Variational approach to the three-particle problem in the Hubbard model: an exact result

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The paper proposes a well-defined procedure, based on the steady-state principle, for linearizing equations of motion. The one-particle Green's function is obtained in the special case of a single flipped spin in the saturated ferromagnetic state (the three-particle problem). It is proved that irrespective of whether the initial (unperturbed) state is a tight binding band (the Bloch representation) or a two-level atomic system (the Hubbard representation), the results for the one-particle Green's function coincide for arbitrary values of the Hamiltonian constants and the electron concentration $n^{\uparrow}$. In the nontrivial limiting case $U=\infty$ this Green's function agrees with the exact result of J. Igarashi [J. Phys. Soc. Jpn. **54**, 260 (1985)] and A. E. Ruckenstein and S. Schmitt-Rink [Int. J. Mod. Phys. **3**, 1089 (1989)] based on the solution of the Faddeev equations.

1. INTRODUCTION

The recent progress in solving the problem of the ground state in the Hubbard model is due to the following results:

(a) Shastry, Krishnamurthy, and Anderson[1] considered the variational problem of the stability of the Stoner–Nagaoka phase (saturated ferromagnet, $U=\infty$) under a single spin flip. They established that such a system becomes unstable at a certain threshold hole concentration depending on the symmetry of the lattice.

(b) Igarashi[2] and Ruckenstein and Schmitt-Rink[3] used a reduced Hubbard Hamiltonian that allowed only for the interaction between an electron and an electron–hole pair with opposite spin. In such an approach the one-particle Green's function is linked to the three-particle Green's function, which in turn satisfies the Lippmann–Schwinger equation. This equation can be separated into two coupled equations (Faddeev equations) describing the scattering in the particle–particle (P–P) and particle–hole (P–h) channels. The equations have yet to be analyzed for the general case ($U\neq\infty$) (Ref. 2 contains only numerical analysis for the one-dimensional case). However, in the nontrivial limit $U=\infty$ the equations have been solved.[3]

In previous papers by the present author and Kuz'min[4,5] the starting point was the site (atomic) representation presupposing the use of Hubbard operators. In this approach a two-level system (ε_a,ε_a+U) was the initial (unperturbed) state, while the transfer integral $b(\mathbf{f}-\mathbf{f}')$ between two nearest atoms acted as the perturbation. The next step was to build a self-consistent kinematic field theory that generalized Nagaoka's assertions to the thermodynamic limit ($N\to\infty$) for macroscopic deviations of the hole concentration from $h=0$. It was found that the resulting equations describe instability in the Stoner–Nagaoka phase at finite hole concentrations, $h\approx 0.2$, a result obtained by integration with a rectangular density of states $\rho=1/2W$. This agrees with the rigorous assertion made in Ref. 3.

In a later paper,[6] a result (which we feel is remarkable) was achieved: within the framework of the kinematic-field approximation in the region where $R=n^{\uparrow}-n^{\downarrow}=0$ ($0.7\leqslant n\leqslant 0$) holds the static susceptibility $\chi(0,0)$ was found to be negative at $U=\infty$?! This fact could indicate a singlet phase in the system.

But how well does the kinematic-field approximation describe physical processes in the region of intermediate and low energy concentrations, where the Bloch representation is the appropriate one? In this representation the unperturbed state is the quasiparticle spectrum calculated in the tight-binding approximation, $\varepsilon(\mathbf{k})=\Sigma_h b(\mathbf{h})\exp(i(\mathbf{kh}))$, and the Coulomb interaction U between two electrons with opposite spins at a single site acts as a perturbation.

The results obtained in this paper are:

(1) The procedure for linearizing equations of motion is substantiated from the standpoint of the steady-state principle.

(2) A one-particle Green's function for which the unperturbed state is the tight binding spectrum is found in the special case of a single "down" spin ($\downarrow$) in a saturated ferromagnetic state with an arbitrary concentration of "up" spins ($\uparrow$). At $U=\infty$ the Green's function coincides with the exact solution of Faddeev equations.

(3) The resulting Green's function is compared with the results of the kinematic-field theory (the atomic approach) and their full equivalence for any Hamiltonian constants and electron concentrations is established. This result, however, is restricted to the problem being considered.

