Dynamical mean-field theory of correlated hopping: A rigorous local approach

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I. INTRODUCTION

A microscopic origin of the different effects and phenomena specific to transition and rare-earth metals and oxides, including high-$T_c$, superconductors is due to the strong local correlations between electrons. The simplest interaction that introduces such local correlations is the Hubbard single-site Coulomb repulsion $U_{ni}n_i$. In addition to such local terms there are others involving neighboring lattice sites that describe the charge-charge hopping:

$$
\sum_{ij\sigma} t_{ij}^{(1)} a_{i\sigma}^\dagger a_{j\sigma} (n_{i\bar{\sigma}} + n_{j\bar{\sigma}}).
$$

In general, an effective model with correlated hopping can be obtained after integrating out additional degrees of freedom or as a phenomenological model. It was first proposed to describe the properties of mixed valence systems, but after the discovery of high-$T_c$ superconductivity the interest in correlated hopping as a possible new mechanism for a superconducting instability and temperature-induced metal-insulator transition increased. In addition correlated hopping is considered an important factor in the stabilization of the ferromagnetism and localization of electrons.

Models with correlated hopping, like other models with strong electron correlations, cannot be solved exactly. However in the last decade, great progress in the description of strongly correlated electron systems was achieved with the development of the dynamical mean-field theory (DMFT).

The main idea of the dynamical mean-field theory, which is exact in the limit of infinite dimensions, is in the local (single-site) nature of the self-energy. But this statement, as shown by Schiller, is violated for systems with correlated hopping, when the self-energy becomes nonlocal that breaks the general DMFT scheme. Now the effect of correlated hopping is similar to the Hartree (mean-field) renormalization of the band energy, as an additional nonlocal contribution to the self-energy.

A possible solution of this problem is in a reformulation of the DMFT approach without introducing the self-energy. It should be noted that self-energy appears in the Dyson equation for the one-electron Green’s function as a correction to the band energy due to many-electron interactions, which are treated as perturbations. On the other hand, one can start, not from one-electron band states, but from many-electron local states, and analyze the influence of the intersite hopping $t_{ij}$ on the creation of the band structure. Such a strong-coupling approach corresponds to the perturbation theory over electron hopping. In this case the one-electron Green’s function can be a solution to the Larkin equation, who proved that it is local in the $D \rightarrow \infty$ limit. Below it will be shown that this statement is more general than the one about the local nature of the self-energy.

In this paper we present a general approach for a description of correlated hopping in infinite dimensions which is based on an expansion over electron hopping around the atomic limit, which keeps the DMFT local ideology, and which allows one to calculate the thermodynamical functions. As a limiting case the Falicov-Kimball model with correlated hopping and a model with broken bonds (“diluted” conductor) are considered. In this case, such a strong coupling approach corresponds
to the generalized locator coherent potential approximation developed by Blackman, Esterling and Berk (BEB CPA) for the description of the binary alloy with off-diagonal disorder.

II. EXPANSION AROUND THE ATOMIC LIMIT

In general, the hopping term of the Hamiltonian with correlated hopping for the Falicov–Kimball and Hubbard models is written

$$H_t = \frac{1}{\sqrt{D}} \sum_{(ij)} \left[ t_1 d_i^\dagger d_j + t_2 d_i^\dagger d_j (n_{ij} + n_{jf}) + t_3 d_i^\dagger d_j n_{if} n_{jf} \right]$$  \hspace{1cm} (2.1)

and

$$H_t = \frac{1}{\sqrt{D}} \sum_{(ij)} \left[ t_1 a_i^\dagger a_{j\sigma} + t_2 a_i^\dagger a_{j\sigma} (n_{i\sigma} + n_{j\bar{\sigma}}) + t_3 a_i^\dagger a_{j\sigma} n_{i\sigma} n_{j\bar{\sigma}} \right]$$  \hspace{1cm} (2.2)

respectively. As a rule, the first two terms with $t_1$ and $t_2$ were considered, but an influence of the last term with $t_3$, that can originate from the nondirect interactions over other degrees of freedom, was also investigated. In Hamiltonians (2.1) and (2.2) the terms $t_1$, $t_2$, and $t_3$ describe hopping between two nearest-neighbor sites $i$ and $j$ irrespective of the occupation of these sites, the hopping between these sites when one of them is occupied by another particle and the hopping between two occupied sites, respectively. One can transfer Hamiltonian (2.1) to the other one that describes the hopping between the sites with the certain occupations,

$$H_t = \frac{1}{\sqrt{D}} \sum_{(ij)} \left[ t_{ij}^{++} P_i^+ d_j^+ P_j^+ + t_{ij}^{--} P_i^- d_j^- P_j^- + t_{ij}^{-+} P_i^+ d_j^- P_j^+ + t_{ij}^{+-} P_i^- d_j^+ P_j^- \right]$$

$$= \frac{1}{\sqrt{D}} \sum_{(ij)} d_i^\dagger t_{ij} d_j,$$

where the projection operators

$$P_i^+ = n_{if}, \quad P_i^- = 1 - n_{if}$$

and matrix notations

$$d_i = \left( \begin{array}{c} P_i^+ \\ P_i^- \end{array} \right) d_i, \quad t_{ij} = \left( \begin{array}{c} t_{ij}^{++} & t_{ij}^{+-} \\ t_{ij}^{-+} & t_{ij}^{--} \end{array} \right)$$

are introduced. For the Hubbard model it corresponds to the transition to the Hubbard operators

$$H_t = \frac{1}{\sqrt{D}} \sum_{(ij)} a_i^\dagger t_{ij} a_{j\sigma}, \quad a_{\sigma} = \left( \begin{array}{c} \bar{X}_i^{\sigma} \\ \bar{X}_i^{\bar{\sigma}} \end{array} \right).$$

It is obvious that

$$t_{ij}^{\alpha\gamma} = (t_{ji}^{\gamma\alpha})^*$$

and hopping integrals in Eqs. (2.1), (2.2), and (2.5) are connected by the following equations

$$t^{--} = t_1, \quad t^+ = t^+ + t_2, \quad t^{++} = t_1 + t_2 + t_3, \quad t^{++} = t_1 + t_2 + t_3.$$  \hspace{1cm} (2.8)

The total Hamiltonian of the electronic system with local correlations and correlated hopping,

$$H = \sum_i H_i + H_t,$$  \hspace{1cm} (2.9)

includes, besides the hopping term $H_t$ that is not local, the single-site contributions $H_i$. Our aim is to consider the $D \to \infty$ limit, and, as mentioned in Sec. I, it is convenient to start not from the Dyson equation, that considers the terms with correlated hopping $t_2$ and $t_3$ as some kind of many-particle interactions, but from the Larkin equation [11, 12] in a coordinate representation,

$$G_{ij}(\omega) = \Xi_{ij}(\omega) + \sum_{lm} \Xi_{il}(\omega) t_{lm} G_{mj}(\omega),$$  \hspace{1cm} (2.10)

that treats all hopping terms in the same manner. Here an irreducible part (irreducible cumulant [13]) \( \Xi_{ij}(\omega) \), that cannot be divided into parts by cutting one hopping line $t_{im}$, is introduced.

