Strong-coupling approach for strongly correlated electron systems

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A perturbation theory scheme in terms of electron hopping, which is based on the Wick theorem for Hubbard operators, is developed. Diagrammatic series contain single-site vertices connected by hopping lines and it is shown that for each vertex the problem splits into the subspaces with ''vacuum states'' determined by the diagonal Hubbard operators and only excitations around these vacuum states are allowed. The rules to construct diagrams are proposed. In the limit of infinite spatial dimensions the total auxiliary single-site problem exactly splits into subspaces that allows to build an analytical thermodynamically consistent approach for a Hubbard model. Some analytical results are given for the simple approximations when the two-pole (alloy-analogy solution) and four-pole (Hartree-Fock approximation) structure for Green's function is obtained. Two poles describe contribution from the Fermi-liquid component, which is dominant for small electron and hole concentrations (''overdoped case'' of high-T_c's), whereas other two describe contribution from the non-Fermi liquid and are dominant close to half-filling (''underdoped case'').

I. INTRODUCTION

Many unconventional properties [e.g., metal-insulator transition, electronic (anti)ferromagnetism] of the narrow-band systems (transition metals and their compounds, some organic systems, high-T_c superconductors, etc.) can be explained only by the proper treatment of the strong local electron correlations. The simplest models allowing for the electron correlations are a single-band Hubbard model with on-site repulsion U and hopping energy t and its strong-coupling limit ($U \gg t$): t-J model. Recent studies of the Hubbard-type models connected mainly with the theory of high-T_c superconductivity and performed in the weak- ($U \leqslant 4t$) and strong- ($U \gg t$) coupling limits, elucidate some important features of these models.[1] But still a lot of problems remains, especially for the $U \gg t$ case where there are no rigorous approaches.

Such approaches can be built using systematic perturbation expansion in terms of the electron hopping[2] using diagrammatic technique for Hubbard operators.[3,4] One of them was proposed for the Hubbard ($U=\infty$ limit) and t-J models.[5,6] The lack of such approach is connected with the concept of a ''hierarchy'' system for Hubbard operators when the form of the diagrammatic series and final results strongly depend on the system of the pairing priority for Hubbard operators. On the other hand it is difficult to generalize it on the case of the arbitrary U.

In the last decade the essential achievements in the theory of the strongly correlated electron systems are connected with the development of the dynamical mean-field theory (DMFT) proposed by Metzner and Vollhardt[7] for the Hubbard model (see also Ref. 8 and references therein). DMFT is a nonperturbative scheme that allows to project the Hubbard model on the single impurity Anderson model and is exact in the limit of infinite space dimensions ($d=\infty$). There are no restrictions on the U value within this theory and it turns out to be useful for intermediate coupling ($U \sim t$) for which it ensures the correct description of the metal-insulator phase transition and determines the region of the Fermi-liquid behavior of the electron subsystem. Moreover, some class of the binary-alloy-type models (e.g., the Falicov-Kimball model) can be studied almost analytically within DMFT.[9] But in the case of the Hubbard model, the treatment of the effective single impurity Anderson model is very complicated and mainly computer simulations [exact diagonalization of the finite-sized systems or quantum Monte Carlo (QMC)] are used, which calls for the development of the analytical approaches.

The first analytical approximation proposed for the Hubbard model was a simple Hubbard-I approximation[10] (see Ref. 11 for its possible improvement) which is correct in the atomic ($t=0$) and band ($U=0$) limits but is inconsistent in the intermediate cases and cannot describe metal-insulator transition. Hubbard's alloy-analogy solution[12] (so-called Hubbard-III approximation) incorporates into the theory an electron scattering on the charge and spin fluctuations that allows us to give qualitative description of the changes of the density-of-state at the metal-insulator transition point. Hubbard-I and Hubbard-III approximations introduces two types of particles (electrons moving between empty sites and electrons moving between sites occupied by electrons of opposite spin) with the different energies that differ by U and form two Hubbard bands. Related schemes of the so-called two-pole approximations,[13,14] which are justified by the $t/U \ll 1$ perturbation theory expansions,[15] are also considered. However, in the recent QMC studies[16,17] it is clearly distinguished four bands in the spectral functions rather than the two bands predicted by the two-pole approximations. Such four-band structure is reproduced by the strong-coupling expansion for the Hubbard model[17] in the one-dimensional case. Within other approaches let us mention non-crossing approximation,[18,19] Edwards-Hertz approach,[20,21] iterative perturbation theory,[22,23] alloy-analogy based approaches,[24,25] and linked cluster expansions,[26,27] which are reliable in certain limits and the construction of the thermodynamically consistent theory still remains open.[28]

The aim of this paper is to develop for Hubbard-type models a rigorous perturbation theory scheme in terms of electron hopping that is based on the Wick theorem for Hubbard operators[3,4] and is valid for arbitrary value of U ($U < \infty$) and does not depend on the ''hierarchy'' system for X operators. In the limit of infinite spatial dimensions, these

analytical schemes allow us to build a self-consistent Kadanoff-Baym type theory[29] for the Hubbard model and some analytical results are given for simple approximations. The Falicov-Kimball model is also considered as an exactly soluble limit of Hubbard model.

II. PERTURBATION THEORY IN TERMS OF ELECTRON HOPPING

We consider the lattice electronic system that can be described by the following statistical operator:

$$\hat{\rho}=e^{-\beta\hat{H}_0}\hat{\sigma}(\beta), \tag{2.1}$$

$$\hat{\sigma}(\beta)=T\exp\left\{-\int_0^\beta d\tau\int_0^\beta d\tau' \times\sum_{ij\sigma} t_{ij}^{\sigma}(\tau-\tau')a_{i\sigma}^{\dagger}(\tau)a_{j\sigma}(\tau')\right\},$$

where

$$\hat{H}_0=\sum_i \hat{H}_i \tag{2.2}$$

is a sum of the single-site contributions and for the Hubbard model we must put

$$H_i=Un_{i\uparrow}n_{i\downarrow}-\mu(n_{i\uparrow}+n_{i\downarrow})-h(n_{i\uparrow}-n_{i\downarrow}),$$

$$t_{ij}^{\sigma}(\tau-\tau')=t_{ij}\delta(\tau-\tau'). \tag{2.3}$$

In addition for the Falicov-Kimball model we must also put

$$t_{ij}^{\sigma}(\tau-\tau')=\begin{cases} t_{ij}\delta(\tau-\tau') & \text{for } \sigma=\uparrow \\ 0 & \text{for } \sigma=\downarrow \end{cases}. \tag{2.4}$$

It is supposed that we know eigenvalues and eigenstates of the zero-order Hamiltonian (2.2),

$$H_i|i,p\rangle=\lambda_p|i,p\rangle \tag{2.5}$$

and one can introduce Hubbard operators

$$\hat{X}_i^{pq}=|i,p\rangle\langle i,q| \tag{2.6}$$

in terms of which zero-order Hamiltonian is diagonal

$$H_0=\sum_i\sum_p \lambda_p\hat{X}_i^{pp}. \tag{2.7}$$

For the Hubbard model we have four states $|i,p\rangle=|i,n_{i\uparrow},n_{i\downarrow}\rangle$: $|i,0\rangle=|i,0,0\rangle$ (empty site), $|i,2\rangle=|i,1,1\rangle$ (double occupied site), $|i,\uparrow\rangle=|i,1,0\rangle$, and $|i,\downarrow\rangle=|i,0,1\rangle$ (sites with spin-up and spin-down electrons) with energies

$$\lambda_0=0,\ \lambda_2=U-2\mu,\ \lambda_\downarrow=h-\mu,\ \lambda_\uparrow=-h-\mu. \tag{2.8}$$

The connection between the electron operators and the Hubbard operators is the following:

$$n_{i\sigma}=X_i^{22}+X_i^{\sigma\sigma};\ \ a_{i\sigma}=X_i^{0\sigma}+\sigma X_i^{\bar{\sigma}2}. \tag{2.9}$$

Our aim is to calculate the grand canonical potential functional

$$\Omega=-\frac{1}{\beta}\ln \mathrm{Sp}\hat{\rho}=\Omega_0-\frac{1}{\beta}\ln\langle\hat{\sigma}(\beta)\rangle_0,$$

$$\Omega_0=-\frac{1}{\beta}\ln \mathrm{Sp}\, e^{-\beta H_0}, \tag{2.10}$$

single-electron Green functions

$$G_{ij\sigma}(\tau-\tau')=\langle Ta_{i\sigma}^{\dagger}(\tau)a_{j\sigma}(\tau')\rangle=\frac{\delta\Omega}{\delta t_{ij}^{\sigma}(\tau-\tau')} \tag{2.11}$$

and mean values

$$n_\sigma=\frac{1}{N}\sum_i\langle n_{i\sigma}\rangle=-\frac{1}{N}\frac{d\Omega}{d\mu_\sigma},$$

$$n=n_\uparrow+n_\downarrow;\ \ m=n_\uparrow-n_\downarrow, \tag{2.12}$$

where $\mu_\sigma=\mu+\sigma h$ is a chemical potential for the electrons with spin σ. Here, $\langle\ldots\rangle=(1/Z)\mathrm{Sp}(\ldots\hat{\rho})$, $Z=\mathrm{Sp}\,\hat{\rho}$, or in interacting representation

$$\langle\ldots\rangle=\frac{1}{\langle\hat{\sigma}(\beta)\rangle_0}\langle\ldots\hat{\sigma}(\beta)\rangle_0=\langle\ldots\hat{\sigma}(\beta)\rangle_{0c}, \tag{2.13}$$

where $\langle\ldots\rangle_0=(1/Z_0)\mathrm{Sp}(\ldots e^{-\beta H_0});\ Z_0=\mathrm{Sp}e^{-\beta H_0}$.

We expand the scattering matrix $\hat{\sigma}(\beta)$ in Eq. (2.1) into the series in terms of electron hopping and for $\langle\sigma(\beta)\rangle_0$ we obtain a series of terms that are products of the hopping integrals and averages of the electron creation and annihilation operators or, using Eq. (2.9), Hubbard operators that will be calculated with the use of the corresponding Wick's theorem.