2. THE VARIATIONAL PRINCIPLE AND THE ONE-PARTICLE GREEN'S FUNCTION

To find the "best" approximation for the Green's function, we must linearize the multiparticle equations of motion according to a variational principle. This means that in the class of quasiparticle states determined by the operator $A=\Sigma_i c_i a_i$, where $\{a_i\}$ is the base set of operators, the quasiparticle energy is found from the steady-state condition, i.e., the condition that variations of the energy $E=\langle[[A,H],A^{+}]_{\pm}\rangle$ vanish under variations of the c_i, where

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$(\delta c_i \equiv (\partial/\partial c_i)\delta c_i)$:

with the constraints $\langle [A,A^+]_\pm \rangle$:

$$\delta\langle [[AH],\ A^+]_\pm - \omega [AA^+]_\pm \rangle = 0. \tag{1}$$

where H the Hamiltonian of the system and ω is a Lagrange multiplier or, in the case at hand, the quasiparticle energy. From (1) it follows that

$$[AH] = \omega A. \tag{2}$$

If, in general, there is a set of operators A_i, the condition

$$\delta \left\langle [[A_i H], A_e^+]_\pm - \sum_j T_{ij} [A_j A_e^+]_\pm \right\rangle = 0, \tag{3}$$

involving the variations in energy $E_{ie} = \langle [[A_i,H], A_e^+]_\pm \rangle$ and the constraints $\langle [A_j,A_e^+]_\pm \rangle$ leads to the following generalization of Eq. (2):

$$[A_i,H] = \sum_j T_{ij} A_j. \tag{4}$$

where T_{ij} is a matrix Lagrange multiplier. If Eq. (4) is obtained, diagonalizing T_{ij} yields the energy of an excited quasiparticle state.

Strictly speaking, the steady-state condition, Eqs. (1) and (3), is the necessary condition for the energy minimum, but the expected value of ω may coincide with the exact value. Ideas concerning the connection between Eq. (4) and the steady-state condition were first expounded in Ref. 7.

The Hubbard Hamiltonian in the Bloch representation has the form:

$$\mathcal{H} = \sum_{k\sigma} \varepsilon(k) c_{k\sigma}^+ c_{k\sigma} + \frac{U}{N} \sum_{p_1,p_2,q} c_{p_1+q\downarrow}^+ c_{p_2-q\uparrow}^+ c_{p_2\uparrow} c_{p_1\downarrow}. \tag{5}$$

Let us examine the problem of a single flipped spin ($\downarrow$) propagating in a Stoner–Nagaoka state (saturated ferromagnetism). First we note that the Green's function for an "up" spin ($\uparrow$) in this case has the simple form

$$\ll c_{k\uparrow};\ c_{k'\uparrow}^+ \gg_\omega = \delta_{kk'} G_{k\uparrow}(\omega) = \delta_{kk'}/(\omega - \varepsilon(k) + i0). \tag{6}$$

We begin the calculation of $G_{k\downarrow}(\omega)$ from the exact equation of motion for the fermion operator $c_{k\downarrow}$:

$$[c_{k\downarrow} H] = (\varepsilon(k) + Un^\uparrow) c_{k\downarrow} + \frac{U}{N} \sum_{k'q}{}' R_k^\downarrow(k'q), \tag{7}$$

$$n^\uparrow = \frac{1}{N} \sum_p n_p{}^\uparrow, \tag{8}$$

where in (7) we have written the Stoner factor $Un^\uparrow$ explicitly, and $R_k^\downarrow(k',q)$ is the "elementary" annihilation operator for a three-particle excitation in an intermediate state of the system,

$$R_k^\downarrow(k',q) = c_{k'\uparrow}^+ c_{q\uparrow} c_{k+k'-q\downarrow}, \qquad k' \neq q. \tag{9}$$

For the basis $\{A_i\}$ for the variational solution we take the one-fermion operator $C_{k\downarrow}$ and the "collective" operator $\Sigma'_{k'q} R_k^\downarrow(k',q)$, where k' and q assume their values inside and outside the Fermi surface, respectively. It can easily be verified that

$$\langle F|\{R_k^\downarrow(k',q),\ c_{k\downarrow}^+\}|F\rangle = 0, \quad c_{k\downarrow}|F\rangle = R_k^\downarrow(k',q)|F\rangle = 0, \tag{10}$$

$$\langle F|\{R_k^\downarrow(k',q),\ R_{k''}^{\downarrow+}(k'',q')\}|F\rangle = \delta_{k'k''}\delta_{qq'} f_{k'}{}^\uparrow (1-f_q{}^\uparrow), \tag{11}$$

where $f_p^\uparrow = \langle F|n_p^\uparrow|F\rangle$, and $|F\rangle$ is a Stoner–Nagaoka state ($|\ \rangle$ in what follows).