For the models with correlated hopping all quantities in Eq. (2.10) are matrices, e.g., the components of the Green’s function $G_{ij}(\omega)$ are constructed by the projected (Hubbard) operators

$$G_{ij}^{\alpha\gamma}(\tau - \tau') = - \left< (P_i^\alpha d_i^\dagger (d_j^\dagger P_j^\gamma)) \right> = \beta \frac{\delta \Omega}{\delta t_{ij}^{\alpha\gamma}(\tau' - \tau)},$$

$$G_{ij}(\tau - \tau') = - \left< (T d_i(\tau) \otimes d_j^\dagger(\tau')) \right> = \beta \frac{\delta \Omega}{\delta t_{ij}(\tau' - \tau)},$$

(2.11)

where $\Omega$ is a grand canonical potential functional and $\delta t_{ij}^{\alpha\gamma}(\tau' - \tau)$ is some auxiliary field.

After the Fourier transformation to the momentum space one can find the Green’s function as a solution of Larkin equation (2.10),

$$G_k(\omega) = \left[ 1 - \Xi_k(\omega) t_k \right]^{-1} \Xi_k(\omega)$$

$$= \Xi_k^{-1}(\omega) - t_k^{-1},$$  \hspace{1cm} (2.12)

and the total physical Green’s function

$$G_{ij}(\tau - \tau') = - \left< (T d_i(\tau) d_j^\dagger(\tau')) \right> = \frac{\delta \Omega}{\delta t_{ij}(\tau' - \tau)},$$

(2.13)

is equal to the sum of all matrix components

$$G_{ij}(\omega) = \sum_{\alpha\gamma} G_{ij}^{\alpha\gamma}(\omega).$$  \hspace{1cm} (2.14)
In general, an irreducible part $\Xi_{ij}(\omega)$ is represented diagrammatically by the single-site vertices (because all interactions in $H_I$ are local) connected by hopping lines\cite{14} and in the $D \to \infty$ limit it can be shown (see, e.g., Ref. 13) that it becomes local

$$\Xi_{ij}(\omega) = \delta_{ij}\Xi(\omega), \quad \Xi_k(\omega) = \Xi(\omega). \quad (2.15)$$

Such a matrix representation allows one to reformulate the dynamical mean-field theory of systems with correlated hopping in terms of local quantities. Indeed, the local irreducible part $\Xi(\omega)$ depends on the electron hopping only via the local coherent potential (auxiliary $\lambda$ field of Brandt and Mielisch\cite{17})

$$J^{\alpha}(\omega) = \sum_{lm\gamma\delta} t_{\alpha l}^\gamma G_{lm}^{\gamma\delta}(\omega) t_{\delta m}^\alpha \quad (2.16)$$
or, in matrix notations,

$$J(\omega) = \sum_{lm} t_{\alpha l} G_{lm}^{\gamma\delta}(\omega) t_{\delta m} \quad (2.17)$$

where $G_{lm}^{\gamma\delta}(\omega)$ is the Green’s function for lattice with the removed site $\alpha$. On the other hand, we can introduce another quantity

$$I(\omega) = \sum_{lm} t_{\alpha l} G_{lm}(\omega) t_{\delta m} = \frac{1}{N} \sum_k t_k G_k(\omega) t_k \quad (2.18)$$

that is connected with coherent potential [Eq. (2.17)] by the equation

$$I(\omega) = [I - J(\omega)\Xi(\omega)]^{-1} J(\omega). \quad (2.19)$$

From Eqs. (2.17), (2.18) and (2.19) we obtain the following equation for the coherent potential $J(\omega)$:

$$\frac{1}{N} \sum_k [\Xi^{-1}(\omega) - t_k]^{-1} = [\Xi^{-1}(\omega) - J(\omega)]^{-1}, \quad (2.20)$$

that is a matrix generalization of the known one (see, e.g., Ref. 9).

The expression in the right-hand side of Eq. (2.20) is the Larkin representation of the Green’s function,

$$G_{\text{imp}}(\omega) = [\Xi^{-1}(\omega) - J(\omega)]^{-1}, \quad (2.21)$$

for the effective single-impurity problem with the statistical operator

$$\hat{\rho}_{\text{imp}} = e^{-\beta H_0} T \exp \left\{ -\int d\tau \int d\tau' d_\alpha(\tau) J(\tau - \tau') d_{\alpha}(\tau') \right\}. \quad (2.22)$$

Equations (2.20) and (2.21) give the closed set of equations for the local coherent potential $J(\omega)$ and irreducible part $\Xi(\omega)$,

$$\frac{1}{N} \sum_k \left[ G_{\text{imp}}^{-1}(\omega) + J(\omega) - t_k \right]^{-1} = G_{\text{imp}}(\omega), \quad (2.23)$$

$$\Xi^{-1}(\omega) = G_{\text{imp}}^{-1}(\omega) + J(\omega), \quad (2.24)$$

that was derived without introducing of the self-energy for the total Green’s function [Eq. (2.14)]. Solution (2.24) is substituted into the expression for the lattice Green’s function [Eq. (2.12)] that allows one to calculate the total Green’s function (2.14). Below it will be shown for the Falicov–Kimball model with correlated hopping how to solve the effective single-impurity problem, to calculate $G_{\text{imp}}(\omega)$, and to derive the self-energy that is now momentum dependent.

Another advantage of such an approach is in the correct analytic properties of all quantities. In the complex plane they behave as

$$G(z) \to \frac{C_{\Xi}}{z}, \quad J(z) \to \frac{C_J}{z}, \quad (2.25)$$

$$\Xi(z) \to \frac{C_{\Xi}}{z} \quad (2.26)$$

for $|z| \to \infty$, that allows one to build the Lehmann representation for the Green’s functions

$$G_{\text{imp}}(z) = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega \frac{\text{Im} G_{\text{imp}}(\omega - i0^+)}{z - \omega}, \quad (2.27)$$

the irreducible part

$$\Xi(z) = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega \frac{\text{Im} \Xi(\omega - i0^+)}{z - \omega}, \quad (2.28)$$

and the coherent potential

$$J(z) = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega \frac{\text{Im} J(\omega - i0^+)}{z - \omega}. \quad (2.29)$$

The last two equations follows from the definitions of the irreducible part [Eq. (2.10)] and the coherent potential [Eq. (2.17)]. It should be noted that we can, if we wish, introduce a matrix of the local (CPA) self-energies\cite{15} in the same way as in Eq. (1.3) by

$$\Sigma(z) = (z + \mu) I - \Xi^{-1}(z), \quad (2.30)$$

but components of such self-energy matrix do not possess correct analytic properties because $C^{\alpha\alpha}_{\Xi} \neq 1$ and they diverge for $|z| \to \infty$ (see below for the Falicov–Kimball model).

## III. SUMMATION OVER WAVE VECTOR

In Eq. (2.20) the sum over wave vector $\mathbf{k}$ can be calculated directly when we put

$$t_{ij} = a_{ij}, \quad (3.1)$$
where \( a \) is a matrix of the correlated hopping constants. In this case, in (2.20), we can replace the sum over \( k \) by the integral with some density of states \( \rho(t) \)

\[
\frac{1}{N} \sum_k [\Xi^{-1}(\omega) - a t_k]^{-1} = \int d\rho(t) [\Xi^{-1}(\omega) - t a]^{-1} = \int d\rho(t) [a^{-1}\Xi^{-1}(\omega) - t t^\dagger]^{-1} a^{-1}. \tag{3.2}
\]

Matrix \( M = a^{-1}\Xi^{-1}(\omega) \) can be diagonalized by some transformation \( V \),

\[
V^{-1} M V = \begin{pmatrix} z_1 & 0 & \cdots & 0 \\ 0 & z_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & z_s \end{pmatrix} \tag{3.3}
\]

and finally we obtain

\[
G_{\text{imp}} a = V \begin{pmatrix} F(z_1) & 0 & \cdots & 0 \\ 0 & F(z_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & F(z_s) \end{pmatrix} V^{-1}, \tag{3.4}
\]

\[
J = a V \begin{pmatrix} z_1 - \frac{1}{F(z_1)} & 0 & \cdots & 0 \\ 0 & z_2 - \frac{1}{F(z_2)} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & z_s - \frac{1}{F(z_s)} \end{pmatrix} V^{-1}, \tag{3.5}
\]

where

\[
F(z) = \int d\rho(t) \frac{e^t}{z-t} \tag{3.6}
\]

is the Hilbert transform of the density of states \( \rho(t) \).