Wick's theorem for Hubbard operators was formulated in Ref. 3 (see also Ref. 4 and references therein). For the Hubbard model we can define four diagonal Hubbard operators X^{pp} $(p=0,2,\downarrow,\uparrow)$ which are of bosonic type, four annihilation $X^{0\downarrow}$, $X^{0\uparrow}$, $X^{\uparrow 2}$, $X^{\downarrow 2}$ and four conjugated creation fermionic operators, and two annihilation $X^{\downarrow\uparrow}$, X^{02} and two conjugated creation bosonic operators. The algebra of $\hat{X}$ operators is defined by the multiplication rule

$$X_i^{rs}X_i^{pq}=\delta_{sp}X_i^{rq}, \tag{2.14}$$

the conserving condition

$$\sum_p X_i^{pp}=1, \tag{2.15}$$

and the commutation relations

$$[X_i^{rs},X_j^{pq}]_\pm=\delta_{ij}(\delta_{sp}X_i^{rq}\pm\delta_{rq}X_i^{ps}), \tag{2.16}$$

where one must use anticommutator when both operators are of the fermionic type and commutator in all other cases. So, commutator or anticommutator of two Hubbard operators is

not a *c* number but a new Hubbard operator. Then the average of a *T* products of *X* operators can be evaluated by the consecutive pairing, while taking into account standard permutation rules for bosonic and fermionic operators, of all off-diagonal Hubbard operators X^{pq} according to the rule (Wick's theorem)

$$\overbrace{X_i^{rs}(\tau_1)X_0^{pq}}(\tau) = -\delta_{0i}g_{pq}(\tau-\tau_1)[X_i^{rs}(\tau_1),X_i^{pq}(\tau_1)]_{\pm} \tag{2.17}$$

until we get the product of the diagonal Hubbard operators only. Here we introduce the zero-order Green's function

$$g_{pq}(\tau-\tau_1)=\frac{1}{\beta}\sum_n g_{pq}(\omega_n)e^{i\omega_n(\tau-\tau_1)} = e^{(\tau-\tau_1)\lambda_{pq}}\begin{cases}\pm n_{\pm}(\lambda_{pq}) & \tau>\tau_1\\ \pm n_{\pm}(\lambda_{pq})-1 & \tau<\tau_1,\end{cases} \tag{2.18}$$

where $\lambda_{pq}=\lambda_p-\lambda_q$ and $n_{\pm}(\lambda)=\dfrac{1}{e^{\beta\lambda}\pm 1}$, and its Fourier transform is equal

$$g_{pq}(\omega_n)=\frac{1}{i\omega_n-\lambda_{pq}}. \tag{2.19}$$

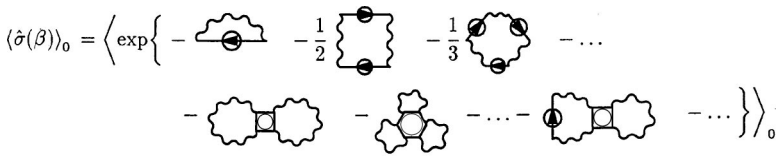
In particular, for the Hubbard model one can introduce the following pairings:

$$\begin{aligned}
&\overbrace{a_{i\sigma}(\tau_1)a_{j\sigma}^{\dagger}}(\tau) = -\delta_{ij}\{g_{\sigma 0}(\tau-\tau_1)(X_i^{00}(\tau_1)+X_i^{\sigma\sigma}(\tau_1))\\
&\qquad\qquad +g_{2\bar{\sigma}}(\tau-\tau_1)(X_i^{22}(\tau_1)+X_i^{\bar{\sigma}\bar{\sigma}}(\tau_1))\},\\
&\overbrace{a_{i\bar{\sigma}}(\tau_1)a_{j\sigma}^{\dagger}}(\tau) = -\delta_{ij}f_{\sigma}(\tau-\tau_1)X_i^{\sigma\bar{\sigma}}(\tau_1),\\
&\overbrace{a_{i\bar{\sigma}}^{\dagger}(\tau_1)a_{j\sigma}^{\dagger}}(\tau) = \delta_{ij}f_{\sigma}(\tau-\tau_1)\cdot\sigma\cdot X_i^{20}(\tau_1),\\
&\overbrace{a_{i\bar{\sigma}}^{\dagger}(\tau_1)X_j^{\sigma\bar{\sigma}}}(\tau) = \delta_{ij}g_{\sigma\bar{\sigma}}(\tau-\tau_1)a_{i\sigma}^{\dagger}(\tau_1),\\
&\overbrace{a_{i\sigma}(\tau_1)X_j^{\sigma\bar{\sigma}}}(\tau) = -\delta_{ij}g_{\sigma\bar{\sigma}}(\tau-\tau_1)a_{i\bar{\sigma}}(\tau_1),\\
&\overbrace{a_{i\sigma}(\tau_1)X_j^{20}}(\tau) = -\delta_{ij}g_{20}(\tau-\tau_1)\cdot\sigma\cdot a_{i\bar{\sigma}}^{\dagger}(\tau_1),
\end{aligned} \tag{2.20}$$

where

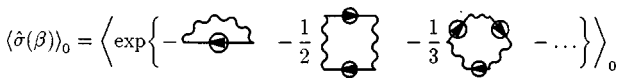
$$f_{\sigma}(\omega_n)\equiv g_{\sigma 0}(\omega_n)-g_{2\bar{\sigma}}(\omega_n)=-Ug_{\sigma 0}(\omega_n)g_{2\bar{\sigma}}(\omega_n). \tag{2.21}$$

Applying such pairing procedure to the expansion of $\langle\hat{\sigma}(\beta)\rangle_0$ we get the following diagrammatic representation:

$\langle\hat{\sigma}(\beta)\rangle_0 =$  (2.22)

where arrows denote the zero-order Green's functions (2.19), wavy lines denote hopping integrals and □, ... stay for some complicated ''*n* vertices,'' which for such type perturbation expansion are an irreducible many-particle single-site Green's functions calculated with single-site Hamiltonian (2.7). Each vertex (Green's function) is multiplied by a diagonal Hubbard operator denoted by a circle and one gets an expression with averages of the products of diagonal Hubbard operators.

For the Falicov-Kimball model, expression (2.22) reduces and contains only single loop contributions

$\langle\hat{\sigma}(\beta)\rangle_0 =$  (2.23)

where


$=\dfrac{\hat{P}_i^{\pm}}{i\omega_n+\mu^*\mp\dfrac{U}{2}}; \hat{P}_i^{+}=\hat{n}_{i\downarrow}; \hat{P}^{-}=1-\hat{n}_{i\downarrow}, \mu^*=\mu-(U/2)$

and by introducing pseudospin variables $S_i^z=\frac{1}{2}(\hat{P}_i^{+}-\hat{P}_i^{-})$ one can transform the Falicov-Kimball model into an Ising-type model with the effective multisite retarded pseudospin interactions. Expression (2.23) can be obtained from the statistical operator (2.1) by performing partial averaging over fermionic variables, which gives an effective statistical operator for pseudospins (ions).

So, after applying Wick's theorem our problem splits into two problems: (i) calculation of the irreducible many-particle Green's functions (vertices) in order to construct expression (2.22) and (ii) calculation of the averages of the products of diagonal Hubbard operators and summing up the resulting series.

III. IRREDUCIBLE MANY-PARTICLE GREEN'S FUNCTIONS

For the Hubbard model by applying the Wick theorem for *X* operators one gets for two-vertex


$= g_{\sigma 0}(\omega_n)(\hat{X}_i^{\sigma\sigma}+\hat{X}_i^{00}) + g_{2\bar{\sigma}}(\omega_n)(\hat{X}_i^{22}+\hat{X}_i^{\bar{\sigma}\bar{\sigma}}),$ (3.1)

for four-vertex

$$
\begin{aligned}
\omega_{n\sigma} \quad \omega_{n'\bar{\sigma}} \quad &= \hat{\Lambda}^{(4)}_{i\sigma\bar{\sigma}}(\omega_n, \omega_{n+m}, \omega_{n'+m}, \omega_{n'}) \\
\omega_{n+m\sigma} \quad \omega_{n'+m\bar{\sigma}} \quad &= \hat{X}^{00}_i g_{\sigma 0}(\omega_n) g_{\sigma 0}(\omega_{n+m}) \left(U + U^2 g_{20}(\omega_{n+n'+m})\right) g_{\bar{\sigma}0}(\omega_{n'}) g_{\bar{\sigma}0}(\omega_{n'+m}) \\
&+ \hat{X}^{22}_i g_{2\bar{\sigma}}(\omega_n) g_{2\bar{\sigma}}(\omega_{n+m}) \left(U - U^2 g_{20}(\omega_{n+n'+m})\right) g_{2\sigma}(\omega_{n'}) g_{2\sigma}(\omega_{n'+m}) \\
&+ \hat{X}^{\sigma\sigma}_i g_{\sigma 0}(\omega_n) g_{\sigma 0}(\omega_{n+m}) \left(U + U^2 g_{\sigma\bar{\sigma}}(\omega_{n-n'})\right) g_{2\sigma}(\omega_{n'}) g_{2\sigma}(\omega_{n'+m}) \\
&+ \hat{X}^{\bar{\sigma}\bar{\sigma}}_i g_{2\bar{\sigma}}(\omega_n) g_{2\bar{\sigma}}(\omega_{n+m}) \left(U - U^2 g_{\sigma\bar{\sigma}}(\omega_{n-n'})\right) g_{\bar{\sigma}0}(\omega_{n'}) g_{\bar{\sigma}0}(\omega_{n'+m}),
\end{aligned}
$$

$$
\hat{\Lambda}^{(4)}_{i\sigma\sigma}(\omega_n, \omega_{n+m}, \omega_{n'+m}, \omega_{n'}) \equiv 0 \tag{3.2}
$$

and so on. Expressions (3.1) and (3.2) and for the vertices of higher order possess one significant feature. They decompose into four terms with different diagonal Hubbard operators X^{pp}, which project our single-site problem on certain ''vacuum'' states (subspaces), and zero-order Green's functions, which describe all possible excitations and scattering processes around these ''vacuum'' states: i.e., creation and annihilation of single electrons and of the doublon (pair of electrons with opposite spins) for subspaces $p=0$ and $p=2$ and creation and annihilation of single electrons with appropriate spin orientation and of the magnon (spin flip) for subspaces $p=\uparrow$ and $p=\downarrow$.

In compact form expressions (3.1) and (3.2) can be written as

$$
\longrightarrow = \sum_p \hat{X}^{pp}_i g_{\sigma(p)}(\omega_n) \tag{3.3}
$$

and

$$
\begin{aligned}
= \sum_p \hat{X}^{pp}_i & g_{\sigma(p)}(\omega_n) g_{\sigma(p)}(\omega_{n+m}) \\
& \times \tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_l | \omega_m) g_{\bar{\sigma}(p)}(\omega_l) g_{\bar{\sigma}(p)}(\omega_{l+m}),
\end{aligned} \tag{3.4}
$$

where

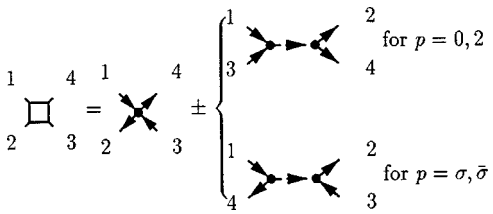
$$
g_{\sigma(p)}(\omega_n) = \begin{cases} g_{\sigma 0}(\omega_n) & \text{for } p = 0, \sigma \\ g_{2\bar{\sigma}}(\omega_n) & \text{for } p = \bar{\sigma}, 2. \end{cases} \tag{3.5}
$$

Here

$$
\tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_l | \omega_m) = \begin{cases} U \pm U^2 g_{20}(\omega_{n+l+m}) & \text{for } p = 0,2 \\ U \pm U^2 g_{\sigma\bar{\sigma}}(\omega_{n-l}) & \text{for } p = \sigma, \bar{\sigma}, \end{cases}
$$

$$
\tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_l | \omega_m) = \tilde{U}_{\bar{\sigma}\sigma(p)}(\omega_l, \omega_n | \omega_m) \tag{3.6}
$$

is a renormalized Coulombic interaction in the subspaces. In diagrammatic notations expressions (3.2) or (3.4) can be represented as



(3.7)

where dots denote Coulombic correlation energy $U=\lambda_2+\lambda_0-\lambda_\uparrow-\lambda_\downarrow$ and dashed arrows denote bosonic zero-order Green's functions: doublon $g_{20}(\omega_m)$ or magnon $g_{\sigma\bar{\sigma}}(\omega_m)$.

