-q))N^{-1}\sum_{\tau}\varepsilon_{\tau}(A^{+-}(-\tau)-B^{+-}(\tau-q))\right\}=0. \tag{49}$$

The spectrum of quasiparticle states consists of two branches:

$$\omega_{1,2}(q)=1/2\{(E_{+}+E_{-}+a_1+b_1)\pm[(E_{+}+E_{-}-a_1-b_1)^2-4cd]^{1/2}\},\quad a_1=\omega-E_{+}-a,\ b_1=\omega-E_{-}-b. \tag{50}$$

Thus, the spectral intensity of the zeroth-order Green's function has two peaks separated by the distance

$$\omega_1(q)-\omega_2(q)=\{(U-a_1-b_1)^2-cd\}^{1/2}\approx U\left(1-\frac{(a_1-b_1)}{U}\right)+O(z). \tag{51}$$

We now consider in more detail a comparison between our initial approximation (47) and the other well-known solutions of the Hubbard Hamiltonian in the case of strong correlation. For this, we rewrite $\bar{G}_{0q}(\omega)$ in the form

$$\bar{G}_{0q}(\omega)=\begin{bmatrix}\left\{\frac{a}{n_{-\sigma}^{+}}-\frac{db^{-1}c}{n_{-\sigma}^{+}}\right\}^{-1} & \frac{d}{a}\left\{\frac{b}{n_{-\sigma}^{-}}-\frac{da^{-1}c}{n_{-\sigma}^{-}}\right\}^{-1}\\ \frac{c}{b}\left\{\frac{a}{n_{-\sigma}^{+}}-\frac{db^{-1}c}{n_{-\sigma}^{+}}\right\}^{-1} & \left\{\frac{b}{n_{-\sigma}^{-}}-\frac{da^{-1}c}{n_{-\sigma}^{-}}\right\}^{-1}\end{bmatrix} \tag{52}$$

from which we obtain for the total zeroth-order Green's function

$$G_{0\sigma}(q,\omega)=\frac{n_{-\sigma}^{+}(1+c/b)}{a-db^{-1}c}+\frac{n_{-\sigma}^{-}(1+d/a)}{b-ca^{-1}d}\approx\frac{n_{-\sigma}^{-}}{\omega-E_{-}-n_{-\sigma}^{+}W_{q,-\sigma}^{-}}+\frac{n_{-\sigma}^{+}}{\omega-E_{+}-n_{-\sigma}^{-}W_{q,-\sigma}^{+}}, \tag{53}$$

where

$$n_{-\sigma}^{+}n_{-\sigma}^{-}W_{q,-\sigma}^{\pm}=N^{-1}\sum_{i\neq j}t_{ij}\exp[-iq(R_i-R_j)]\{(\langle a_{i-\sigma}^{+}n_{i\sigma}^{\mp}a_{j-\sigma}\rangle+\langle a_{i-\sigma}n_{i\sigma}^{\mp}a_{j-\sigma}^{+}\rangle)+(\langle n_{j-\sigma}^{\pm}n_{i-\sigma}^{\pm}\rangle+$$

$$\langle a_{i\sigma}a_{i-\sigma}^{+}a_{j-\sigma}a_{j\sigma}^{+}\rangle-\langle a_{i\sigma}a_{i-\sigma}a_{j-\sigma}^{+}a_{j\sigma}^{+}\rangle)\} \tag{54}$$

are the shifts for the upper and lower bands due to the correlation of the electrons. In this form, the solution (53) is very close to the solution obtained in the case of strong correlation by Roth's method [21, 22] and the method of moments [23, 24]. The expression (54) for the band shift obtained by the method of irreducible Green's functions coincides with the results obtained by these methods except that the band shift (54) is different for the upper and lower sub-bands and does not contain terms independent of the quasimomentum. The reason for this is that the expression (47) takes into account more accurately the nondiagonal structure of the solution since all the renormalizations of the average field are summed. Usually, in the atomic limit in Roth's method and the method of moments one retains in the band shift only the part that does not depend on the quasimomentum, which corresponds precisely to the neglect of the nonlocal terms.