Now, let us consider some popular densities of states. The Hilbert transform of the Lorentzian density of states

\[
\rho(t) = \frac{W}{\pi} \frac{1}{W^2 + t^2} \tag{3.7}
\]

is equal to

\[
F(z) = \frac{1}{z + iW}, \tag{3.8}
\]

that immediately gives

\[
J(\omega) = \pm iW a. \tag{3.9}
\]

For a Bethe lattice with a semielliptic density of states\(^9\)

\[
\rho(t) = \frac{2}{\pi W^2} \sqrt{W^2 - t^2}, \tag{3.10}
\]

we have

\[
F(z) = \frac{2}{W^2} \left( z - \sqrt{z^2 - W^2} \right), \tag{3.11}
\]

\[
z = \frac{1}{F(z)} = \frac{W^2}{4} F(z) \tag{3.12}
\]

that gives a matrix generalization of the known relation\(^{18}\)

\[
J(\omega) = \frac{W^2}{4} a G_{\text{imp}}(\omega) a. \tag{3.13}
\]

It should be noted that Eqs. (3.4) and (3.5) are correct only when \( \det a \neq 0 \). In other case, a direct decomposition of Eq. (3.2) into simple fractions over \( t_k \) must be used. But results for the particular cases [Eqs. (3.9) and (3.13)] are always correct.

For a density of states different than the Lorentzian and semielliptic ones the iterative procedure is as follows. We start from the initial value for the coherent potential \( J(\omega) \), e.g., that of the Lorentzian density of states [Eq. (3.9)], that is used to calculate the Green’s matrix \( G_{\text{imp}}(\omega) \) for the single impurity problem [Eq. (2.22)] (see below for the Falicov-Kimball model). Then Eq. (2.24) is used to find an irreducible part \( \Xi(\omega) \), Eq. (2.23) is employed to find a new value of \( G_{\text{imp}}(\omega) \), and then Eq. (2.24) is used to find a new coherent potential \( J(\omega) \) value. The algorithm is then repeated until its converges.

**IV. THERMODYNAMICS AND \( \Phi \)-DERIVATIBLE THEORY**

One can see that the DMFT system of equations presented above is a matrix generalization of the known equations for the systems without correlated hopping, with the replacement of the local self-energy by the local irreducible part

\[
\Sigma(\omega) = \omega + \mu - \Xi^{-1}(\omega). \tag{4.1}
\]

However, there are principal difficulties in obtaining expression for the grand canonical potential (free energy). The main idea in derivation of a grand canonical potential in the DMFT is the following.\(^9,\)\(^{17}\) We start from the Baym–Kadanoff functionals for the lattice,

\[
\frac{\Omega_{\text{lat}}}{N} = -\frac{1}{\beta} \sum_{\nu} \frac{1}{N} \sum_k \ln \left[ i\omega_{\nu} + \mu - \Sigma(i\omega_{\nu}) - t_k \right] - \frac{1}{\beta} \sum_{\nu} \frac{1}{N} \sum_k G_k(i\omega_{\nu}) \Sigma(i\omega_{\nu}) + \frac{\Phi_{\text{lat}}}{N}, \tag{4.2}
\]

and the effective single-impurity problem:

\[
\Omega_{\text{imp}} = -\frac{1}{\beta} \sum_{\nu} \ln \left[ i\omega_{\nu} + \mu - \Sigma(i\omega_{\nu}) - J(i\omega_{\nu}) \right] - \frac{1}{\beta} \sum_{\nu} G_{\text{imp}}(i\omega_{\nu}) \Sigma(i\omega_{\nu}) + \Phi_{\text{imp}}. \tag{4.3}
\]

In the case of the absence of correlated hopping the self-energies for the lattice and impurity are local and the same. In addition

\[
\frac{\Phi_{\text{lat}}}{N} = \Phi_{\text{imp}}. \tag{4.4}
\]
and
\[
\frac{1}{N} \sum_k G_k(i\omega) = G_{\text{imp}}(i\omega),
\]
that allows one to exclude an unknown Luttinger–Ward functional and to find the final expression
\[
\frac{\Omega_{\text{lat}}}{N} = \Omega_{\text{imp}} - \frac{1}{\beta} \sum_\nu \left\{ \frac{1}{N} \sum_k \ln |i\omega_{\nu} + \mu - \Sigma(i\omega_{\nu}) - t_k| + \ln G_{\text{imp}}(i\omega_{\nu}) \right\},
\]
But in the case of correlated hopping the self-energy is momentum dependent and it is impossible to write down the Baym–Kadanoff functional for the impurity in the form of Eq. (4.3), and that is the main problem.