For six-verticies one can get

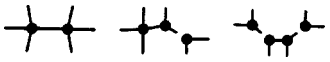
$$
\hat{\Lambda}^{(6)}_{i\sigma\sigma\sigma}(\omega_n, \omega_{n_1}, \omega_{n_2}, \omega_{n_3}, \omega_{n_4}, \omega_{n_5}) \equiv 0,
$$

$$
\begin{aligned}
\hat{\Lambda}^{(6)}_{i\sigma\sigma\sigma}(\omega_n, \omega_{n_1}, \omega_{n_2}, \omega_{n_3}, \omega_{n_4}, \omega_{n_5}) &= \delta(\omega_n - \omega_{n_1} + \omega_{n_2} - \omega_{n_3} + \omega_{n_4} - \omega_{n_5}) \\
&\times \sum_p \hat{X}^{pp}_i g_{\sigma(p)}(\omega_n) g_{\sigma(p)}(\omega_{n_1}) g_{\bar{\sigma}(p)}(\omega_{n_2}) g_{\bar{\sigma}(p)}(\omega_{n_3}) g_{\bar{\sigma}(p)}(\omega_{n_4}) g_{\bar{\sigma}(p)}(\omega_{n_5}) \\
&\times \{ \tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_{n_3} | \omega_{n_2 - n_3}) g_{\bar{\sigma}(p)}(\omega_{n+n_2-n_3}) \tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_{n_1}, \omega_{n_4} | \omega_{n_5 - n_4}) \\
&- \tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_{n_5} | \omega_{n_2 - n_5}) g_{\bar{\sigma}(p)}(\omega_{n+n_2-n_5}) \tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_{n_1}, \omega_{n_4} | \omega_{n_3 - n_4}) \\
&- \tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_{n_3} | \omega_{n_4 - n_3}) g_{\bar{\sigma}(p)}(\omega_{n+n_4-n_3}) \tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_{n_1}, \omega_{n_2} | \omega_{n_5 - n_2}) \\
&+ \tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_{n_5} | \omega_{n_4 - n_5}) g_{\bar{\sigma}(p)}(\omega_{n+n_4-n_5}) \tilde{U}_{\sigma\bar{\sigma}(p)}(\omega_{n_1}, \omega_{n_2} | \omega_{n_3 - n_2}) \\
&+ \Upsilon_{\sigma\bar{\sigma}\sigma(p)}(\omega_n, \omega_{n_1}, \omega_{n_2}, \omega_{n_3}, \omega_{n_4}, \omega_{n_5}) \},
\end{aligned} \tag{3.8}
$$

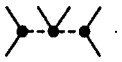
where

$$\Upsilon_{\sigma\sigma\overline{\sigma}(p)}(\omega_n,\omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4},\omega_{n_5})=\begin{cases}\pm U^3[g_{20}(\omega_{n+n_2})-g_{20}(\omega_{n+n_4})][g_{20}(\omega_{n_1+n_3})-g_{20}(\omega_{n_1+n_5})] & \text{for } p=0,2\\ \pm U^3[g_{\sigma\overline{\sigma}}(\omega_{n-n_3})-g_{\sigma\overline{\sigma}}(\omega_{n-n_5})][g_{\sigma\overline{\sigma}}(\omega_{n_1-n_2})-g_{\sigma\overline{\sigma}}(\omega_{n_1-n_4})] & \text{for } p=\sigma,\overline{\sigma}.\end{cases} \tag{3.9}$$

In expression (3.8) the contributions of the first four terms in braces can be presented by the following diagrams:

 (3.10)

with the internal vertices of the same type as in Eq. (3.7), whereas the contribution of the last term can be presented diagrammatically as

 (3.11)

So, we can introduce primitive vertices

 (3.12)

by which one can construct all n vertices in expansion (2.22) according to the following rules:

(1) n vertices are constructed by the diagonal Hubbard operator X^{pp} and zero-order fermionic and bosonic lines connected by primitive vertices (3.12) specific for each subspace p.

(2) External lines of n vertices must be of the fermionic type.

(3) Diagrams with the loops formed by zero-order fermionic and bosonic Green's functions are not allowed because they are already included into the formalism, e.g.,

gives

For n vertices of higher order a new primitive vertex can appear but we do not check this due to the rapid increase of the algebraic calculations with the increase of n. Diagrams (3.7), (3.10), and (3.11) topologically are truncated Bethe-lattices constructed by the primitive vertices (3.12) and can be treated as some generalization of the Hubbard stars[30,31] in the thermodynamical perturbation theory.

It should be noted that each n vertex contains Coulombic interaction U as in primitive vertices (3.12) (denoted by dots) as in the denominators of the zero-order Green's functions (2.19). In the $U\rightarrow\infty$ limit, each term in the expressions for n vertices can diverge but total vertex possesses finite $U\rightarrow\infty$ limit when diagrammatic series of Ref. 5 are reproduced.

The second problem of calculation of the averages of diagonal X operators is more complicated. One of the ways to solve it is to use semi-invariant (cumulant) expansions as was done in Refs. 5 and 6 for the $U=\infty$ limit. Another way is to consider the $d=\infty$ limit where new simplifications appear.

IV. DYNAMICAL MEAN-FIELD THEORY

Within the frames of the considered perturbation theory in terms of electron hopping a single-electron Green's function (2.11) can be presented in a form

$$G_\sigma(\omega_n,\mathbf{k})=\frac{1}{\Xi_\sigma^{-1}(\omega_n,\mathbf{k})-t_{\mathbf{k}}}, \tag{4.1}$$

where we introduce an irreducible part $\Xi_\sigma(\omega_n,\mathbf{k})$ of Green's function which, in general, is not local. In the case of infinite dimensions $d\rightarrow\infty$ one should scale the hopping integral according to

$$t_{ij}\rightarrow\frac{t_{ij}}{\sqrt{d}} \tag{4.2}$$

in order to obtain finite density of states and it was shown by Metzner in his pioneer work[26] that in this limit the irreducible part become local

$$\Xi_{ij\sigma}(\tau-\tau')=\delta_{ij}\Xi_\sigma(\tau-\tau') \quad \text{or} \quad \Xi_\sigma(\omega_n,\mathbf{k})=\Xi_\sigma(\omega_n) \tag{4.3}$$

and such a site-diagonal function, as it was shown by Brandt and Mielsch,[9] can be calculated by mapping the infinite-dimensional lattice problem (2.1) with $t_{ij}^\sigma(\tau-\tau')=1/\sqrt{d}\,t_{ij}\delta(\tau-\tau')$ on the atomic model with the auxiliary Kadanoff-Baym field

$$t_{ij}^\sigma(\tau-\tau')=\delta_{ij}J_\sigma(\tau-\tau'), \tag{4.4}$$

which has to be self-consistently determined from the condition that the same function $\Xi_\sigma(\omega_n)$ defines Green's functions for the lattice and atomic limit. The self-consistent set of equations for $\Xi_\sigma(\omega_n)$ and $J_\sigma(\omega_n)$ (e.g., see Ref. 8 and references therein) is the following:

$$\frac{1}{N}\sum_{\mathbf{k}}\frac{1}{\Xi_\sigma^{-1}(\omega_n)-t_{\mathbf{k}}}=\frac{1}{\Xi_\sigma^{-1}(\omega_n)-J_\sigma(\omega_n)}=G_\sigma^{(a)}(\omega_n,\{J_\sigma(\omega_n)\}), \tag{4.5}$$

where $G_\sigma^{(a)}(\omega_n,\{J_\sigma(\omega_n)\})$ is a Green's function for atomic limit (4.4).

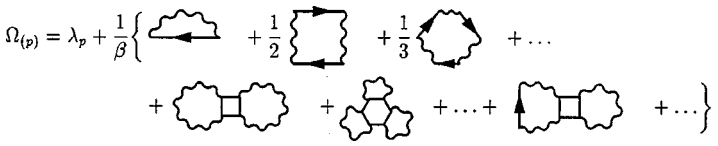
Grand canonical potential for lattice is connected with the one for atomic limit by the expression[9]

$$\frac{\Omega}{N}=\Omega_a-\frac{1}{\beta}\sum_{n\sigma}\left\{\ln G_\sigma^{(a)}(\omega_n)-\frac{1}{N}\sum_{\mathbf{k}}\ln G_\sigma(\omega_n,\mathbf{k})\right\}. \tag{4.6}$$

On the other hand, we can write for the grand canonical potential for atomic limit Ω_a the same expansion as in Eq. (2.22) but now we have averages of the products of diagonal X operators at the same site. According to Eq. (2.14) we can multiply them and reduce their product to a single X operator that can be taken outside of the brackets and exponent in (2.22) and its average is equal to $\langle X^{pp}\rangle_0=e^{-\beta\lambda_p}/\Sigma_q e^{-\beta\lambda_q}$. Finally, for the grand canonical potential for the atomic limit we get

$$\Omega_a=-\frac{1}{\beta}\ln\sum_p e^{-\beta\Omega_{(p)}}, \tag{4.7}$$

where



(4.8)

are the ''grand canonical potentials'' for the subspaces.

Now we can find single-electron Green's function for atomic limit by

$$G_\sigma^{(a)}(\tau-\tau')=\frac{\delta\Omega_a}{\delta J_\sigma(\tau-\tau')}=\sum_p w_p G_{\sigma(p)}(\tau-\tau'), \tag{4.9}$$

where

$$G_{\sigma(p)}(\tau-\tau')=\frac{\delta\Omega_{(p)}}{\delta J_\sigma(\tau-\tau')} \tag{4.10}$$

are single-electron Green functions for the subspaces characterized by the ''statistical weights''

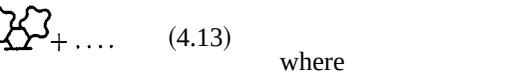
$$w_p=\frac{e^{-\beta\Omega_{(p)}}}{\sum_q e^{-\beta\Omega_{(q)}}} \tag{4.11}$$

and our single-site atomic problem exactly (naturally) splits into four subspaces $p=0,2,\downarrow,\uparrow$.