In our approach, to obtain further approximate solutions from the representation (54) it is necessary to compare the collective correlation functions on the right-hand side of (54). For $z\to 0$ and $n_{\sigma}+n_{-\sigma}<1$ we can, following [25], assume that the correlation functions $\langle a_{i-\sigma}^{+}n_{i\sigma}^{\pm}a_{j-\sigma}\rangle$, $\langle a_{i-\sigma}n_{i\sigma}^{\pm}a_{j-\sigma}^{+}\rangle$, and $\langle a_{i\sigma}a_{j-\sigma}^{+}a_{j-\sigma}a_{j\sigma}^{+}\rangle$ are small. From (54) we then obtain the band shift

$$n_{-\sigma}^{+}n_{-\sigma}^{-}W_{q,-\sigma}^{\pm}=N^{-1}\sum_{i\neq j}t_{ij}\langle n_{j-\sigma}^{\pm}n_{i-\sigma}^{\pm}\rangle\exp[-iq(R_i-R_j)]. \tag{55}$$

The solution (55) goes over into the Hubbard I solution [7] if we make the additional approximation $\langle n_{j-\sigma}n_{i-\sigma}\rangle\approx n_{-\sigma}^{2}$; we then obtain

$$G_{\sigma\sigma}(q,\omega)\cong\frac{n_{-\sigma}}{\omega-U-\varepsilon_q n_{-\sigma}}+\frac{1-n_{-\sigma}}{\omega-\varepsilon_q(1-n_{-\sigma})} \tag{56}$$

Thus, the use of the representation (47) as the Green's function of the "zeroth" order makes it possible to obtain the well-known solutions of the Hubbard model as special cases; the conditions of applicability of these solutions are discussed in the quoted references. The approximations used in the present paper to obtain these solutions are always associated with the standard decoupling procedure that expresses the higher correlation functions in terms of the lower ones. Namely, the use of the method of two-time Green's function

makes it possible to see clearly what correlations are omitted in the total correlation function to obtain any particular well-known approximation, and this makes it possible to construct approximate solutions systematically. Note that the parameters $\lambda_i(q)$ in (48) do not depend on the frequency. Such a dependence, due to inelastic scattering processes, arises, as will be shown below, on account of the mass operator.

7. Let us consider the corrections due to the mass operator. The renormalized spectrum of the system will be given by the equation

$$\left\{\left(\frac{a}{n_{-\sigma}^{+}}M_{q\sigma}^{++}\right)\left(\frac{b}{n_{-\sigma}^{-}}-M_{q\sigma}^{--}\right)-\left(\frac{c}{n_{-\sigma}^{-}}+M_{q\sigma}^{+-}\right)\left(\frac{d}{n_{-\sigma}^{+}}+M_{q\sigma}^{+-}\right)\right\}=0, \tag{57}$$

and is essentially determined by the nature of the approximations used to calculate the mass operator. The total Green's function $G_\sigma(q, \omega)$ has the form

$$G_\sigma(q,\omega)=\frac{1}{\det(\bar{G}_{ij}^{-1}-\bar{M}_{q\sigma})}\left\{\frac{1}{n_{-\sigma}^{+}}(a-n_{-\sigma}^{+}M_{q\sigma}^{++})+\frac{1}{n_{-\sigma}^{-}}(b-n_{-\sigma}^{-}M_{q\sigma}^{--})+\frac{1}{n_{-\sigma}^{+}}(d+n_{-\sigma}^{+}M_{q\sigma}^{+-})+\right.$$

$$\left.\frac{1}{n_{-\sigma}^{-}}(c+n_{-\sigma}^{-}M_{q\sigma}^{-+})\right\}=[\omega-(n_{-\sigma}^{+}E_{-}+n_{-\sigma}^{-}E_{+})-\bar{\lambda}(q,\omega)]\cdot[(\omega-E_{+}-n_{-\sigma}^{-}\bar{\lambda}_1(q,\omega))(\omega-E_{-}-n_{-\sigma}^{+}\bar{\lambda}_2(q,\omega))-$$