In order to solve this problem let us construct the Baym–Kadanoff-type functional without introducing the self-energy. To do this we start from the expression for the Green’s function (2.12) and (2.11) in the Larkin representation
\[
\|G_{\nu}^{\gamma}(\omega)\| = \left\| \frac{\beta}{\delta t_{k_{\nu}}^{\alpha}(\omega)} \right\| = \left[ \mathbb{I} - \Xi_k(\omega) t_k(\omega) \right]^{-1} \Xi_k(\omega),
\]
where we introduce an auxiliary field \( t_k(\omega) = t_k + \delta t_k(\omega) \), and a known relation
\[
\delta \ln \det A = \text{Tr} \left( A^{-1} \delta A \right).
\]
That gives
\[
\frac{\Omega_{\text{lat}}}{N} = \Omega_0 + \frac{\Omega'}{N} - \frac{1}{\beta} \sum_\nu \frac{1}{N} \sum_k \ln \det \left[ \mathbb{I} - \Xi_k(\omega_{\nu}) t_k(\omega_{\nu}) \right],
\]
where \( \Omega_0 \) is the grand canonical potential for the single-site Hamiltonian \( H_i \) (\( t_{ij} = 0 \)) and
\[
\beta \frac{\delta \Omega'}{\delta t_{k_{\nu}}^{\alpha}(i\omega_{\nu})} = - \sum_{k', \nu'} \text{Tr} \left\{ \frac{\delta \Xi_{k'}(i\omega_{\nu})}{\delta t_{k_{\nu}}^{\alpha}(i\omega_{\nu})} t_{k'(i\omega_{\nu})} \right\} + \Xi_{k'(i\omega_{\nu})} \mathbb{I} \Xi_{k(i\omega_{\nu})}^{-1} \left[ \mathbb{I} - \Xi_{k(i\omega_{\nu})} t_k(i\omega_{\nu}) \right]^{-1} \right\}.
\]
As mentioned above, the irreducible part \( \Xi_k(\omega_{\nu}) \) can be diagrammatically represented by the single-site vertices connected by hopping lines \( t_k(i\omega_{\nu}) \). On the other hand, by summing up the series of the diagrams of the same topology, one can see that hopping lines are collected into chains,
\[
\tilde{t}_k(i\omega_{\nu}) = t_k(i\omega_{\nu}) + t_k(i\omega_{\nu}) \Xi_k(i\omega_{\nu}) t_k(i\omega_{\nu}) + \cdots = t_k(i\omega_{\nu}) \left[ \mathbb{I} - \Xi_k(i\omega_{\nu}) t_k(i\omega_{\nu}) \right]^{-1},
\]
and the irreducible part can be represented by some skeletal diagrams with the \( t_k(i\omega_{\nu}) \) replaced by \( \tilde{t}_k(i\omega_{\nu}) \) (spreading of lines). Now we can represent \( \Omega' \) as
\[
\frac{\Omega'}{N} = -\frac{1}{\beta} \sum_\nu \frac{1}{N} \sum_k \text{Tr} \left[ \Xi_k(i\omega_{\nu}) \tilde{t}_k(i\omega_{\nu}) \right] + \frac{\Phi_{\text{lat}}}{N},
\]
where \( \Phi_{\text{lat}} \) is a Luttinger–Ward-type functional:
\[
\beta \frac{\delta \Phi_{\text{lat}}}{\delta \tilde{t}_k^{\alpha}(i\omega_{\nu})} = \Xi_k^{\alpha\gamma}(i\omega_{\nu}).
\]
Finally, for the grand canonical potential functional for the lattice we obtain
\[
\frac{\Omega_{\text{lat}}}{N} = \Omega_0 - \frac{1}{\beta} \sum_\nu \frac{1}{N} \sum_k \ln \det \left[ \mathbb{I} - \Xi_k(i\omega_{\nu}) t_k(i\omega_{\nu}) \right] - \frac{1}{\beta} \sum_\nu \frac{1}{N} \sum_k \text{Tr} \left[ \Xi_k(i\omega_{\nu}) \tilde{t}_k(i\omega_{\nu}) \right] + \frac{\Phi_{\text{lat}}}{N}.
\]
In the limit of infinite dimensions an irreducible part becomes local [Eq. (2.15)], and from Eq. (2.20) it follows that
\[
\frac{1}{N} \sum_k \tilde{t}_k(i\omega_{\nu}) = \tilde{J}(i\omega_{\nu}),
\]
where
\[
\tilde{J}(i\omega_{\nu}) = J(i\omega_{\nu}) \left[ \mathbb{I} - \Xi(i\omega_{\nu}) J(i\omega_{\nu}) \right]^{-1}.
\]
On the other hand, we can write a functional for the impurity in the same form,
\[
\Omega_{\text{imp}} = \Omega_0 - \frac{1}{\beta} \sum_\nu \ln \det \left[ \mathbb{I} - \Xi(i\omega_{\nu}) J(i\omega_{\nu}) \right] - \frac{1}{\beta} \sum_\nu \text{Tr} \left[ \Xi(i\omega_{\nu}) \tilde{J}(i\omega_{\nu}) \right] + \Phi_{\text{imp}},
\]
where
\[
\beta \frac{\delta \Phi_{\text{imp}}}{\delta \tilde{J}^{\alpha}(i\omega_{\nu})} = \Xi^{\alpha\gamma}(i\omega_{\nu}).
\]
From Eqs. (2.15), (4.13), (4.18), and (4.15) it is easy to prove that
\[
\frac{\Phi_{\text{lat}}}{N} = \Phi_{\text{imp}},
\]
and finally we obtain an expression for the grand canonical potential for the lattice in terms of the quantities for the impurity problem
\[
\frac{\Omega_{\text{lat}}}{N} = \Omega_{\text{imp}} - \frac{1}{\beta} \sum_\nu \left\{ \frac{1}{N} \sum_k \ln \det \left[ \mathbb{I} - \Xi(i\omega_{\nu}) t_k \right] - \ln \det \left[ \mathbb{I} - \Xi(i\omega_{\nu}) J(i\omega_{\nu}) \right] \right\},
\]
In the absence of correlated hopping this reduces to the known expression [Eq. (4.6)].

Logarithms in Eq. (4.20) originate from the sum of the loop diagrams,

\[ \text{Tr} \sum_l \frac{1}{T} [\bar{\xi}(i\omega_n)\bar{t}_k]_l \]

and

\[ \text{Tr} \sum_l \frac{1}{T} [\bar{\xi}(i\omega_n)\bar{J}(i\omega_n)]_l, \]

and using analytic properties of the irreducible part [Eq. (2.28)] and the coherent potential [Eq. (2.29)], in Eq. (4.20) one can replace the sum over Matsubara’s frequencies by an integral over real axis, that gives

\[ \frac{\Omega_{\text{lat}}}{N} = \Omega_{\text{imp}} - \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{e^{\beta\omega} + 1} \times \left\{ \frac{1}{N} \sum_k \text{ln} \det \left[ 1 - \bar{\xi}(\omega - i\nu^+)\bar{t}_k \right] \right\} \]

Expression (4.14) and (4.13) are very similar to the one known in the Baym–Kadanoff approach but now, instead of the conjugated quantities the Green’s function \( G_k(i\omega_n) \) and self-energy \( \Sigma_k(i\omega_n) \), we have the renormalized hopping \( \bar{t}_k(i\omega_n) \) and the irreducible part \( \bar{\xi}_k(i\omega_n) \). Such a formal analogy allows us to build a \( \Phi \)-derivable theory starting from functional (4.14) in the same way as done by Baym and Kadanoff.

First of all, for the electron concentration we have

\[ n_1 = -\frac{1}{N} \frac{d\Omega_{\text{lat}}}{d\mu_1} = -\frac{d\Omega_{\text{imp}}}{d\mu_1} \bigg|_{\mu = \text{const}} \]

where a partial derivative is taken over \( \mu \) not in chains \( \bar{t}_k(i\omega_n) \) [Eq. (4.11)]:

\[ \frac{d}{d\mu} = \frac{\partial}{\partial \mu} + \sum_{\alpha,\gamma,\nu_k} \frac{d\bar{t}_k^{\alpha\gamma}(i\omega_n)/d\mu}{\delta t_k^{\alpha\gamma}(i\omega_n)}. \]

Next, for the correlation function (dynamical susceptibility)

\[ \chi_{12} = \frac{dn_1}{d\mu_2} = \frac{dn_2}{d\mu_1} = \frac{1}{N} \frac{d^2\Omega_{\text{lat}}}{d\mu_1 d\mu_2} \]

we obtain an expression that can be represented diagrammatically as

\[ \chi_{12} = \frac{1}{2} - 1 \times 2 + 1 \times 2 = 2, \]

where the full four-vertex is a solution of the Bethe–Salpeter type equation

\[ \text{Here the thick wavy lines represent the renormalized hopping } \bar{t}_k(i\omega_n) [\text{Eq. (4.11)], and} \]

\[ 1 \times 2 = -\frac{d^2\Omega_0}{d\mu_1 d\mu_2} - \frac{1}{N} \frac{d^2\Phi_{\text{lat}}}{d\mu_1 d\mu_2} = \frac{dn_1}{d\mu_2} = \frac{dn_2}{d\mu_1}. \]

\[ \begin{aligned}
1 & \times 2 = -\frac{d^2\Phi_{\text{lat}}}{d\mu_1 d\mu_2} \quad \frac{\omega}{\bar{J}(i\omega_n)} \quad \frac{\delta t_{32}}{\delta t_{32}} = \frac{\delta n_1}{\delta t_{32}} = \frac{\delta n_2}{\delta t_{32}}, \\
1 & \times 3 = -\frac{\delta^2 \Phi_{\text{lat}}}{\delta t_{21} \delta t_{43}} = \frac{\delta^2 \Xi_{12}}{\delta t_{43}} = \frac{\delta^2 \Xi_{34}}{\delta t_{21}}.
\end{aligned} \]

are irreducible vertices that can not be divided into parts by cutting two hopping lines, and it can be shown that in the \( D \rightarrow \infty \) limit all irreducible vertices become local.20