We can introduce irreducible parts of Green's functions in subspaces $\Xi_{\sigma(p)}(\omega_n)$ by

$$G_{\sigma(p)}(\omega_n)=\frac{1}{\Xi^{-1}_{\sigma(p)}(\omega_n)-J_\sigma(\omega_n)}, \tag{4.12}$$

where



(4.13)

According to the rules of the introduced diagrammatic technique, n vertices are terminated by the fermionic Green's functions [see diagrams (3.7), (3.10), and (3.11)] and this allows us to write a Dyson equation for the irreducible parts and to introduce a self-energy in subspaces

$$\Xi^{-1}_{\sigma(p)}(\omega_n)=g^{-1}_{\sigma(p)}(\omega_n)-\Sigma_{\sigma(p)}(\omega_n), \tag{4.14}$$

where self-energy

$$\Sigma_{\sigma(p)}(\omega_n)$$

depends on the hopping integral $J_{\sigma'}(\omega_{n'})$ only through quantities

$$\begin{aligned}\Psi_{\sigma'(p)}(\omega_{n'})&=G_{\sigma'(p)}(\omega_{n'})-\Xi_{\sigma'(p)}(\omega_{n'})\\&\equiv\Xi^2_{\sigma'(p)}(\omega_{n'})J_{\sigma'}(\omega_{n'})\\&\quad\times\{1+\Xi_{\sigma'(p)}(\omega_{n'})J_{\sigma'}(\omega_{n'})+\cdots\}.\end{aligned} \tag{4.15}$$

It should be noted, that the total self-energy of the atomic problem is connected with the total irreducible part by the expression

$$\Sigma_\sigma(\omega_n)=i\omega_n+\mu-\Xi^{-1}_\sigma(\omega_n) \tag{4.16}$$

and it has no direct connection with the self-energies in the subspaces.

The fermionic zero-order Green's function (3.5) can be also represented in the following form:

$$g_{\sigma(p)}=\frac{1}{i\omega_n+\mu_\sigma-Un^{(0)}_{\sigma(p)}}, \tag{4.17}$$

where

$$n^{(0)}_{\sigma(p)}=-\frac{d\lambda_p}{d\mu_\sigma}=\begin{cases}0 & \text{for } p=0,\overline{\sigma}\\ 1 & \text{for } p=2,\sigma\end{cases} \tag{4.18}$$

is an occupation of the state $|p\rangle$ by the electron with spin σ, and Green's function (4.12) can be written as

$$G_{\sigma(p)}(\omega_n)=\frac{1}{i\omega_n+\mu_\sigma-Un^{(0)}_{\sigma(p)}-\Sigma_{\sigma(p)}(\omega_n)-J_\sigma(\omega_n)}. \tag{4.19}$$

Now, one can reconstruct expressions for the grand canonical potentials $\Omega_{(p)}$ in subspaces from the known structure of Green's functions. To do this, we scale hopping integral

$$J_\sigma(\omega_n)\rightarrow\alpha J_\sigma(\omega_n),\quad \alpha\in[0,1] \tag{4.20}$$

which allows to define the grand canonical potential as

$$\Omega_{(p)}=\lambda_p+\int_0^1 d\alpha\frac{1}{\beta}\sum_{n\sigma}\ J_\sigma(\omega_n)G_{\sigma(p)}(\omega_n,\alpha) \tag{4.21}$$

and after some transformations one can get

$$\Omega_{(p)}=\lambda_p-\frac{1}{\beta}\sum_{n\sigma}\ \ln\frac{\Xi^{-1}_{\sigma(p)}(\omega_n)-J_\sigma(\omega_n)}{\Xi^{-1}_{\sigma(p)}(\omega_n)}$$

$$-\frac{1}{\beta}\sum_{n\sigma}\ \Sigma_{\sigma(p)}(\omega_n)\Psi_{\sigma(p)}(\omega_n)+\Phi_{(p)}, \tag{4.22}$$

where

$$\Phi_{(p)}=\frac{1}{\beta}\sum_{n\sigma}\ \int_0^1 d\alpha\Sigma_{\sigma(p)}(\omega_n,\alpha)\frac{d\Psi_{\sigma(p)}(\omega_n,\alpha)}{d\alpha} \tag{4.23}$$

is some functional, such that its functional derivative with respect to Ψ produces self-energy:

$$\frac{\delta\Phi_{(p)}}{\delta\Psi_{\sigma(p)}(\omega_n)}=\Sigma_{\sigma(p)}(\omega_n). \tag{4.24}$$

So, if one can find or construct self-energy

$$\Sigma_{\sigma(p)}(\omega_n)$$

he can find Green's functions and grand canonical potentials for subspaces and, according to (4.7) and (4.9), solve atomic problems.

Starting from the grand canonical potential (4.7) and (4.22) one can get for mean values (2.12),

$$n_\sigma=\sum_p\ w_p n_{\sigma(p)}, \tag{4.25}$$

$$n_{\sigma(p)}=n^{(0)}_{\sigma(p)}+\frac{1}{\beta}\sum_n\ [G_{\sigma(p)}(\omega_n)-\Xi_{\sigma(p)}(\omega_n)]-\frac{\partial\Phi_{(p)}}{\partial\mu_\sigma},$$

where in the last term the partial derivative is taken over the μ_σ not in the chains (4.15). The second term on the right-hand side of Eq. (4.25) can be represented diagrammatically as

 (4.26)

and the first contributions into the last term are the following

 (4.27)

where double lines denote quantities $\Psi_{\sigma(p)}(\omega_n)$. Loop

is connected with the superconducting or magnon susceptibilities for subspaces $p=0,2$ or $p=\sigma,\overline{\sigma}$, respectively.

For the single atom $[J_\sigma(\omega_n)=0]$ we have $\Phi_{(p)}=0$, $G_{\sigma(p)}(\omega_n)=\Xi_{\sigma(p)}(\omega_n)=g_{\sigma(p)}(\omega_n)$, and

$$n_\sigma=\sum_p\ w_p\frac{1}{\beta}\sum_n\ g_{\sigma(p)}(\omega_n)=\sum_p\ w_p n^{(0)}_{\sigma(p)}, \tag{4.28}$$

but in the general case $[J_\sigma(\omega_n)\neq0]$ we cannot prove that the sum rule

$$n_\sigma=\frac{1}{\beta}\sum_n\ G^{(a)}_\sigma(\omega_n) \tag{4.29}$$

is fulfilled.

A. Falicov-Kimball model

For the Falicov-Kimball model $J_\downarrow(\omega_n)=0$ and according to Eqs. (3.2) and (3.8),

$$\Sigma_{\uparrow(p)}(\omega_n)\equiv0;\quad \Xi_{\uparrow(p)}(\omega_n)=g_{\uparrow(p)}(\omega_n) \tag{4.30}$$

and

$$\Omega_{(p)}=\lambda_p-\frac{1}{\beta}\sum_n\ \ln[1-J_\uparrow(\omega_n)g_{\uparrow(p)}(\omega_n)], \tag{4.31}$$

$$G^{(a)}_\uparrow(\omega_n)=\frac{1-n_\downarrow}{i\omega_n-\lambda_{\uparrow0}-J_\uparrow(\omega_n)}+\frac{n_\downarrow}{i\omega_n-\lambda_{2\downarrow}-J_\uparrow(\omega_n)}, \tag{4.32}$$

$$n_\uparrow=\frac{1}{\beta}\sum_n\ G^{(a)}_\uparrow(\omega_n),\quad n_\downarrow=w_2+w_\downarrow \tag{4.33}$$

which immediately gives results of Ref. 9 (see also Ref. 32).

For the Hubbard model there are no exact expressions for self-energy but the set of Eqs. (4.12), (4.14), and (4.22) allows one to construct different self-consistent approximations.

B. Alloy-analogy approximation

The simplest approximation, which can be done, is to put

$$\Sigma_{\sigma(p)}(\omega_n)=0, \tag{4.34}$$

which gives

$$\Xi_{\sigma(p)}(\omega_n)=g_{\sigma(p)}(\omega_n) \tag{4.35}$$

and

$$\Omega_{(p)}=\lambda_p-\frac{1}{\beta}\sum_{n\sigma}\ \ln[1-J_\sigma(\omega_n)g_{\sigma(p)}(\omega_n)] \tag{4.36}$$

and for the Green's function for the atomic problem one can obtain a two-pole expression

$$G_{\sigma}^{(a)}(\omega_n)=\frac{w_0+w_{\sigma}}{i\omega_n-\lambda_{\sigma 0}-J_{\sigma}(\omega_n)}+\frac{w_2+w_{\sigma}^{-}}{i\omega_n-\lambda_{2\sigma}^{-}-J_{\sigma}(\omega_n)} \tag{4.37}$$

of the alloy-analogy solution for the Hubbard model, which is a zero-order approximation within the considered approach and is exact for the Falicov-Kimball model. For this approximation, mean values (2.12) are equal to

$$n_{\sigma}=\frac{1}{\beta}\sum_n G_{\sigma}^{(a)}(\omega_n)+w_2+w_{\sigma}-\frac{w_0+w_{\sigma}}{e^{\beta\lambda_{\sigma 0}}+1}-\frac{w_2+w_{\sigma}^{-}}{e^{\beta\lambda_{2\sigma}^{-}}+1}$$

$$\neq\frac{1}{\beta}\sum_n G_{\sigma}^{(a)}(\omega_n) \tag{4.38}$$

and, for some values of the chemical potential, they can get unphysical values: negative or greater than one.