$$n_{-\sigma}^{-}n_{-\sigma}^{+}\bar{\lambda}_3(q,\omega)\bar{\lambda}_4(q,\omega)]^{-1}, \tag{58}$$

where

$$\bar{\lambda}_1(q,\omega)=\lambda_1(q)-(n^{\pm}/n_{-\sigma}^{\mp})M_{q\sigma}^{\pm\pm}(\omega),\quad \bar{\lambda}_3(q,\omega)=\lambda_3(q)+(n_{-\sigma}^{\mp}/n_{-\sigma}^{\pm})M_{q\sigma}^{\pm\mp}(\omega),$$
$$\bar{\lambda}(q,\omega)=\lambda(q)+n_{-\sigma}^{+}n_{-\sigma}^{-}(M_{q\sigma}^{++}(\omega)+M_{q\sigma}^{--}(\omega)-M_{q\sigma}^{-+}(\omega)-M_{q\sigma}^{+-}(\omega)). \tag{59}$$

The corrections due to the mass operator occur in (59) as additive corrections, which is very convenient for estimating the contributions of different scattering effects. The solution (58) is an exact representation for the total Green's function $G_\sigma(q, \omega)$ of the Hubbard model. Here, no approximations have yet been made; all the average-field effects have merely been separated in the zeroth Green's function. The use of projection operators has made it possible to cast this exact representation in the two-pole form. Therefore, this representation is more convenient for obtaining approximate solutions in the region of strong correlation, where a decoupling into two sub-bands occurs. To find (58), we write the exact mass operator in terms of the correlation functions:

$$\{\bar{\Phi}\bar{M}_{q\sigma}\bar{\Phi}\}_{\alpha\beta}=\int_{-\infty}^{\infty}\frac{d\omega'}{\omega-\omega'}(e^{\omega'/\vartheta}+1)\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{i\omega' t}N^{-1}\sum_{ijlm}e^{-iq(R_l-R_j)}t_{il}t_{mj}\langle D_{mj,\beta}^{+1r}D_{il,\alpha}^{1r}(t)\rangle^{c}. \tag{60}$$

By introducing irreducible parts, we have separated all the equal-time pairings. As in the preceding case, we now perform the possible different-time pairings for the correlation function on the right-hand side of (60), obtaining

$$\langle D_{mj,\beta}^{+1r}D_{il,\alpha}(t)\rangle^{c}\approx\langle a_{m\sigma}^{+}a_{l\sigma}(t)\rangle\langle n_{j-\sigma}^{\beta}n_{i-\sigma}^{\alpha}(t)\rangle+\langle a_{m\sigma}^{+}n_{l-\sigma}^{\alpha}(t)\rangle\langle n_{j-\sigma}^{\beta}a_{l\sigma}(t)\rangle+\beta\langle b_{mj,-\sigma}^{+}a_{l\sigma}(t)\rangle\times$$
$$\langle a_{j\sigma}^{+}n_{i-\sigma}^{\alpha}(t)\rangle+\beta\langle b_{mj,-\sigma}^{+}n_{i-\sigma}^{\alpha}(t)\rangle\langle a_{j\sigma}^{+}a_{l\sigma}(t)\rangle+\alpha\langle a_{m\sigma}^{+}a_{i\sigma}(t)\rangle\langle n_{j-\sigma}^{\beta}b_{il,-\sigma}(t)\rangle+\alpha\langle a_{m\sigma}^{+}b_{il,-\sigma}(t)\rangle\times$$
$$\langle n_{j-\sigma}^{\beta}b_{il,-\sigma}(t)\rangle+\alpha\beta\langle b_{mj,-\sigma}^{+}a_{i\sigma}(t)\rangle\langle a_{j\sigma}^{+}b_{il,-\sigma}(t)\rangle+\alpha\beta\langle b_{mj,-\sigma}^{+}b_{il,-\sigma}(t)\rangle\langle a_{j\sigma}^{+}a_{i\sigma}(t)\rangle. \tag{61}$$