V. FALICOV–KIMBALL MODEL

Now let us apply the developed above approach to the Falicov–Kimball model with correlated hopping. In this case the single-site Hamiltonian \( H_i \) is written as

\[ H_i = -\mu_f n_{if} - \mu_d n_{id} + U n_{id} n_{if} \]

or

\[ H_i = [(U - \mu_d)n_{id} - \mu_f] P_1^+ - \mu_d n_{id} P_2^- = H_1^+ P_1^+ + H_1^- P_2^-. \]

Projection operators \( P_1^+ \) and \( P_2^- \) commute with the total Hamiltonian [Eq. (2.9)] and the statistical operator for the effective single-impurity model [Eq. (2.22)] can be represented as

\[ \hat{\rho}_i = P_1^+ \hat{\rho}_i + P_2^- \hat{\rho}_i, \]

where

\[ \hat{\rho}_i = e^{-\beta H_o^\text{imp}} T \exp \left\{ -\int_0^\beta \int_0^\beta d\tau d\tau' \xi_n^{\alpha}(\tau) J_{\alpha\beta}(\tau - \tau') d_{\alpha}(\tau') \right\} \]

are statistical operators for the noninteracting \( d \) electrons placed in the different fields for the different subspaces \( \alpha = \pm \). As a result, the partition function for the impurity is a sum of the partition functions for the subspaces:

\[ \text{Z}_{\text{imp}} = \text{Tr} \hat{\rho}_{\text{imp}} = e^{-\beta Q_+} + e^{-\beta Q_-}, \]

\[ Q_+ = -\mu_f - \frac{1}{\beta} \ln \left( 1 + e^{\beta(U - \mu_d)} \right) \]

\[ -\frac{1}{\beta} \sum_\nu \ln \left( 1 + \frac{J_{\alpha\beta}^{\text{imp}}(\nu)}{J_{\alpha\beta}^{\text{imp}}(\nu)} \right), \]

\[ Q_- = -\frac{1}{\beta} \ln \left( 1 + e^{\beta U} \right) - \frac{1}{\beta} \sum_\nu \ln \left( 1 + \frac{J_{\alpha\beta}^{\text{imp}}(\nu)}{J_{\alpha\beta}^{\text{imp}}(\nu)} \right), \]
that gives, for the grand canonical potential of the impurity, the following expression
\[ \Omega_{\text{imp}} = -\frac{1}{\beta} \ln \left( e^{-\beta Q_+} + e^{-\beta Q_-} \right). \] (5.7)

From Eq. (5.3) it also follows that components of the Green’s function for the impurity are equal
\[ G_{\text{imp}}^{++}(\omega) = \frac{\langle P^+ \rangle}{\omega + \mu_d - U - J^{++}(\omega)}, \]
\[ G_{\text{imp}}^{--}(\omega) = \frac{\langle P^- \rangle}{\omega + \mu_d - J^{--}(\omega)}, \]
\[ G_{\text{imp}}^{+-}(\omega) = G_{\text{imp}}^{-+}(\omega) = 0. \] (5.8)

The inverse matrix of the irreducible part is equal,
\[ \Xi^{-1}(\omega) = \begin{pmatrix} \frac{\langle P^+ \rangle}{\omega + \mu_d - U - J^{++}(\omega)} & -\frac{\langle J^{--}(\omega) - t_k^+ \rangle}{\langle P^- \rangle} \\ J^{--}(\omega) & \frac{\langle P^- \rangle}{\omega + \mu_d - J^{--}(\omega)} \end{pmatrix}, \]
\[ D_{\text{k}}(\omega) = \begin{pmatrix} \omega + \mu_d - J^{--}(\omega) & -\frac{\langle J^{--}(\omega) - t_k^+ \rangle}{\langle P^- \rangle} \\ J^{--}(\omega) & \omega + \mu_d - J^{--}(\omega) \end{pmatrix}. \] (5.9)

and one can see that in the \(|\omega| \to \infty\) limit its diagonal components diverge faster than \(\omega\) that does not allow to introduce a matrix of the local (CPA) self-energies with correct analytic properties by Eq. (2.30). As a rule, the behavior of the CPA self-energy at the \(\omega \to \pm \infty\) limit is not analyzed considering analytic properties of the BEB CPA.\(^{21,22}\) On the other hand, the components of the irreducible part matrix at \(|\omega| \to \infty\) behave as
\[ \Xi^{++}(\omega) \to \frac{\langle P^+ \rangle}{\omega}; \quad \Xi^{--}(\omega) \to \frac{\langle P^- \rangle}{\omega}, \]
\[ \Xi^{+-}(\omega), \Xi^{-+}(\omega) \to \mathcal{O} \left( \frac{1}{\omega^2} \right). \] (5.10)

that is in agreement with Eq. (2.25).

In the absence of \(f\) particles \(\langle P^+ \rangle = 0\) and \(\langle P^- \rangle = 1\), and we obtain solution for the free electrons,
\[ G_{\text{k}}(\omega) = G_{\text{imp}}^{--}(\omega) = \frac{1}{\omega + \mu_d - t_k^+}, \] (5.11)
whereas for the opposite case, when all sites are occupied by \(f\)-particles \(\langle P^+ \rangle = 1\) and \(\langle P^- \rangle = 0,\)
\[ G_{\text{k}}(\omega) = G_{\text{imp}}^{++}(\omega) = \frac{1}{\omega + \mu_d - U - t_k^+}. \] (5.12)

Here
\[ n_f = \langle P^+ \rangle = \frac{e^{-\beta Q_+}}{e^{-\beta Q_+} + e^{-\beta Q_-}} \] (5.13)
is the \(f\)-particle concentration. In addition, for the \(d\)-particle concentration we have
\[ n_d = \langle d^d \rangle = \frac{1}{\beta} \sum \left[ G_{\text{imp}}^{++}(i\omega_n) + G_{\text{imp}}^{--}(i\omega_n) \right]. \] (5.14)

The coherent potential \(\mathbf{J}(\omega)\) is a solution of Eq. (2.23), and finally for the Green’s function of the lattice we obtain
\[ \mathbf{G}(\omega) = \frac{1}{\mathcal{D}(\omega)} \begin{pmatrix} \omega + \mu_d - U - J^{++}(\omega) & -\frac{\langle J^{--}(\omega) - t_k^+ \rangle}{\langle P^- \rangle} \\ J^{--}(\omega) & \omega + \mu_d - J^{--}(\omega) \end{pmatrix} \]
\[ \mathcal{D}(\omega) = \begin{pmatrix} \omega + \mu_d - J^{--}(\omega) & -\frac{\langle J^{--}(\omega) - t_k^+ \rangle}{\langle P^- \rangle} \\ J^{--}(\omega) & \omega + \mu_d - J^{--}(\omega) \end{pmatrix}. \] (5.15)