C. Hartree-Fock approximation

The next possible approximation is to take into account the contribution from diagram (4.26) and to construct the equation for the self-energy in the following form:

$$\Sigma_{\sigma(p)}(\omega_n)=\frac{1}{\beta}\sum_{n'} U\Psi_{\overline{\sigma}(p)}(\omega_{n'}), \tag{4.39}$$

which, together with the expression for mean values

$$n_{\sigma(p)}=n_{\sigma(p)}^{(0)}+\frac{1}{\beta}\sum_n \Psi_{\sigma(p)}(\omega_n)$$

$$=n_{\sigma(p)}^{(0)}-\frac{1}{2}+\frac{1}{2}\tanh\frac{\beta}{2}[Un_{\overline{\sigma}(p)}-\mu_{\sigma}]$$

$$+\frac{1}{\beta}\sum_{n'} G_{\sigma(p)}(\omega_{n'}), \tag{4.40}$$

gives for the Green's function in the subspaces expression in the Hartree-Fock approximation:

$$G_{\sigma(p)}(\omega_n)=\frac{1}{i\omega_n+\mu_{\sigma}-Un_{\overline{\sigma}(p)}-J_{\sigma}(\omega_n)}. \tag{4.41}$$

Now, grand canonical potentials in the subspaces are equal

$$\Omega_{(p)}=\lambda_p-\frac{1}{\beta}\sum_{n\sigma}\ln[1-J_{\sigma}(\omega_n)\Xi_{\sigma(p)}(\omega_n)]$$

$$-U(n_{\sigma(p)}-n_{\sigma(p)}^{(0)})(n_{\overline{\sigma}(p)}-n_{\overline{\sigma}(p)}^{(0)}) \tag{4.42}$$

and for the Green's function for the atomic problem (4.9) one can obtain four-pole structure

$$G_{\sigma}^{(a)}(\omega_n)=\sum_p \frac{w_p}{i\omega_n+\mu_{\sigma}-Un_{\overline{\sigma}(p)}-J_{\sigma}(\omega_n)}. \tag{4.43}$$

Expression (4.43), in contrast to the alloy-analogy solution (4.37), possesses the correct Hartree-Fock limit for small Coulombic interaction $U\ll t$:

$$G_{\sigma}^{(a)}(\omega_n)=\frac{1}{i\omega_n+\mu_{\sigma}-Un_{\overline{\sigma}}-J_{\sigma}(\omega_n)} \tag{4.44}$$

when $w_p\approx\frac{1}{4}$ and

$$n_{\sigma(p)}\approx n_{\sigma}=\frac{1}{\beta}\sum_n G_{\sigma}^{(a)}(\omega_n).$$

On the other hand, in the same way as an alloy-analogy solution, it describes the metal-insulator transition with the change of U.

In Fig. 1 the frequency distribution of the total spectral weight function

$$\rho_{\sigma}(\omega)=\frac{1}{\pi}\Im G_{\sigma}^{(a)}(\omega-i0^{+}) \tag{4.45}$$

as well as contributions into it from the subspaces [separate terms in Eq. (4.43)] are presented for the different electron concentration (chemical potential) values. One can see, that the spectral weight function contains two peaks, which correspond to the two Hubbard bands. Each band is formed by the two close peaks: $p=0$ and σ for the lower Hubbard band and $p=2$ and $\overline{\sigma}$ for the upper one, with weights w_p Eq. (4.11). The main contributions come (see Fig. 2) from the subspaces $p=0$ for the low-electron concentrations ($n<\frac{2}{3},\mu<0$), $p=2$ for the low-hole concentrations ($2-n<\frac{2}{3},\mu>U$) and $p=\sigma,\overline{\sigma}$ for the intermediate values. For the small electron or hole concentrations, the Green's function for the atomic problem (4.43) possesses correct Hartree-Fock limits too.

Such four-pole structure of the single-electron Green's function can be obtained also for the one-dimensional chain with the $N=2$ periodic boundary condition (see the Appendix), which is equivalent to the two-site problem considered by Harris and Lange.[15] Here, two poles correspond to the noninteracting electrons or holes, which hope over the empty sites, and give the main contribution for small concentrations. The other two poles give the main contribution close to half-filling and correspond to the hopping of the strongly-correlated electrons over the resonating valence bond (RVB) states.

So, one can suppose that the Hubbard model describes strongly-correlated electronic systems that contain four components (subspaces). Subspaces $p=0$ and $p=2$ describe the Fermi-liquid component (electron and hole, respectively) which is dominant for the small electron and hole concentrations, when the chemical potential is close to the bottom of the lower band and top of the upper one. On the other hand, subspaces $p=\uparrow$ and $\downarrow$ describe the non-Fermi-liquid (strongly correlated, e.g., RVB) component, which is dominant close to half-filling. Within the considered Hartree-Fock approximation, at $n\approx\frac{2}{3}$ and $2-n\approx\frac{2}{3}$ we have transition between these two regimes: Fermi liquid and non-Fermi liquid. It reminds us that the known properties of the high-T_c compounds, where for the nondoped case ($n=1$) compounds are in the antiferroelectric dielectric state, then for small doping the non-Fermi-liquid behavior is observed (underdoped case $n\lesssim 1$) and after some optimal doping value the properties of the compound sharply change from the non-Fermi to the Fermi liquid (overdoped case).

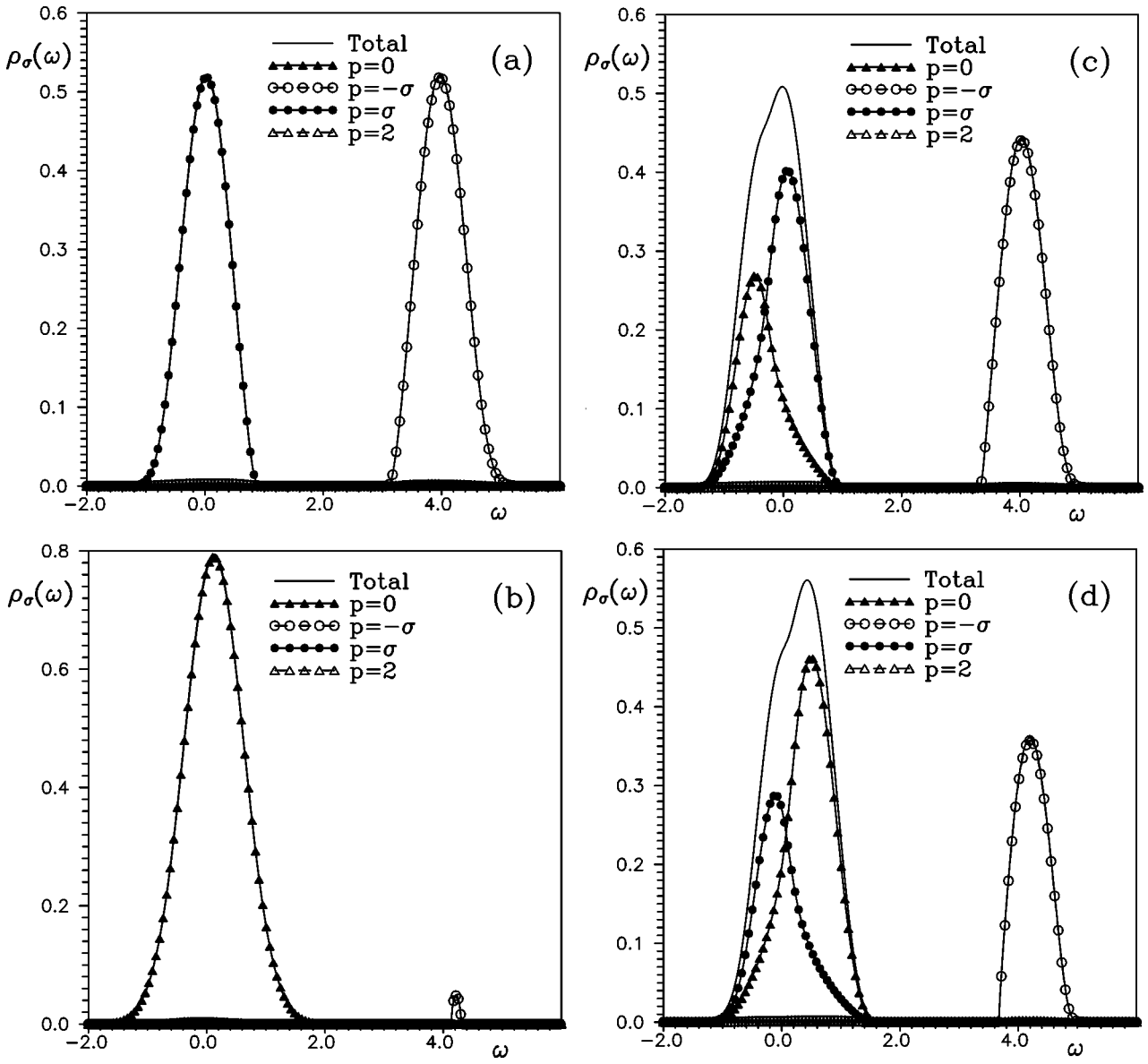


FIG. 1. Spectral weight function $\rho_\sigma(\omega)$ (4.45); total and for each subspace, for the different chemical potential values: (a) $\mu=U/2, n=1$; (b) $\mu=-1, n=0.07$; (c) $\mu=0.01, n=0.72$; (d) $\mu=-0.01, n=0.66$ ($U=4, T=0.2$).

The results presented in Figs. 1 and 2 are obtained for relatively high temperature. With the temperature decrease, on the one hand, the transition between the Fermi and non-Fermi liquid becomes sharp and, on the other hand, for some chemical potential values there can be three solutions of Eq. (4.40) with two of them corresponding to the phase-separated states. The consideration of the phase separation in the Hubbard model is not a topic in this paper and will be the subject of further investigations.

D. Beyond the Hartree-Fock approximation

Self-energy in the Hartree-Fock approximation [see Eq. (4.41)] describes some self-consistent shift of the initial energy levels and does not depend on the frequency. All other improvements of the expression for self-energy add the frequency dependent contributions. To see this, let us consider the contribution into the mean values from the first diagram in (4.27). This diagram originates from the following skeletal diagram

(4.46)

in the diagrammatic expansion for functional $\Phi_{(p)}$. On the other hand, such a skeletal diagram produces additional contribution into the self-energy

(4.47)

which is frequency dependent. Also, in order to get a self-consistent set of equations, we introduce renormalized bosonic Green's functions

$$D_{20}(\omega_m)=\frac{1}{i\omega_m-\tilde{\lambda}_{20}};\quad D_{\sigma\bar{\sigma}}(\omega_m)=\frac{1}{i\omega_m-\tilde{\lambda}_{\sigma\bar{\sigma}}}, \tag{4.48}$$

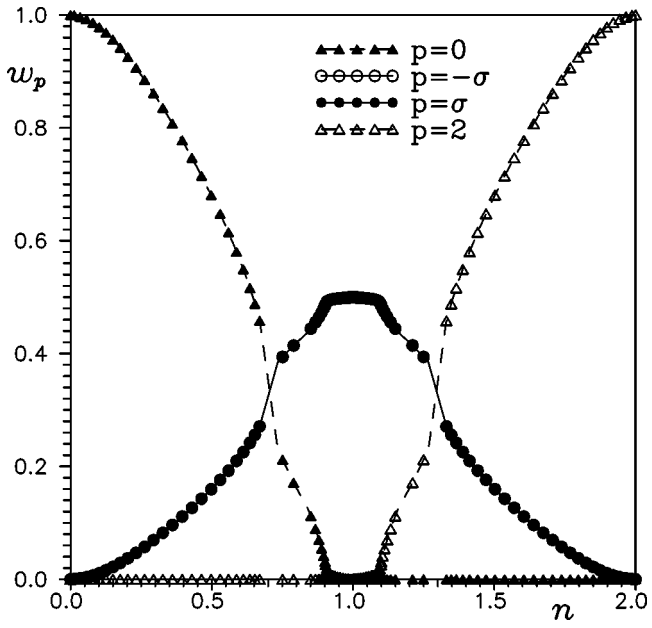


FIG. 2. Statistical weights of the subspaces w_p (4.11) as functions of the electron concentration ($U=4, T=0.2$).