The quantities in (61) can be interpreted in the language of the theory of alloys as scattering corrections, resonance-broadening corrections, and interference corrections [10]. As an example, we calculate the simplest scattering correction, i.e., we shall assume that

$$\langle D_{mj,\beta}^{+1r}D_{il,\alpha}^{1r}\rangle\approx\langle a_{m\sigma}^{+}a_{l\sigma}(t)\rangle\langle n_{j-\sigma}^{\beta}n_{i-\sigma}^{\alpha}\rangle=\langle a_{m\sigma}^{+}a_{l\sigma}(t)\rangle\{n_{-\sigma}^{\beta}n_{-\sigma}^{\alpha}+K_{ij}^{\alpha\beta}(t)\},\quad K_{ij}^{\alpha\beta}(t)=\langle(n_{j-\sigma}^{\beta}-n_{-\sigma}^{\beta})(n_{i-\sigma}^{\alpha}(t)-n_{-\sigma}^{\alpha})\rangle. \tag{62}$$

The first term in Eq. (62) describes the scattering of quasiparticle excitations with spin σ in the average field, and the second the additional momentum transfer on scattering. For qualitative estimate of the second effect, we use, as in (29), the static approximation $K_{ij}^{\alpha\beta}(t)\approx K_{ij}^{\alpha\beta}(0)$. Substituting (62) in (60), we obtain

$$\{\bar{\Phi}\bar{M}_{q\sigma}\Phi\}_{\alpha\beta}=\int_{-\infty}^{\infty}\frac{d\omega'}{\omega-\omega'}(e^{\omega'/\vartheta}+1)\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{i\omega' t}N^{-1}\sum_{ijlm}\exp[-iq(R_i-R_j)]\times$$
$$t_{il}t_{mj}\int_{-\infty}^{\infty}d\omega_1 n(\omega_1)e^{i\omega_1 t}\left\{-\frac{1}{\pi}\operatorname{Im}G_{ml,\sigma}(\omega_1+i\varepsilon)\right\}(n_{-\sigma}^{\beta}n_{-\sigma}^{\alpha}+K_{ij}^{\alpha\beta}(0)). \tag{63}$$

Equations (63) and (58) are a self-consistent system of equations for the single-particle Green's function $G_{ij\sigma}(\omega)$. For a simple estimate, we take the expression (56) as initial approximation. We then have

$$\{\Phi\overline{M}_{q\sigma}\Phi\}_{\alpha\beta}\approx N^{-1}\sum_{q'}|\varepsilon_{q-q'}|^2\{K_{q'}{}^{\alpha\beta}+n_{-\sigma}{}^{\beta}n_{-\sigma}{}^{\alpha}\}\left\{\frac{n_{-\sigma}}{\omega-U-\varepsilon_{q-q'}n_{-\sigma}}+\frac{1-n_{-\sigma}}{\omega-\varepsilon_{q-q'}(1-n_{-\sigma})}\right\}. \quad (64)$$

On the basis of the mass operator (64), we can explicitly find the energy shift and damping due to inelastic scattering of quasiparticle excitations, which has significant advantages over [20], in which explicit calculation of the analytic form of the mass operator for different corrections was very difficult. Note that for the systematic construction of solutions it is necessary to calculate the collective correlation functions of the electron density, the spin density, and the pair density. We propose to consider this question separately.