In general the total Green’s function [Eq. (2.14)] for a Falicov–Kimball model with correlated hopping can be written in the Dyson representation as
\[ G_{\text{k}}(\omega) = \frac{1}{\omega + \mu_d - \Sigma_{\text{k}}(\omega) - t_k}, \] (5.16)
where
\[ \tilde{t}_k = t_k^{++} \langle P^+ \rangle^2 + t_k^{--} \langle P^- \rangle^2 + (t_k^{+-} + t_k^{-+}) \langle P^+ \rangle \langle P^- \rangle \] (5.17)
is the Hartree (mean-field) renormalized hopping already introduced by Schiller,\(^{10}\) and
\[ \Sigma_{\text{k}}(\omega) = U \langle P^+ \rangle + J_3(\omega) \langle P^+ \rangle \langle P^- \rangle \]
\[ + \frac{U_{1k}(\omega)U_{2k}(\omega) \langle P^+ \rangle \langle P^- \rangle}{\omega + \mu_d - U \langle P^- \rangle - J(\omega) - t_{3k} \langle P^+ \rangle \langle P^- \rangle}, \] (5.18)
is a momentum-dependent (nonlocal) self-energy. Here
\[ U_{1k}(\omega) = U + \left[ t_k^{++} - t_k^{--} \right] \langle P^+ \rangle \langle P^- \rangle \]
\[ + \left[ t_k^{+-} - t_k^{-+} \right] \langle P^+ \rangle \langle P^- \rangle \] (5.19)
\[ U_{2k}(\omega) = U + \left[ t_k^{++} - t_k^{--} \right] \langle P^+ \rangle \langle P^- \rangle \]
\[ + \left[ t_k^{+-} - t_k^{-+} \right] \langle P^+ \rangle \langle P^- \rangle \] (5.20)
describe renormalization of the interaction $U$, and

$$
\tilde{J}(\omega) = J^{++}(\omega)(P^-)^2 + J^{--}(\omega)(P^+)^2
$$

and from Eq. (5.19) we obtain the same result for the self-energy,

$$
\Sigma_k(\omega) = \Sigma_0(\omega) + \Sigma_1(\omega)t_k + \Sigma_2(\omega)t_k^2,
$$

that for the nearest-neighbor hopping $t_k$ contains only local, nearest-neighbor and next-nearest-neighbor contributions. The connection with Schiller’s approach for this case is given in the Appendix. But in a general case of $t_{3k} \neq 0$, when Schiller’s approach is not applied, the self-energy is extended over the whole lattice, see Ref. 22 for a comparison with the BEB CPA.

In Fig. 1 we present the spectral function (imaginary part of the Green’s function) and its components for different relations $t_2/t_1$ ($t_3 = 0$) for the $D = \infty$ hypercubic lattice with nearest-neighbor hopping ($W = 1$, $U = 2$, $T = 0.01$) at half-filling $\mu_d = \mu_f$, $n_f + n_d = 1$.

![Figure 1](image1.png)

**FIG. 1.** (Color online) The spectral function (imaginary part of the Green’s function) and its components for different relations $t_2/t_1$ ($t_3 = 0$) for the $D = \infty$ hypercubic lattice with nearest-neighbor hopping ($W = 1$, $U = 2$, $T = 0.01$) at half-filling $\mu_d = \mu_f$, $n_f + n_d = 1$.

In his paper Schiller\textsuperscript{10} considered the case of

$$
t_{3k} = 0,
$$

and from [Eq. (5.19)] we obtain the same result for the self-energy,

$$
\Sigma_k(\omega) = \Sigma_0(\omega) + \Sigma_1(\omega)t_k + \Sigma_2(\omega)t_k^2,
$$

that for the nearest-neighbor hopping $t_k$ contains only local, nearest-neighbor and next-nearest-neighbor contributions. The connection with Schiller’s approach for this case is given in the Appendix. But in a general case of $t_{3k} \neq 0$, when Schiller’s approach is not applied, the self-energy is extended over the whole lattice, see Ref. 22 for a comparison with the BEB CPA.

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![Figure 2](image2.png)

**FIG. 2.** (Color online) Deviation from the half-filling of the $f$-state occupation as a function of $t_2/t_1$. Parameter values are the same as in Fig. 1.

achieves its maximum at low temperatures. On the other hand, at high temperature $n_f \rightarrow \frac{1}{2}$ for $T \rightarrow \infty$. The gap in the spectrum is at a maximum at $n_f \approx \frac{1}{2}$, and with the decrease of the temperature such a deviation from the half-filling of the $f$ states can lead to a shutdown of the gap and a Mott transition (see Fig. 3).

Now let us consider some limiting cases. In the absence of correlated hopping ($t_2 = t_3 = 0$),

$$
t_{k}^{++} = t_{k}^{--} = t_{k}^{--} = t_{k}^{++} = t_{k}
$$

and

$$
J^{++}(\omega) = J^{--}(\omega) = J^{-+}(\omega) = J^{+-}(\omega) = J(\omega),
$$

that follows from definition (2.17), and we obtain the known result for the Falicov–Kimball model,

$$
\Sigma(\omega) = U \langle P^+ \rangle + \frac{U^2 \langle P^+ \rangle \langle P^- \rangle}{\omega + \mu_d - U \langle P^- \rangle - J(\omega)}
$$

with local self-energy.
Another symmetric point $t_2/t_1 = -1$ corresponds to the case of diagonal hopping matrix ($t_k^- = t_k^+ = 0$) when hopping is allowed only between sites with the same occupancy. In this case we have a binary alloy with atoms of two types distributed stochastically over the lattice, and hopping is restricted between atoms of different types. Now atoms of one subsystem can be treated as impurities for the other subsystem, and it was supposed in Ref. 15 that this case corresponds to two independent bands (independent band limit). In this limit the particular case of $t_3 = 0$ was considered for the one-dimensional Hubbard model when exact results can be obtained.\textsuperscript{23} In Ref. 24 it was shown for the Hubbard model, by the slave-boson mean-field approach, that in this case a direct transition from the superconducting state to the Mott insulator takes place.

A coherent potential matrix in this case is also diagonal ($J^+(\omega) = J^-(\omega) = 0$) and for the Falicov–Kimball model and the semielliptic density of states [Eq. (3.10)] we can obtain analytic expressions

\[ J^{+} (\omega) = \frac{a_{++}^2 W^2}{4} \text{Im} G^{++} (\omega) \]  \hspace{1cm} (5.31)

\[ = \frac{1}{2} \left[ \omega + \mu_d - U \pm i \sqrt{W_+^2 - (\omega + \mu_d - U)^2} \right], \]

\[ J^{-} (\omega) = \frac{a_{--}^2 W^2}{4} \text{Im} G^{--} (\omega) \]  \hspace{1cm} (5.32)

\[ = \frac{1}{2} \left[ \omega + \mu_d \pm i \sqrt{W_-^2 - (\omega + \mu_d)^2} \right], \]

\[ W_{\pm}^2 = a_{\pm\pm}^2 W^2 \langle P^{\pm} \rangle. \]

The Green’s function for the lattice contains two contributions

\[ G^+_{\mathbf{k}} = \frac{\langle P^+ \rangle}{\omega + \mu_d - U - J^+ (\omega) \langle P^- \rangle - t_k \langle P^+ \rangle}, \]  \hspace{1cm} (5.33)

\[ G^-_{\mathbf{k}} = \frac{\langle P^- \rangle}{\omega + \mu_d - J^-(\omega) \langle P^+ \rangle - t_k \langle P^- \rangle} \]  \hspace{1cm} (5.34)

that describe two independent bands originating from two disordered subsystems characterized by their own coherent potentials. The spectral weight function contains two bands

\[ \rho (\omega) = \frac{1}{\pi} \text{Im} G_{\text{imp}} (\omega - \mu - i 0^+) \]

\[ = \langle P^+ \rangle \frac{2}{\pi W_+^2} \sqrt{W_+^2 - (\omega - U)^2} \]

\[ + \langle P^- \rangle \frac{2}{\pi W_-^2} \sqrt{W_-^2 - \omega^2} \]  \hspace{1cm} (5.35)

separated by the gap

\[ \Delta = U - |W_+| - |W_-|, \]  \hspace{1cm} (5.36)

that, in general, is temperature dependent and disappears at some critical value

\[ U_c = |W_+| + |W_-| = W \left( |a_{++}| \sqrt{\langle P^+ \rangle} + |a_{--}| \sqrt{\langle P^- \rangle} \right) \]  \hspace{1cm} (5.37)