$$\tilde{\lambda}_{20}=\lambda_{20}+U\frac{1}{\beta}\sum_{n\sigma}\Psi_{\sigma(p)}(\omega_n),$$

$$\tilde{\lambda}_{\sigma\bar{\sigma}}=\lambda_{\sigma\bar{\sigma}}-U\frac{1}{\beta}\sum_{n\sigma}\sigma\Psi_{\sigma(p)}(\omega_n).$$

Finally, for the Green's function (4.19) we get the general representation

$$G_{\sigma(p)}(\omega_n)=\frac{1}{i\omega_n+\mu_\sigma-Un_{\bar{\sigma}(p)}-\tilde{\tilde{\Sigma}}_{\sigma(p)}(\omega_n)-J_\sigma(\omega_n)}, \tag{4.49}$$

where the Hartree-Fock contribution $Un_{\bar{\sigma}(p)}$ is extracted and

$$\tilde{\tilde{\Sigma}}_{\sigma(p)}(\omega_n)$$

is a frequency dependent part of the self-energy, which within the considered approximation is equal

$$\tilde{\tilde{\Sigma}}_{\sigma(p)}(\omega_n)=US_{\sigma(p)}(\omega_n), \tag{4.50}$$

where

$$S_{\sigma(p)}(\omega_n)=\pm\frac{U}{\beta}\sum_{n'}D_{\sigma\bar{\sigma}(p)}(\omega_n,\omega_{n'})\Psi_{\bar{\sigma}(p)}(\omega_{n'}) \tag{4.51}$$

and

$$D_{\sigma\bar{\sigma}(p)}(\omega_n,\omega_{n'})=\begin{cases}D_{20}(\omega_{n+n'}) & \text{for } p=0,2\\ D_{\sigma\bar{\sigma}}(\omega_{n-n'}) & \text{for } p=\sigma\bar{\sigma}.\end{cases} \tag{4.52}$$

Now, mean values (4.25) are equal

$$n_{\sigma(p)}=n^{(0)}_{\sigma(p)}+\frac{1}{\beta}\sum_n\Psi_{\sigma(p)}(\omega_n)$$
$$\pm\frac{1}{\beta^2}\sum_{nn'}U^2D^2_{\sigma\bar{\sigma}(p)}(\omega_n,\omega_{n'})\Psi_{\sigma(p)}(\omega_n)\Psi_{\bar{\sigma}(p)}(\omega_{n'}) \tag{4.53}$$

and for the grand canonical potentials in the subspaces we obtain the following expressions:

$$\Omega_{(p)}=\lambda_p-\frac{1}{\beta}\sum_{n\sigma}\ln[1-J_\sigma(\omega_n)\Xi_{\sigma(p)}(\omega_n)]$$
$$-\frac{1}{\beta^2}\sum_{nn'}U[1\pm UD^2_{20}(\omega_{n+n'})g^{-1}_{20}(\omega_{n+n'})]$$
$$\times\Psi_{\sigma(p)}(\omega_n)\Psi_{\bar{\sigma}(p)}(\omega_{n'}) \tag{4.54}$$

for $p=0,2$, and

$$\Omega_{(p)}=\lambda_p-\frac{1}{\beta}\sum_{n\sigma}\ln[1-J_\sigma(\omega_n)\Xi_{\sigma(p)}(\omega_n)]$$
$$-\frac{1}{\beta^2}\sum_{nn'}U[1\pm UD^2_{\sigma\bar{\sigma}}(\omega_{n-n'})g^{-1}_{\sigma\bar{\sigma}}(\omega_{n-n'})]$$
$$\times\Psi_{\sigma(p)}(\omega_n)\Psi_{\bar{\sigma}(p)}(\omega_{n'}) \tag{4.55}$$

for $p=\sigma,\bar{\sigma}$.

In order to analyze the structure of the poles in Eq. (4.49), an analytical continuation of the expression for

$$\tilde{\tilde{\Sigma}}_{\sigma(p)}(\omega_n)$$

from the imaginary axis to the real one should be done. To do it, we use the well-known identity

$$\frac{1}{\beta}\sum_n\frac{e^{i\omega_n0^+}}{i\omega_n-\lambda}=\pm n_\pm(\lambda), \tag{4.56}$$

which follows from Eq. (2.18), and analytical properties of the Green's function

$$G_\sigma(z)=\frac{1}{\pi}\int_{-\infty}^{+\infty}d\omega\frac{\Im G_\sigma(\omega-i0^+)}{z-\omega}. \tag{4.57}$$

Green's functions in the subspaces $G_{\sigma(p)}(z)$, irreducible parts $\Xi_{\sigma(p)}(z)$, and dynamical mean-field $J_\sigma(z)$ all possess the same analytical properties. Finally, for $S_{\sigma(p)}(z)$ we get the following expressions:

$$S_{\sigma(p)}(z)=\pm\frac{U}{\pi}\mathcal{P}\int_{-\infty}^{+\infty}d\omega n_+(\omega)\frac{\Im\Psi_{\bar{\sigma}(p)}(\omega-i0^+)}{z+\omega-\tilde{\lambda}_{20}}$$
$$\pm n_-(\tilde{\lambda}_{20})U\Psi_{\bar{\sigma}(p)}(\tilde{\lambda}_{20}-z) \tag{4.58}$$

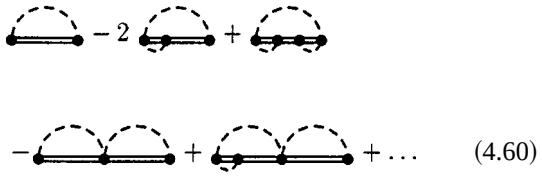
for subspaces $p=0,2$ and

$$S_{\sigma(p)}(z)=\pm\frac{U}{\pi}\mathcal{P}\int_{-\infty}^{+\infty}d\omega n_{+}(\omega)\frac{\Im\Psi_{\bar{\sigma}(p)}(\omega-i0^{+})}{z-\omega-\tilde{\lambda}_{\sigma\bar{\sigma}}}$$

$$\mp[n_{-}(\tilde{\lambda}_{\sigma\bar{\sigma}})+1]U\Psi_{\bar{\sigma}(p)}(z-\tilde{\lambda}_{\sigma\bar{\sigma}}) \qquad (4.59)$$

for $p=\sigma,\bar{\sigma}$. Analytical continuation of the expressions (4.53), (4.54), and (4.55) can be done in the same way. One can see that contributions (4.58) and (4.59) diverge when $\tilde{\lambda}_{20}=0$ and $\tilde{\lambda}_{\sigma\bar{\sigma}}=0$, respectively, which is an unphysical result.

So, we cannot include into the consideration only one contribution from diagram (4.47) but must sum up all diagrams of the following type:



(4.60)

which gives an expression free from the above-mentioned divergences

$$\tilde{\Sigma}_{\sigma(p)}(\omega_n)=U[1+S''_{\sigma(p)}(\omega_n)]-U\frac{[1+S'_{\sigma(p)}(\omega_n)]^2}{1+S_{\sigma(p)}(\omega_n)}, \qquad (4.61)$$

where $S_{\sigma(p)}(\omega_n)$ is defined above and

$$S'_{\sigma(p)}(\omega_n)=\frac{U}{\beta}\sum_{n'}D_{\sigma\bar{\sigma}(p)}(\omega_n,\omega_{n'})\Psi_{\bar{\sigma}(p)}(\omega_{n'})\times\frac{S_{\bar{\sigma}(p)}(\omega_{n'})-S'_{\bar{\sigma}(p)}(\omega_{n'})}{1+S_{\bar{\sigma}(p)}(\omega_{n'})}, \qquad (4.62)$$

$$S''_{\sigma(p)}(\omega_n)=\frac{U}{\beta}\sum_{n'}D_{\sigma\bar{\sigma}(p)}(\omega_n,\omega_{n'})\Psi_{\bar{\sigma}(p)}(\omega_{n'})\times\left(\frac{S_{\bar{\sigma}(p)}(\omega_{n'})-S'_{\bar{\sigma}(p)}(\omega_{n'})}{1+S_{\bar{\sigma}(p)}(\omega_{n'})}\right)^2.$$

Such diagram resummation must be also done in the expression for the mean values (4.53), where the last term must be replaced by

$$\pm\frac{1}{\beta^2}\sum_{nn'}U^2D^2_{\bar{\sigma}\sigma(p)}(\omega_n,\omega_{n'})\Psi_{\sigma(p)}(\omega_n)\Psi_{\bar{\sigma}(p)}(\omega_{n'})\times\left(\frac{1+S'_{\sigma(p)}(\omega_n)}{1+S_{\sigma(p)}(\omega_n)}+\frac{1+S'_{\bar{\sigma}(p)}(\omega_{n'})}{1+S_{\bar{\sigma}(p)}(\omega_{n'})}-1\right)^2. \qquad (4.63)$$

Besides diagram (4.47), there are a lot of other diagrams that diverge and need additional resummation of the diagrammatic series. But now it is difficult to clear out what types of diagrams are leading in different case, which calls for additional investigation. But it is, obviously, that such contributions will shift the boundary between the Fermi and non-Fermi-liquid behavior.

V. SUMMARY

A finite-temperature perturbation theory scheme in terms of electron hopping, which is based on the Wick theorem for Hubbard operators and is valid for arbitrary values of U ($U<\infty$) has been developed for Hubbard-type models. Diagrammatic series contain single-site vertices, which are irreducible many-particle Green's functions for unperturbated single-site Hamiltonian, connected by hopping lines. Applying the Wick theorem for Hubbard operators has allowed us to calculate these vertices and it is shown that for each vertex the problem splits into subspaces with ''vacuum states'' determined by the diagonal (projection) operators and only excitations around these ''vacuum states'' are allowed. The vertices possess finite $U\to\infty$ limit when diagrammatic series of the strong-coupling approach[5,6] are reproduced. The rules to construct diagrams by the primitive vertices are proposed.

In the limit of infinite spatial dimensions the total auxiliary single-site problem exactly (naturally) splits into subspaces (four for Hubbard model) and a considered analytical scheme allows to build a self-consistent Kadanoff-Baym-type theory for the Hubbard model. Some analytical results are given for simple approximations: an alloy-analogy approximation, when two-pole structure for Green's function is obtained, which is exact for the Falicov-Kimball model, and the Hartree-Fock-type approximation, which results in the four-pole structure for the Green's function. Expanding beyond the Hartree-Fock approximation calls for considering the frequency dependent contributions into the self-energy and resummation of the diagrammatic series.