In accordance with Eq. (4), we seek an expression for $[c_{k\downarrow},H]$ in the form

$$[c_{k\downarrow} H] = T_{11}(k) c_{k\downarrow} + T_{12} \sum_{k'q}{}' R_k^\downarrow(k',q). \tag{12}$$

Using the properties (10) and (11) and Eq. (7), we obtain

$$T_{11}(k) = \langle\{[c_{k\downarrow}H],\ c_{k\downarrow}^+\}\rangle = \varepsilon_k + U\langle n^\uparrow\rangle, \tag{13}$$

$$T_{12} = \frac{\sum_{k'',q'}{}' \langle\{[c_{k\downarrow}H], R_{k''}^{\downarrow+}(k'',q')\}\rangle}{\sum_{k'q}{}' \sum_{k''q'}{}' \langle\{R_k^\downarrow(k',q), R_{k''}^{\downarrow+}(k'',q')\}\rangle} = \frac{U}{N}. \tag{14}$$

Thus, the linearized equation (12) is identical with the exact equation (7) in which the Stoner factor is averaged over the ground state, $Un^\uparrow \to U\langle n^\uparrow\rangle$.

The equation of motion for $R_k^\downarrow(k',q)$ has the form

$$[R_k^\downarrow(k',q), H] = \Omega_k(k',q,U) R_k^\downarrow(k',q) + \frac{U}{N}(c_{k'\uparrow}^+ c_{q\uparrow} R_{k'+k-q}^\downarrow + c_{k'\uparrow}^+ R_q{}^\uparrow c_{k+k'-q'} - R_{k'}^{\uparrow+} c_{q\uparrow} c_{k+k'-q\downarrow}), \tag{15}$$

$$\Omega_k(k',q,U) = \Omega_k(k',q) + Un^\uparrow,$$

$$\Omega_k(k',q) = \varepsilon(k+k'-q) + \varepsilon(q) - \varepsilon(k'),$$

$$R_k^{\downarrow(\uparrow)} = \sum_{k'q}{}' R_k^{\downarrow(\uparrow)}(k',q). \tag{16}$$

Note that the last two terms on the right-hand side of (15) are annihilation operators for a five-particle excitation in the intermediate state with two flipped spins. The dynamics of such excited states is, obviously, "cut out" from the linearized equation of motion in terms of the chosen basis. Indeed, according to Eq. (4), the equations for $[R_k^\downarrow(k',q),H]$ are found in the form

$$[R_k^\downarrow(k',q), H] = T_{21}(k',q) c_{k\downarrow} + T_{22}(k) \sum_{k'',q'}{}' R_k^\downarrow(k'',q'). \tag{17}$$

After calculations similar to (13) and (14) we get

$$T_{21}(k',q) = \frac{U}{N} f_{k'}{}^\uparrow (1-f_q{}^\uparrow), \tag{18}$$

$$T_{22}(k)=\frac{1}{\langle n^{\uparrow}\rangle\langle 1-n^{\uparrow}\rangle}\frac{1}{N^2}\sum_{k'',q}{}'$$

$$\times\Big[\delta_{k'k''}\delta_{qq'}\Omega_k(k',q,U)f_{k'}{}^{\uparrow}(1-f_q{}^{\uparrow})$$

$$+\frac{U}{N}(\delta_{k'k''}f_{k'}{}^{\uparrow}(1-f_q{}^{\uparrow})(1-f_{q'}{}^{\uparrow})-\delta_{qq'}f_{k'}{}^{\uparrow}f_{k''}{}^{\uparrow}(1-f_q{}^{\uparrow}))\Big]. \tag{19}$$