(the Mott transition point) that achieves its maximum

\[ U_c^\text{max} = W \sqrt{a_{++}^2 + a_{--}^2} \]  \hspace{1cm} (5.38)

at

\[ n_f = \frac{a_{++}^2}{a_{++}^2 + a_{--}^2}. \]  \hspace{1cm} (5.39)

At half-filling ($\mu_f = \mu_d$, $n_f + n_d = 1$) and for the case $t_3 = 0$, when $a_{--} = 1$, $a_{++} = -1$, and $n_f = n_d = \frac{1}{2}$, the gap does not depend on temperature and disappears at $U_c = W \sqrt{2}$.

The same features can be observed in Fig. 1 [case (d) $t_2/t_1 = -1$] for the Gaussian density of states too, when
different subspaces contribute to different independent subbands. In this case there are no well-defined band edges and there are no exact gap for any value of $U$.

The next simplification of the model corresponds to a system with broken bonds when we have hopping only between the sites not occupied by $f$ particles

$$t^{++}_k = t^{+-}_k = t^{-+}_k = 0, \quad J^{++}(\omega) = J^{+-}(\omega) = J^{-+}(\omega) = 0. \quad (5.41)$$

In other words, lattice sites are occupied stochastically by atoms of two types ("conducting" and "isolating"), and electron hopping is allowed only between atoms of the first type and the influence of other subsystem is considered as disorder (the case of the "diluted" conductor).

Now the total Green’s function [Eq. (5.17)] contains the renormalized hopping

$$\tilde{t}_k = t^{--}_k \langle P^- \rangle^2,$$

and some momentum-dependent (nonlocal) self-energy

$$\Sigma_k(\omega) = U \langle P^+ \rangle + J^{--}(\omega) \langle P^+ \rangle \langle P^- \rangle \quad (5.42)$$
$$+ \frac{[U - J^{--}(\omega) \langle P^+ \rangle - t^{--}_k \langle P^- \rangle]^2 \langle P^+ \rangle \langle P^- \rangle}{\omega + \mu_d - U \langle P^- \rangle - J^{--}(\omega) \langle P^+ \rangle^2 - t^{--}_k \langle P^- \rangle^2 \langle P^- \rangle}.$$

But, in fact, these quantities have no any physical sense. Indeed, in this case the total Green’s function contains two contributions

$$G_k(\omega) = G^{++}_k(\omega) + G^{--}_k(\omega), \quad (5.43)$$
$$G^{++}_k(\omega) = \frac{\langle P^+ \rangle}{\omega + \mu_d - U}, \quad (5.44)$$
$$G^{--}_k(\omega) = \frac{\langle P^- \rangle}{\omega + \mu_d - J^{--}(\omega) \langle P^+ \rangle - t^{--}_k \langle P^- \rangle}, \quad (5.45)$$

where $G^{++}_k(\omega)$ originates from the localized levels of the isolating atoms and $G^{--}_k(\omega)$ describes the one-electron excitations in the disordered conducting system characterized by the coherent potential $J^{--}(\omega)$. For the semielliptic density of states [Eq. (3.10)], we have

$$J^{--}(\omega) = \frac{1}{2} \left[ \omega + \mu_d \pm i \sqrt{W^2 - \langle P^- \rangle - (\omega + \mu_d)^2} \right], \quad (5.46)$$

and the one-particle spectral weight function

$$\rho(\omega) = \frac{1}{\pi} \text{Im}G_{\text{imp}}(\omega - \mu - i 0^+) \quad (5.47)$$
$$= \langle P^+ \rangle \delta(\omega - U) + \langle P^- \rangle \frac{2}{\pi W^2} \sqrt{W^2 - \omega^2}$$

contains the $\delta$-peak from the localized levels and conducting band of the half-width $W_- = W \sqrt{\langle P^- \rangle}$ and their statistical weights are equal to the concentrations of the isolating $\langle P^+ \rangle = n_f$ and conducting $\langle P^- \rangle = 1 - n_f$ atoms, respectively. A critical value of $U$ when a "gap" develops is equal,

$$U_c = W_- = W \sqrt{\langle P^- \rangle}, \quad (5.48)$$

and is a function of the temperature. This limiting case of the Falicov–Kimball model with correlated hopping shows that the explanation of the model behavior in terms of the CPA approach is more appropriate than in the Fermi-liquid language.

VI. SUMMARY

In this paper we presented a general approach to the description of correlated hopping in dynamical mean-field theory, whose application is not limited by the case of the Falicov–Kimball model and can be applied to other models, e.g., Hubbard, $t$-$J$, etc. It is based on the Larkin equation (an expansion over electron hopping around the atomic limit) that considers all hopping terms, including correlated hopping, in the same manner. Another starting point is the local character of the irreducible part (irreducible cumulant) of the Green’s functions, constructed by the projected (Hubbard) operators, in the $D \to \infty$ limit, that is a more general statement than the one about the local character of the self-energy, which in the case of correlated hopping is nonlocal. Such an approach keeps the dynamical mean-field theory local ideology, and allows one to calculate the thermodynamical functions. To do this a grand canonical potential functional of the Baym–Kadanoff-type, that allows one to build a $\Phi$-derivatible theory without introducing the self-energy, was proposed.

As an example, a Falicov–Kimball model with correlated hopping, and its limiting case of a model with broken bonds ("diluted" conductor), were considered when exact analytic results can be obtained. In particular, the temperature-driven Mott transition in the Falicov–Kimball model with correlated hopping was investigated. Such a strong coupling approach for the Falicov–Kimball model with correlated hopping corresponds to the BEB CPA approach for a binary alloy with off-diagonal disorder, and it follows that the BEB CPA becomes exact in the $D = \infty$ limit. In addition, analytic properties of the local self-energies in the BEB theory were considered.