8. Thus, in this paper, using the method of irreducible Green's functions, we have obtained for the mass operator the general expressions (14) and (60), which enable us to construct interpolation solutions of the Hubbard model systematically in a wide range of the parameter z from the atomic to the band limits. In particular, one can directly separate the approximations for the mass operator that do not violate the quasimomentum conservation law in the system. This is particularly important in the band limit, i.e., for the metallic phase [26]. Indeed, in the case of very weak correlation, when there is no decoupling into sub-bands, one can determine the Fermi surface in the manner of Luttinger [27]. If when ω tends to some fixed value ε_f the damping $\Gamma_{k\sigma}(\omega)=-\operatorname{Im}M_{k\sigma}(\omega+i\varepsilon)$ tends to zero, then

$$g_{k\sigma}(\omega)=\frac{\Gamma_{k\sigma}(\omega)}{[\omega-\varepsilon_{k\sigma}{}^{HF}-\Delta_{k\sigma}(\omega)]^2+\Gamma_{k\sigma}{}^2(\omega)}\approx\delta(\omega-\varepsilon_{k\sigma}{}^{HF}-\Delta_{k\sigma}(\varepsilon_f))|_{\omega\to\varepsilon_f}. \quad (65)$$

In the general case, the set of quasimomentum values k satisfying the equation

$$\varepsilon_f-\varepsilon_{k\sigma}{}^{HF}-\Delta_{k\sigma}(\varepsilon_f)=0, \quad (66)$$

belongs to a surface in the momentum space, which is called the Fermi surface of the interacting system [27]. In [26], Edwards and Hewson asserted that the Hubbard I solution does not enable one to introduce a well-defined Fermi surface because the mass operator does not contain a dependence on the quasimomentum. However, in our opinion, it is incorrect to speak of a Fermi surface of the interacting system in the sense of Luttinger [27] when there is a splitting into sub-bands. The finite lifetime of quasiparticles on the Fermi surface obtained by Edwards and Hewson for the Hubbard I solution indicates this. For the single-band solution of the Hubbard model in the band limit one can determine a well-defined Fermi surface for the local mass operator as well if the solution is constructed in such a way that the damping on the Fermi surface is zero. In this case, the quasimomentum-independent correction to (66) leads to a shift of the center of gravity and a deformation of the ideal Fermi sphere; a more accurate description of course requires allowance for the quasimomentum dependence. Our approach enables us, on the basis of the solution (14) in the band limit, to describe the case of nonsplit sub-bands and introduce a Fermi surface in a natural manner on the basis of the definition (66). For the mass operator in the binary approximation (18), the proof that a well-defined Fermi surface exists can be found in [28].

Thus, the self-consistent method developed here for constructing generalized interpolation solutions of the Hubbard model is very general, does not use a definite zeroth approximation, and makes it possible to calculate in a unified scheme the spectrum of quasiparticle excitations of the system in both the band and the atomic limit. It may be hoped that this method will be useful for the concrete systems for which the Hubbard model applies. For example, the results of [9] have already been used to investigate a Hubbard antiferromagnet [29], and also in some other problems.

I am grateful to N. M. Plakida and W. Goetz for helpful discussions.

LITERATURE CITED

1. N. N. Bogolyubov and S. V. Tyablikov, Dokl. Akad. Nauk SSSR, **126**, 53 (1959).
2. S. V. Tyablikov, Methods of Quantum Theory of Magnetism, Plenum Press, New York (1967).
3. N. M. Plakida, Teor. Mat. Fiz., **5**, 147 (1970).
4. N. M. Plakida, Fiz. Tverd. Tela (Leningrad), **14**, 2841 (1972).
5. N. M. Plakida, Phys. Lett. A, **43**, 481 (1973).
6. G. Konwent, N. M. Plakida, and F. Vukailovich, Preprint JINR R4-7145 [in Russian], Dubna (1973); Z. Petru and G. L. Mailyan, Preprint JINR R4-8893 [in Russian], Dubna (1975).
7. J. Hubbard, Proc. R. Soc. London, Ser.A, **276**, 1963).
8. D. I. Khomskii, Fiz. Met. Metalloved., **29**, 31 (1970).
9. A. L. Kuzemskii, Preprint JINR R4-7225 [in Russian], Dubna (1973).

