DYNAMICAL MEAN FIELD THEORY OF CORRELATED HOPPING*

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The general Dynamical Mean-Field Theory approach based on the expansion over electron hopping and local nature of the irreducible parts (cumulants) of the Green's functions in infinite dimensions is developed for the description of correlated hopping. In order to calculate the thermodynamical functions the new grand canonical potential functional is proposed that allows to build the Φ-derivatible theory without introducing self-energy.

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It is known that correlated hopping in infinite dimensions leads to the nonlocal self-energy [1]. This result breaks the basic statements of the Dynamical Mean Field Theory (DMFT), which is exact in the limit of infinite dimensions, about the local (single-site) nature of the self-energy [2]. In our report we present an alternative approach to build Dynamical Mean Field Theory of systems with correlated hopping that is based on the expansion over electron hopping around the atomic limit, keeps the DMFT local ideology and allows to calculate the thermodynamical functions.

In general, the hopping term of the Hamiltonian with correlated hopping for the Falicov–Kimball models can be written

$$H_t = \frac{1}{\sqrt{D}} \sum_{\langle ij \rangle} \boldsymbol{d}_i^\dagger \boldsymbol{t}_{ij} \boldsymbol{d}_j, \quad \boldsymbol{d}_i = \begin{pmatrix} P_i^+ \\ P_i^- \end{pmatrix} d_i, \quad \boldsymbol{t}_{ij} = \begin{pmatrix} t_{ij}^{++} & t_{ij}^{+-} \\ t_{ij}^{-+} & t_{ij}^{--} \end{pmatrix}, \tag{1}$$

where the projection operators $P_i^+ = n_{if}$ and $P_i^- = 1 - n_{if}$ are introduced. For the Hubbard model the hopping part of the Hamiltonian can be rewritten in terms of the Hubbard operators

$$H_t = \frac{1}{\sqrt{D}} \sum_{\langle ij \rangle \sigma} \boldsymbol{a}_{i\sigma}^\dagger \boldsymbol{t}_{ij} \boldsymbol{a}_{j\sigma}, \quad \boldsymbol{a}_{i\sigma} = \begin{pmatrix} \sigma X_i^{\bar{\sigma}2} \\ X_i^{0\sigma} \end{pmatrix}. \tag{2}$$

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The total Hamiltonian of the electronic system with local correlations and correlated hopping $H = \sum_i H_i + H_t$ includes, besides the hopping term H_t that is not local, also the single-site contributions H_i and it is convenient to start not from the Dyson equation, that considers the terms with correlated hopping as some kind of many-particle interactions, but from the Larkin equation [3,4] in coordinate representation

$$\begin{aligned} \boldsymbol{G}_{ij}(\omega) &= \boldsymbol{\Xi}_{ij}(\omega) + \sum_{lm} \boldsymbol{\Xi}_{il}(\omega)\boldsymbol{t}_{lm}\boldsymbol{G}_{mj}(\omega), \\ \boldsymbol{G}_{\boldsymbol{k}}(\omega) &= \left[1 - \boldsymbol{\Xi}_{\boldsymbol{k}}(\omega)\boldsymbol{t}_{\boldsymbol{k}}\right]^{-1} \boldsymbol{\Xi}_{\boldsymbol{k}}(\omega) = \left[\boldsymbol{\Xi}_{\boldsymbol{k}}^{-1}(\omega) - \boldsymbol{t}_{\boldsymbol{k}}\right]^{-1} \end{aligned} \tag{3}$$

that treats all hopping terms in a same manner. Here, an irreducible part (irreducible cumulant [5]) $\boldsymbol{\Xi}_{ij}(\omega)$, that can not be divided into parts by cutting one hopping line $\boldsymbol{t}_{lm}$, is introduced.

For the models with correlated hopping all quantities in (3) are matrices and for the Green's functions $\boldsymbol{G}_{ij}(\omega)$ we have the following components constructed by the projected (Hubbard) operators

$$G_{ij}^{\alpha\gamma}(\omega) = -\left\langle T P_i^{\alpha} d_i d_j^{\dagger} P_j^{\gamma} \right\rangle_{\omega} = \beta \frac{\delta\Omega}{\delta t_{ji}^{\gamma\alpha}(\omega)}, \tag{4}$$

where Ω is the grand canonical potential functional.