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Appendix: Equivalence to Schiller’s approach

For the case $t_{3k} = 0$ we can find a connection between components of $\Sigma^S$ and $J$ (here and below we use $J^{+-} = J^{++} = J^{--}$ and $\Sigma_{\psi d}^S = \Sigma_{d\psi}^S$) by comparison of Eqs. (5.25) and
(S.8) here and below (S.8) indicates Eq. (8) in the paper by Schiller^10^:

\[ J^{++} = \omega - U + \left( \Sigma_{dd}^S - U - \frac{(\Sigma_{\psi d}^S - t_2)^2}{\Sigma_{\psi \psi}^S} \right) \frac{n_f}{1 - n_f}, \]

\[ J^{--} = \omega + \left( \Sigma_{dd}^S - U - \frac{(\Sigma_{\psi d}^S)^2}{\Sigma_{\psi \psi}^S} \right) \frac{1 - n_f}{n_f}, \quad (A.1) \]

\[ J^{+-} = \omega - \Sigma_{dd}^S + \frac{\Sigma_{\psi d}^S}{\Sigma_{\psi \psi}^S} (\Sigma_{\psi d}^S - t_2). \]

In addition, according to their definition the components of the Green’s function (S.9) are not independent and satisfy the following relation:

\[ (\omega - \Sigma_{dd}^S)G_{dd} - (t_1 + 2\Sigma_{\psi d}^S)G_{\psi d} - \Sigma_{\psi \psi}^S G_{\psi \psi} = 1. \quad (A.2) \]

of the Green’s functions

\[ G^{++} = \frac{\Sigma_{\psi \psi}^S}{t_2^2} \left[ \left( \omega - \Sigma_{dd}^S + \frac{(\Sigma_{\psi d}^S)^2}{\Sigma_{\psi \psi}^S} \right) G_{dd} - t_1 G_{\psi d} \right] \]

\[ = \frac{1 - n_f}{U - \Sigma_{dd}^S + \frac{(\Sigma_{\psi d}^S - t_2)^2}{\Sigma_{\psi \psi}^S}}. \]

\[ G^{--} = \frac{\Sigma_{\psi \psi}^S}{t_2^2} \left[ \left( \omega - \Sigma_{dd}^S + \frac{(\Sigma_{\psi d}^S - t_2)^2}{\Sigma_{\psi \psi}^S} \right) G_{dd} - (t_1 + 2t_2) G_{\psi d} \right] = \frac{n_f}{(\Sigma_{\psi \psi}^S)^2 - \Sigma_{dd}^S}. \]

\[ G^{+-} = \frac{\Sigma_{\psi \psi}^S}{t_2^2} \left[ (t_1 + t_2) G_{\psi d} - \left( \omega - \Sigma_{dd}^S + \frac{\Sigma_{\psi d}^S}{\Sigma_{\psi \psi}^S} (\Sigma_{\psi d}^S - t_2) \right) G_{dd} \right] = 0. \]

A solution of this system of equations with the use of Eq. (A.2) gives

\[ G_{dd} = G^{++} + G^{--}, \]

\[ G_{\psi d} = -\frac{\Sigma_{\psi d}^S}{\Sigma_{\psi \psi}^S} G^{++} - \frac{\Sigma_{\psi d}^S}{\Sigma_{\psi \psi}^S} G^{--}, \]

\[ G_{\psi \psi} = \frac{\Sigma_{\psi d}^S}{\Sigma_{\psi \psi}^S} G^{++} + \frac{\Sigma_{dd}^S}{\Sigma_{\psi \psi}^S} G^{--}. \]

that is equivalent to the solution of Eqs. (S.5) and (S.10) with respect to \( G \):

\[ \hat{G} = -n_f \left( \hat{\Sigma}_{\psi \psi}^S \right)^{-1} - (1 - n_f) \left[ \hat{\Sigma}^S - \left( \begin{array}{cc} U & t_2 \\ t_2 & 0 \end{array} \right) \right]^{-1}. \quad (A.5) \]

For the \( f \)-particle occupation number \( n_f = 1/(e^{\beta \epsilon} + 1) \), where \( \epsilon \) is defined by Eq. (S.11), we have

\[ \epsilon - E_f + \mu - \frac{U}{2} = -\frac{1}{\beta} \sum_{\nu} \ln \left[ \frac{\det \left( U \begin{array}{cc} t_2 \\ 0 \end{array} \right) - \hat{\Sigma}^S(i\omega_{\nu})}{(1 - n_f)^2 \det \hat{\Sigma}^S(i\omega_{\nu})} \right] \]

\[ = -\frac{1}{\beta} \sum_{\nu} \ln \left[ \frac{i\omega_{\nu} + \mu - U - J^{++}(i\omega_{\nu})}{i\omega_{\nu} + \mu - J^{--}(i\omega_{\nu})} \right]. \quad (A.6) \]

On the other hand, from Eqs. (5.9) and (5.6) we have

\[ \epsilon = Q_+ - Q_- = -\mu_f - \frac{1}{\beta} \ln \frac{1 + e^{-\beta(U - \mu_d)}}{1 + e^{\beta \mu_d}} \]

\[ -\frac{1}{\beta} \sum_{\nu} \ln \frac{i\omega_{\nu} + \mu_d - U - J^{++}(i\omega_{\nu})}{i\omega_{\nu} + \mu_d - J^{--}(i\omega_{\nu})} \]

that gives the same result if we use

\[ \frac{1}{\beta} \sum_{\nu} \ln \frac{i\omega_{\nu} + \mu_d - U}{i\omega_{\nu} + \mu_d} = \frac{1}{\beta} \ln \frac{1 + e^{-\beta(U - \mu_d)}}{1 + e^{\beta \mu_d}}. \quad (A.8) \]
J. Hubbard, Proc. Roy. Soc. London, Ser. A 276, 238 (1963).

2 M.E. Foglio and L.M. Falicov, Phys. Rev. B 20, 4554 (1979).

3 M.E. Simon and A.A. Aligia, Phys. Rev. B 48, 7471 (1993).

4 J.E. Hirsch, Physica C 158, 236 (1989); Physica B 199–200, 366 (1994).

5 L. Didukh, Yu. Skorenkyy, Yu. Dovhopaty, and V. Hankevych, Phys. Rev. B 61, 7893 (2000).

6 M.E. Simon, A.A. Aligia, and E.R. Gagliano, Phys. Rev. B 56, 5637 (1997).

7 M. Kollar and D. Vollhardt, Phys. Rev. B 63, 045107 (2001).

8 W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989).

9 A. Georges, G. Kotliar, W. Krauth, and M.J. Rosenberg, Rev. Mod. Phys. 68, 13 (1996).

10 A. Schiller, Phys. Rev. B 60, 15660 (1999).

11 A.I. Larkin, Zh. Eksp. Teor. Fiz. 37, 264 (1959) [Sov. Phys. JETP 37, 186 (1960)].

12 V.G. Vaks, A.I. Larkin, and S.A. Pikin, Zh. Eksp. Teor. Fiz. 53, 281 (1967) [Sov. Phys. JETP 26, 188 (1968)]; 53, 1089 (1967) [ibid. 26, 647 (1968)].

13 W. Metzner, Phys. Rev. B 43, 8549 (1991).

14 A.M. Shvaika, Phys. Rev. B 62, 2358 (2000).

15 J.A. Blackman, D.M. Esterling, and N.F. Berk, Phys. Rev. B 4, 2412 (1971); D.M. Esterling, ibid. 12, 1596 (1975).

16 J. Wojtkiewicz and R. Lemański, Acta Physica Polonica B 32, 3467 (2001).

17 U. Brandt and C. Mielsch, Z. Phys. B 75, 365 (1989); 79, 295 (1990); 82, 37 (1991).

18 H. Kajueter and G. Kotliar, Phys. Rev. Lett. 77, 131 (1996).

19 G. Baym and L.P. Kadanoff, Phys. Rev. 124, 287 (1961); G. Baym, ibid. 127, 1391 (1962).

20 A.M. Shvaika, Physica C 341–348, 177 (2000); J. Phys. Studies 5, 349 (2001).

21 A. Gonis and J.W. Garland, Phys. Rev. B 16, 1495 (1977).

22 K. Koepernik, B. Velický, R. Hayn, and H. Eschrig, Phys. Rev. B 58, 6944 (1998).

23 R. Strack and D. Vollhardt, Phys. Rev. Lett. 70, 2637 (1993).

24 B.R. Bulka, Phys. Rev. B 57, 10303 (1998).