In general, the expression

$$G^{(a)}_{\sigma}(\omega_n)=\sum_{p}\frac{w_p}{i\omega_n+\mu_{\sigma}-Un_{\bar{\sigma}(p)}-\tilde{\Sigma}_{\sigma(p)}(\omega_n)-J_{\sigma}(\omega_n)}, \qquad (5.1)$$

gives an exact four-pole structure for the single-electron Green's function of the effective atomic problem. In Eq. (4.14) zero-order Green's functions (3.5) are the same for the subspaces $p=0,\sigma$ and $p=2,\bar{\sigma}$, respectively, and correspond to the two-pole solution of the one-site problem without hopping. Switching on of the electron hopping splits these two poles and the value of splitting is determined by the values of the self-energy parts in the subspaces, which describe the contributions from the different scattering processes. Alloy-analogy approximation neglects by the such scattering processes

$$\Sigma_{\sigma(p)}(\omega_n)=0$$

which results in the two-pole structure for the Green's functions (4.37). But, in general, Green's functions possesses four-pole structure and even the Hartree-Fock approximation (4.43) clearly shows it.

It should be noted that the four-pole structure of the Green's function for the atomic problem might not result in the four bands of the spectral weight function (see Fig. 1). The presented consideration allows us to suppose that each pole describes contributions from the different components

(subspaces) of the electronic system: Fermi liquid (subspaces $p=0,2$) and non-Fermi liquid ($p=\uparrow,\downarrow$), and for small electron and hole concentrations ($n<\frac{2}{3}$ and $2-n<\frac{2}{3}$) the Fermi-liquid component gives the main contribution (''overdoped regime'' of high-T_c's), whereas in other cases the non-Fermi liquid one (''underdoped regime'').

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APPENDIX: TWO-SITE PROBLEM

Let us consider an infinite one-dimensional chain with the $N=2$ periodic boundary condition. Mathematically it is equivalent to the two-site problem considered by Harris and Lange,[15] but now we can introduce the lattice Fourier transformation, with two wave-vector values in the first Brillouin zone $q=0$ and $q=\pi$, and perform all calculations for the grand canonical ensemble. The Hamiltonian of the model is the following:

$$H=\sum_{i=1,2}\left(Un_{i\uparrow}n_{i\downarrow}-\mu\sum_{\sigma}n_{i\sigma}\right)+t\sum_{\sigma}(a_{1\sigma}^{\dagger}a_{2\sigma}+a_{2\sigma}^{\dagger}a_{1\sigma}). \tag{A1}$$

We can introduce the Fourier transform of the electron hopping

$$t_q=t\cos q=\begin{cases}t & \text{for } q=0\\ -t & \text{for } q=\pi\end{cases} \tag{A2}$$

and our aim is to calculate the single-electron Green's function

$$G_{\sigma}(\omega,t_q)=\begin{cases}G_{11\sigma}(\omega_n)+G_{12\sigma}(\omega_n) & \text{for } q=0\\ G_{11\sigma}(\omega_n)-G_{12\sigma}(\omega_n) & \text{for } q=\pi,\end{cases} \tag{A3}$$

where $G_{ij\sigma}(\tau-\tau')=\langle Ta_{i\sigma}^{\dagger}(\tau)a_{j\sigma}(\tau')\rangle$.

The initial basis of states contains 16 many-electron two-site states $|p_1,p_2\rangle$, where $p_i=\{n_{i\uparrow}n_{i\downarrow}\}$, i.e.,

$$\begin{aligned}
|1\rangle&=|0,0\rangle,\\
|2\rangle&=|\downarrow,0\rangle=a_{1\downarrow}^{\dagger}|1\rangle,\\
|3\rangle&=|0,\downarrow\rangle=a_{2\downarrow}^{\dagger}|1\rangle,\\
|4\rangle&=|\uparrow,0\rangle=a_{1\uparrow}^{\dagger}|1\rangle,\\
|5\rangle&=|0,\uparrow\rangle=a_{2\uparrow}^{\dagger}|1\rangle,\\
|6\rangle&=|\downarrow,\downarrow\rangle=a_{2\downarrow}^{\dagger}|2\rangle=-a_{1\downarrow}^{\dagger}|3\rangle,\\
|7\rangle&=|\uparrow,\uparrow\rangle=a_{2\uparrow}^{\dagger}|4\rangle=-a_{1\uparrow}^{\dagger}|5\rangle,\\
|8\rangle&=|2,0\rangle=a_{1\uparrow}^{\dagger}|2\rangle=-a_{1\downarrow}^{\dagger}|4\rangle,\\
|9\rangle&=|\uparrow,\downarrow\rangle=a_{1\uparrow}^{\dagger}|3\rangle=-a_{2\downarrow}^{\dagger}|4\rangle,\\
|10\rangle&=|\downarrow,\uparrow\rangle=a_{2\uparrow}^{\dagger}|2\rangle=-a_{1\downarrow}^{\dagger}|5\rangle,\\
|11\rangle&=|0,2\rangle=a_{2\uparrow}^{\dagger}|3\rangle=-a_{2\downarrow}^{\dagger}|5\rangle,\\
|12\rangle&=|2,\downarrow\rangle=a_{1\uparrow}^{\dagger}|6\rangle=a_{1\downarrow}^{\dagger}|9\rangle=-a_{2\downarrow}^{\dagger}|8\rangle,\\
|13\rangle&=|\downarrow,2\rangle=a_{2\uparrow}^{\dagger}|6\rangle=a_{1\downarrow}^{\dagger}|11\rangle=-a_{2\downarrow}^{\dagger}|10\rangle,\\
|14\rangle&=|2,\uparrow\rangle=a_{1\downarrow}^{\dagger}|7\rangle=a_{2\uparrow}^{\dagger}|8\rangle=-a_{1\uparrow}^{\dagger}|10\rangle,\\
|15\rangle&=|\uparrow,2\rangle=a_{2\downarrow}^{\dagger}|7\rangle=a_{2\uparrow}^{\dagger}|9\rangle=-a_{1\uparrow}^{\dagger}|11\rangle,\\
|16\rangle&=|2,2\rangle=a_{1\uparrow}^{\dagger}|13\rangle=-a_{2\uparrow}^{\dagger}|12\rangle=a_{1\downarrow}^{\dagger}|15\rangle=a_{2\downarrow}^{\dagger}|14\rangle
\end{aligned} \tag{A4}$$

and one can introduce Hubbard operators $X^{p,q}=|p\rangle\langle q|$ acting in the space of these states. Now, electron creation operators can be presented in the following form:

$$\begin{aligned}
a_{1\uparrow}^{\dagger}&=X^{4,1}-X^{7,5}+X^{8,2}+X^{9,3}+X^{12,6}-X^{14,10}-X^{15,11}+X^{16,13},\\
a_{1\downarrow}^{\dagger}&=X^{2,1}-X^{6,3}-X^{8,4}-X^{10,5}+X^{12,9}+X^{13,11}+X^{14,7}+X^{16,15},\\
a_{2\uparrow}^{\dagger}&=X^{5,1}+X^{7,4}+X^{10,2}+X^{11,3}+X^{13,6}+X^{14,8}+X^{15,9}-X^{16,12},\\
a_{2\downarrow}^{\dagger}&=X^{3,1}+X^{6,2}-X^{9,4}-X^{11,5}-X^{12,8}-X^{13,10}+X^{15,7}-X^{16,14}.
\end{aligned} \tag{A5}$$

By transformations

$$\begin{pmatrix}|2\rangle & |4\rangle & |12\rangle & |14\rangle\\ |3\rangle & |5\rangle & |13\rangle & |15\rangle\end{pmatrix}=\begin{Vmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{Vmatrix}\times\begin{pmatrix}|\tilde{2}\rangle & |\tilde{4}\rangle & |\widetilde{12}\rangle & |\widetilde{14}\rangle\\ |\tilde{3}\rangle & |\tilde{5}\rangle & |\widetilde{13}\rangle & |\widetilde{15}\rangle\end{pmatrix} \tag{A6}$$

and

$$\begin{pmatrix}|8\rangle\\ |9\rangle\\ |10\rangle\\ |11\rangle\end{pmatrix}=\begin{Vmatrix}\frac{1}{\sqrt{2}}\cos\phi & \frac{-1}{\sqrt{2}}\sin\phi & 0 & \frac{-1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\sin\phi & \frac{1}{\sqrt{2}}\cos\phi & \frac{-1}{\sqrt{2}} & 0\\ \frac{1}{\sqrt{2}}\sin\phi & \frac{1}{\sqrt{2}}\cos\phi & \frac{1}{\sqrt{2}} & 0\\ \frac{1}{\sqrt{2}}\cos\phi & \frac{-1}{\sqrt{2}}\sin\phi & 0 & \frac{1}{\sqrt{2}}\end{Vmatrix}\begin{pmatrix}|\tilde{8}\rangle\\ |\tilde{9}\rangle\\ |\widetilde{10}\rangle\\ |\widetilde{11}\rangle\end{pmatrix}, \tag{A7}$$

where $\sin 2\phi(t)=\dfrac{2t}{\sqrt{U^2/4+4t^2}}$, the Hamiltonian (A1) can be diagonalized

$$H=\sum_{\tilde{p}}\lambda_{\tilde{p}}X^{\tilde{p},\tilde{p}}. \tag{A8}$$

Here

$$\begin{aligned}
\lambda_{\tilde{1}}&=0,\\
\lambda_{\tilde{2}}&=\lambda_{\tilde{4}}=-\mu+t,\\
\lambda_{\tilde{3}}&=\lambda_{\tilde{5}}=-\mu-t,\\
\lambda_{\tilde{6}}&=\lambda_{\tilde{7}}=\lambda_{\tilde{10}}=-2\mu,\\
\lambda_{\tilde{8}}&=U+J-2\mu,\\
\lambda_{\tilde{9}}&=-J-2\mu,\\
\lambda_{\tilde{11}}&=U-2\mu,\\
\lambda_{\tilde{12}}&=\lambda_{\tilde{14}}=U-3\mu+t,\\
\lambda_{\tilde{13}}&=\lambda_{\tilde{15}}=\mathrm{U}-3\mu-\mathrm{t},\\
\lambda_{\tilde{16}}&=2U-4\mu
\end{aligned} \tag{A9}$$

are eigenvalues and

$$J=\frac{4t^2}{\sqrt{U^2/4+4t^2}+U/2}\rightarrow\frac{4t^2}{U}\ (U\gg t). \tag{A10}$$