10. A. L. Kuzemskii, Preprint JINR R17-9239 [in Russian], Dubna (1975).
11. A. L. Kuzemskii, Preprint JINR R17-10695 [in Russian], Dubna (1977).
12. W. D. Langer, Phys. Lett. A, **35**, 45 (1971).
13. N. M. Plakida and P. R. Rusek, Preprint JINR R4-8032 [in Russian], Dubna (1974).
14. R. M. White, The Quantum Theory of Magnetism, McGraw-Hill, New York (1970).
15. A. L. Kuzemskii, Acta Phys. Pol. A, **49**, 169 (1976).
16. K. S. Schönhammer, J. Phys. C, **7**, 3520 (1974).
17. K. Elk, Phys. Status Solidi, **64**, 489 (1974).
18. D. M. Esterling, Phys. Rev. B, **2**, 4686 (1970).
19. V. A. Kapustin, Fiz. Tverd. Tela (Leningrad), **16**, 804 (1974); Teor. Mat. Fiz., **21**, 118 (1974).
20. J. Hubbard, Proc. R. Soc. A, **281**, 401 (1964).
21. L. M. Roth, Phys. Rev., **184**, 451 (1969).
22. O. Krisement, Z. Phys., **270**, 383 (1974).
23. W. Holting, Z. Phys., **255**, 25 (1972).
24. O. K. Kalashnikov and E. S. Fradkin, Zh. Eksp. Teor. Fiz., **55**, 607 (1968); Teor. Mat. Fiz., **5**, 417 (1970).
25. R. A. Tahir-Kheli and H. S. Jarrett, Phys. Rev., **180**, 544 (1969).
26. D. M. Edwards and A. C. Hewson, Rev. Mod. Phys., **40**, 810 (1968).
27. J. M. Luttinger, Phys. Rev., **119**, 1153 (1960).
28. V. M. Galitskin, in: Application of the Methods of Quantum Field Theory to Many-Body Problems [in Russian], Atomizdat (1963).
29. E. V. Kuz'min and S. G. Ovchinnikov, Teor. Mat. Fiz., **31**, 379 (1977); Fiz. Tverd. Tela (Leningrad), **19**, 1127 (1977).

STOCHASTIC APPROACH AND FUNCTIONAL MODELS IN THE KINETIC THEORY OF GASES

O. A. Grechannyi

The stochastic approach [1] is applied to the theory of nonequilibrum processes in a correlated and fluctuating gas with binary collisions. Markov processes are considered that make it possible to treat in a unified manner the fluctuation and dissipation properties of a nonequilibrium system when its evolution is described on space-time scales characteristic of the kinetic theory. A nonlinear stochastic equation is obtained for the single-particle density that is suitable for describing large fluctuations in unstable and strongly correlated states of a nonequilibrium gas.

1. Introduction

Allowance for long-wavelength statistical connections in a rarefied nonequilibrium gas is necessary for the investigation of nonequilibrium fluctuations [2] and the description of the hydrodynamics of turbulent flows [3, 4, 5]. In the general case, the kinetic stage in the evolution of a monatomic gas with allowance for large-scale fluctuations in the approximation of binary collisions is described by a system of irreversible kinetic equations for the partial distribution functions [6, 7]:

$$\frac{\partial F_s}{\partial t}=\sum_{j=1}^{s}[H_1(x_j);F_s]+\sum_{i<j=1}^{s}J_{x_ix_j}[F_s]+n\sum_{j=1}^{s}\int dx_{s+1}J_{x_jx_{s+1}}[F_{s+1}]. \tag{1.1}$$

where

$$J_{x_j}=\int dx_iJ_{x_ix_j}=\int dx_iJ_{x_jx_i} \tag{1.2}$$

is the Boltzmann collision integral, $x_j = (\mathbf{r}_j, \mathbf{p}_j)$, H_1 is the single-particle Hamiltonian, N and V are the

Institute of Technical High-Temperature Physics, Academy of Sciences of the Ukrainian SSR. Translated from Teoreticheskaya i Matematicheskaya Fizika, Vol. 36, No. 2, pp. 224-239, August, 1978. Original article submitted June 17, 1977.

 0040-5779/78/3602-0702$07.50