To find $G_{k\downarrow}(\omega)$ we will need Eq. (17) summed over k' and q, that is,

$$[R_k{}^{\downarrow}H]=UN\langle n^{\uparrow}\rangle\langle 1-n^{\uparrow}\rangle c_{k\downarrow}+(U\langle 1-n^{\uparrow}\rangle+\bar{\Omega}_k)R_k{}^{\uparrow}, \tag{20}$$

where

$$\bar{\Omega}_k=\frac{1}{\langle n^{\uparrow}\rangle\langle 1-n^{\uparrow}\rangle}\frac{1}{N^2}\sum_{k'q}{}'\Omega_k(k',q)f_{k'}{}^{\uparrow}(1-f_q{}^{\uparrow}) \tag{21}$$

is the three-particle excitation energy averaged over all electron and hole states. As a result we get

$$[\omega-\varepsilon(k)-\Sigma_{\downarrow}^{var}(k,\omega)]G_{k\downarrow}(\omega)=1,$$

$$\Sigma_{\downarrow}^{var}(k,\omega)=U\langle n^{\uparrow}\rangle\Big[1+\frac{U\langle 1-n^{\uparrow}\rangle}{\omega-U\langle 1-n^{\uparrow}\rangle-\bar{\Omega}_k}\Big]. \tag{22}$$

3. COMPARISON WITH OTHER RESULTS

The one-particle Green's function in the kinematic-field (*kf*) approximation, where we start from the atomic representation, can be transformed into[4,5]

$$[\omega-\varepsilon(k)-\Sigma_{\downarrow}^{kf}(k,\omega)]G_{k\downarrow}(\omega)=1, \tag{23}$$

$$\Sigma_{\downarrow}^{kf}(k,\omega)=U\langle n^{\uparrow}\rangle\Big[1+\frac{U\langle 1-n^{\uparrow}\rangle}{\omega-U\langle 1-n^{\uparrow}\rangle-\Omega_{\uparrow}(k)}\Big], \tag{24}$$

$$\langle n^{\uparrow}\rangle\langle 1-n^{\uparrow}\rangle\Omega_{\uparrow}(k)=\varepsilon(k)K_{\uparrow}-W\Delta_{\uparrow}, \tag{25}$$

$$K_{\uparrow}=\langle n_0{}^{\uparrow}n_h{}^{\uparrow}\rangle-\langle n^{\uparrow}\rangle^2+\langle c_{h\uparrow}{}^{+}c_{h\downarrow}c_{0\downarrow}{}^{+}c_{0\uparrow}\rangle-\langle c_{h\uparrow}{}^{+}c_{h\downarrow}{}^{+}c_{0\downarrow}c_{0\uparrow}\rangle, \tag{26}$$

$$\Delta_{\uparrow}=\langle c_{0\uparrow}{}^{+}n_0{}^{\downarrow}c_{h\uparrow}\rangle-\langle c_{h\uparrow}{}^{+}c_{0\uparrow}(1-n_0{}^{\downarrow})\rangle. \tag{27}$$

In the Stoner–Nagaoka phase, after a Fourier transformation, Eq. (25) assumes the form

$$\langle n^{\uparrow}\rangle\langle 1-n^{\uparrow}\rangle\Omega_{\uparrow}(k)=-\frac{1}{N}\sum_{k'}\varepsilon(k')f_{k'}{}^{\uparrow}$$

$$+\frac{1}{N^2}\sum_{k'q}\varepsilon(k+k'-q)f_{k'}{}^{\uparrow}(1-f_q{}^{\uparrow}). \tag{28}$$

Comparing (21) with (28), we see that

$$\Sigma_{\downarrow}^{kf}(k,\omega)=\Sigma_{\downarrow}^{var}(k,\omega) \tag{29}$$

valid for all values of the constants in the Hamiltonian (5) and of the electron concentrations $n^{\uparrow}$.

The importance of this result is also seen from the fact that at $U\to\infty$ the self-energy part (29) coincides with the exact solution obtained by Igarashi[1] and Ruckenstein and Schmitt-Rink[2]; specifically,

$$\Sigma_{U=\infty}^{kf}(k,\omega)=\Sigma_{U=\infty}^{var}(k,\omega)=\Sigma_{U=\infty}^{exact}(k,\omega)=-\frac{\langle n^{\uparrow}\rangle}{\langle 1-n^{\uparrow}\rangle}\omega$$

$$+\frac{1}{(\langle 1-n^{\uparrow}\rangle N)^2}\sum_{k'q}\Omega_k(k',q)f_{k'}{}^{\uparrow}(1-f_q{}^{\uparrow}). \tag{30}$$

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