Finally, with the use of the Wick theorem (2.17) for the Hubbard operators acting in the space of eigenstates $|\tilde{p}\rangle$, for the single-electron Green's function (A3) we obtain

$$\begin{aligned}
G_\sigma(\omega,t_q)=&\frac{A_1(t_q)}{\omega-t_q}+\frac{B_1(t_q)}{\omega+J+t_q}+\frac{A_2(t_q)}{\omega-U-t_q}\\
&+\frac{B_2(t_q)}{\omega-U-J+t_q},
\end{aligned} \tag{A11}$$

where

$$\begin{aligned}
A_1(t)=&\frac{1}{Z}\Bigg[1+e^{\beta(\mu-t)}+e^{\beta(\mu+t)}+e^{2\beta\mu}+\frac{1}{2}(e^{\beta(\mu+t)}+e^{2\beta\mu}\\
&+e^{-\beta(U-2\mu)}+e^{-\beta(U-3\mu+t)})\Bigg],\\
A_2(t)=&\frac{1}{Z}\Bigg[e^{-\beta(2U-4\mu)}+e^{-\beta(U-3\mu+t)}+e^{-\beta(U-3\mu-t)}+e^{2\beta\mu}\\
&+\frac{1}{2}(e^{\beta(\mu+t)}+e^{2\beta\mu}+e^{-\beta(U-2\mu)}+e^{-\beta(U-3\mu+t)})\Bigg],
\end{aligned} \tag{A12}$$

$$\begin{aligned}
B_{1,2}(t)=&\frac{1}{2Z}\left(1\pm\frac{2t}{\sqrt{U^2/4+4t^2}}\right)[e^{\beta(\mu-t)}+e^{\beta(2\mu+J)}\\
&+e^{-\beta(U-2\mu+J)}+e^{-\beta(U-3\mu-t)}]
\end{aligned}$$

and

$$Z=\sum_p e^{-\beta\lambda_{\tilde{p}}}.$$

One can see, that Green's function (A11) possesses a four-pole structure and the spectrum contains four ''bands'' grouped near the initial energy levels of the one-site problem 0 and U. The distance between the centers of gravity of the grouped bands is equal to J [Eq. (A10)] and is of the order of magnitude of the effective exchange interaction. It is obvious that the weights of the bands satisfy the sum rule

$$A_1(t_q)+A_2(t_q)+B_1(t_q)+B_2(t_q)=1. \tag{A13}$$

The spectral weight function is equal

$$\begin{aligned}
\rho_\sigma(E)=&\frac{1}{\pi N}\sum_q \Im G_\sigma(E-i0^+,t_q)\\
=&\frac{1}{2}[A_1(t)\,\delta(E-t)\\
&+A_1(-t)\,\delta(E+t)+A_2(t)\,\delta(E-U-t)\\
&+A_2(-t)\,\delta(E-U+t)+B_1(t)\,\delta(E+J+t)\\
&+B_1(-t)\,\delta(E+J-t)+B_2(t)\,\delta(E-U-J+t)\\
&+B_2(-t)\,\delta(E-U-J-t)]
\end{aligned} \tag{A14}$$

contains the same eight energies obtained by Harris and Lange[15] but with different weights and originates from the four poles (bands) of the Green's function (A11) for the two-site problem.

The nature of these peaks is clear from the ground-state properties of the model. At zero temperature, depending on the value of the chemical potential or electron concentration, the ground states are the following ($U\gg t$): empty state $n=0$ ($\mu<-t$):

$$\begin{aligned}
|\tilde{1}\rangle&=|0,0\rangle,\\
\lambda_{\tilde{1}}&=0,\\
G_\sigma(\omega,q)&=\frac{1}{\omega-t_q},
\end{aligned} \tag{A15}$$

one-electron states $n=\frac{1}{2}$ ($-t<\mu<t-J$):

$$\begin{aligned}
|\tilde{3}\rangle&=\frac{1}{\sqrt{2}}(a^\dagger_{2\downarrow}-a^\dagger_{1\downarrow})|0,0\rangle,\\
|\tilde{5}\rangle&=\frac{1}{\sqrt{2}}(a^\dagger_{2\uparrow}-a^\dagger_{1\uparrow})|0,0\rangle,\\
\lambda_{\tilde{3}}&=\lambda_{\tilde{5}}=-\mu-t,\\
G_\sigma(\omega,q=0)&=\frac{3/4}{\omega-t}+\frac{1/4}{\omega-U-t},
\end{aligned} \tag{A16}$$

$$G_\sigma(\omega,q=\pi)=\frac{1/2}{\omega+t}+\frac{1/4(1+\sin 2\phi)}{\omega+J-t}+\frac{1/4(1-\sin 2\phi)}{\omega-U-J-t},$$

two-electron states $n=1$ ($t-J<\mu<U+J-t$):

$$|\tilde{9}\rangle=\frac{1}{\sqrt{2}}\cos\phi(a^{\dagger}_{1\uparrow}a^{\dagger}_{2\downarrow}-a^{\dagger}_{1\downarrow}a^{\dagger}_{2\uparrow})|0,0\rangle$$

$$-\frac{1}{\sqrt{2}}\sin\phi(a^{\dagger}_{1\uparrow}a^{\dagger}_{1\downarrow}-a^{\dagger}_{2\downarrow}a^{\dagger}_{2\uparrow})|0,0\rangle,$$

$$\lambda_{\tilde{9}}=-2\mu-J,$$

$$G_{\sigma}(\omega,q)=\frac{1/2(1+\sin 2\phi_q)}{\omega+J+t_q}+\frac{1/2(1-\sin 2\phi_q)}{\omega-U-J+t_q}, \tag{A17}$$

three-electron states $n=\frac{3}{2}(U+J-t<\mu<U+t)$:

$$|\widetilde{13}\rangle=\frac{1}{\sqrt{2}}(a_{1\uparrow}+a_{2\uparrow})|2,2\rangle,$$

$$|\widetilde{15}\rangle=\frac{1}{\sqrt{2}}(a_{1\downarrow}+a_{2\downarrow})|2,2\rangle,$$

$$\lambda_{\widetilde{13}}=\lambda_{\widetilde{15}}=U-3\mu-t,$$

$$G_{\sigma}(\omega,q=0)=\frac{1/4\,(1-\sin 2\phi)}{\omega+J+t}+\frac{1/4(1+\sin 2\phi)}{\omega-U-J+t}$$

$$+\frac{1/2}{\omega-U-t}, \tag{A18}$$

$$G_{\sigma}(\omega,q=\pi)=\frac{1/4}{\omega+t}+\frac{3/4}{\omega-U+t},$$

and four-electron states $n=2$ $(\mu>U+t)$:

$$|\widetilde{16}\rangle=|2,2\rangle,$$

$$\lambda_{\widetilde{16}}=2U-4\mu,$$

$$G_{\sigma}(\omega,q)=\frac{1}{\omega-U-t_q}. \tag{A19}$$

For small electron ($n\approx 0$ or hole $n\approx 2$) concentrations we get Green's functions (A15) and (A19), respectively, which describe hopping of the noninteracting particles over empty states.

On the other hand, for the half-filled (symmetric) case $n\approx 1$, the ground state $|\tilde{9}\rangle$ is mainly a RVB-type state. Now, Green's function (A17) possesses two-poles shifted by the value of the effective exchange interaction J from the one-site levels and describes the electron transfer over the RVB states. The weight of each pole depends on the hopping value, but its total contribution into the spectral weight function (A14) is equal to $\frac{1}{2}$ as it should be for the symmetric case.

For other cases the number and weights of the poles in the spectral weight function (A14) strongly depend on the electron concentration (chemical potential) and wave-vector values and contain contributions from the noninteracting electrons (holes) and the strongly hybridized RVB states.

[1] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
[2] Yu. A. Izyumov, S. P. Cojocaru, and V. A. Moskalenko, Teor. Mat. Fiz. **97**, 270 (1993) [Theor. Math. Phys. **97**, 1290 (1993)]; V. A. Moskalenko and L. Z. Kon, Condens. Matter Phys. **1**(13), 41 (1998).
[3] P. M. Slobodjan and I. V. Stasyuk, Teor. Mat. Fiz. **19**, 423 (1974) [Theor. Math. Phys. **19**, 616 (1974)].
[4] Yu. A. Izyumov and Yu. N. Skryabin, *Statistical Mechanics of Magnetically Ordered Systems* (Consultants Bureau, New York, 1989).
[5] Yu. A. Izyumov and B. M. Letfulov, J. Phys.: Condens. Matter **2**, 8905 (1990).
[6] Yu. A. Izyumov, B. M. Letfulov, E. V. Shipitsyn, M. Bartkowiak, and K. A. Chao, Phys. Rev. B **46**, 15 697 (1992).
[7] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[8] A. Georges, G. Kotliar, W. Krauth, and M. J. Rosenberg, Rev. Mod. Phys. **68**, 13 (1996).
[9] U. Brandt and C. Mielsch, Z. Phys. B: Condens. Matter **75**, 365 (1989); **79**, 295 (1990); **82**, 37 (1991).
[10] J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963).
[11] A. Dorneich, M. G. Zacher, C. Gröber, and R. Eder, cond-mat/9909352 (unpublished).
[12] J. Hubbard, Proc. R. Soc. London, Ser. A **281**, 401 (1964).
[13] L. M. Roth, Phys. Rev. **184**, 451 (1969).
[14] W. Nolting and W. Borgiel, Phys. Rev. B **39**, 6962 (1989).
[15] A. B. Harris and R. V. Lange, Phys. Rev. **157**, 295 (1967).
[16] C. Gröber, M. G. Zacher, and R. Eder, cond-mat/9902015 (unpublished).
[17] S. Pairault, D. Sénéchal, and A.-M. S. Tremblay, Phys. Rev. Lett. **80**, 5389 (1998); cond-mat/9905245 (unpublished).
[18] T. Pruschke, D. L. Cox, and M. Jarrell, Phys. Rev. B **47**, 3553 (1993).
[19] T. Obermeier, T. Pruschke, and J. Keller, Phys. Rev. B **56**, 8479 (1997).
[20] D. M. Edwards and J. A. Hertz, Physica B **163**, 527 (1990).
[21] S. Wermbter and G. Czycholl, J. Phys.: Condens. Matter **6**, 5439 (1994); **7**, 7335 (1995).
[22] H. Kajueter and G. Kotliar, Phys. Rev. Lett. **77**, 131 (1996).
[23] T. Wegner, M. Potthoff, and W. Nolting, Phys. Rev. B **57**, 6211 (1998).
[24] T. Herrmann and W. Nolting, Phys. Rev. B **53**, 10 579 (1996).
[25] M. Potthoff, T. Herrmann, and W. Nolting, Eur. Phys. J. B **4**, 485 (1998).
[26] W. Metzner, Phys. Rev. B **43**, 8549 (1991).
[27] V. Janiš, cond-mat/9704076 (unpublished).
[28] F. Gebhard, *The Mott Metal-Insulator Transition: Models and Methods* (Springer-Verlag, Berlin, 1997).
[29] G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961); G. Baym, *ibid.* **127**, 1391 (1962).
[30] P. G. J. van Dongen, J. A. Vergés, and D. Vollhardt, Z. Phys. B: Condens. Matter **84**, 383 (1991).
[31] C. Gros, W. Wenzel, R. Valentí, G. Hülsenbeck, and J. Stolze, Europhys. Lett. **27**, 299 (1994); C. Gros and W. Wenzel, Eur. Phys. J. B **8**, 569 (1999).
[32] I. V. Stasyuk and A. M. Shvaika, J. Phys. Stud. **3**, 177 (1999).