In the $D \to \infty$ limit it can be shown (see, *e.g.* [5]) that all irreducible parts become local $\boldsymbol{\Xi}_{ij}(\omega) = \delta_{ij}\boldsymbol{\Xi}(\omega)$, $\boldsymbol{\Xi}_{\boldsymbol{k}}(\omega) = \boldsymbol{\Xi}(\omega)$ and such matrix representation allows to reformulate the DMFT of correlated hopping in the terms of local quantities. Indeed, the local irreducible part $\boldsymbol{\Xi}(\omega)$ depends on the electron hopping only through the local coherent potential $\boldsymbol{J}(\omega) = \sum_{lm} \boldsymbol{t}_{ol}\, \boldsymbol{G}_{lm}^{[o]}(\omega)\, \boldsymbol{t}_{mo}$, where $\boldsymbol{G}_{lm}^{[o]}(\omega)$ is the Green's function for the lattice with the removed site o, and both $\boldsymbol{\Xi}(\omega)$ and $\boldsymbol{J}(\omega)$ are solutions of the following system of equations

$$\frac{1}{N}\sum_{\boldsymbol{k}} \left[\boldsymbol{\Xi}^{-1}(\omega) - \boldsymbol{t}_{\boldsymbol{k}}\right]^{-1} = \left[\boldsymbol{\Xi}^{-1}(\omega) - \boldsymbol{J}(\omega)\right]^{-1} = \boldsymbol{G}_{\rm imp}(\omega). \tag{5}$$

Here $\boldsymbol{G}_{\rm imp}(\omega)$ is the Green's function for the effective single-impurity problem with the statistical operator

$$\hat{\rho}_{\rm imp} = \mathrm{e}^{-\beta H_{\rm o}} T \exp\left\{ -\int_0^{\beta} d\tau \int_0^{\beta} d\tau' \boldsymbol{d}_{\rm o}^{\dagger}(\tau) \boldsymbol{J}(\tau - \tau') \boldsymbol{d}_{\rm o}(\tau') \right\}. \tag{6}$$

One can see that the presented above DMFT system of equations is a matrix generalization of the known equations with the replacement of the

self-energy by the irreducible part: $\Sigma(\omega) = \omega + \mu - \Xi^{-1}(\omega)$. But now, the total Green's function $G_{\boldsymbol{k}}(\omega) = \sum_{\alpha\gamma} G_{\boldsymbol{k}}^{\alpha\gamma}(\omega) = [\omega + \mu - \Sigma_{\boldsymbol{k}}(\omega) - \bar{t}_{\boldsymbol{k}}]^{-1}$ can be written in the Dyson representation with nonlocal self-energy and Hartree renormalized hopping in agreement with [1] and it is impossible to derive the grand canonical potential (free energy) functional in the same way as it was done for the systems without correlated hopping [2]. In order to solve this problem we construct the Baym–Kadanoff-type functional without introducing the self-energy starting from the expressions for the Green's function (3) and (4):

$$\Omega_{\rm lat} = -\frac{1}{\beta}\sum_{\nu\boldsymbol{k}} \left\{\ln\det\left[1 - \boldsymbol{\Xi}_{\boldsymbol{k}}(i\omega_\nu)\boldsymbol{t}_{\boldsymbol{k}}(i\omega_\nu)\right] + \mathrm{Tr}\left[\boldsymbol{\Xi}_{\boldsymbol{k}}(i\omega_\nu)\tilde{\boldsymbol{t}}_{\boldsymbol{k}}(i\omega_\nu)\right]\right\} + \tilde{\Phi}. \tag{7}$$

Here
$$\tilde{\boldsymbol{t}}_{\boldsymbol{k}}(i\omega_\nu) = \boldsymbol{t}_{\boldsymbol{k}}(i\omega_\nu)\left[1 - \boldsymbol{\Xi}_{\boldsymbol{k}}(i\omega_\nu)\boldsymbol{t}_{\boldsymbol{k}}(i\omega_\nu)\right]^{-1} \tag{8}$$

and $\tilde{\Phi}$ is the Luttinger–Ward type functional

$$\beta\frac{\delta\tilde{\Phi}}{\delta\tilde{t}_{\boldsymbol{k}}^{\gamma\alpha}(i\omega_\nu)} = \Xi_{\boldsymbol{k}}^{\alpha\gamma}(i\omega_\nu). \tag{9}$$

In the limit of infinite dimensions the irreducible part becomes local and by writing down the grand canonical potential functional for the impurity we obtain the expression for the grand canonical potential of the lattice in terms of the quantities for the impurity model

$$\frac{\Omega_{\rm lat}}{N} = \Omega_{\rm imp} - \frac{1}{\beta N}\sum_{\nu\boldsymbol{k}}\Big\{\ln\det\left[1 - \boldsymbol{\Xi}(i\omega_\nu)\boldsymbol{t}_{\boldsymbol{k}}\right] - \ln\det\left[1 - \boldsymbol{\Xi}(i\omega_\nu)\boldsymbol{J}(i\omega_\nu)\right]\Big\}. \tag{10}$$

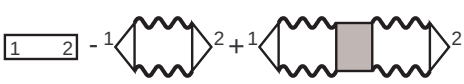
Expressions (7) and (9) are very similar to the one known in the Baym–Kadanoff approach [6], but now instead of the conjugated quantities the Green's function $G_{\boldsymbol{k}}(i\omega_\nu)$ and self-energy $\Sigma_{\boldsymbol{k}}(i\omega_\nu)$ we have the renormalized hopping $\tilde{\boldsymbol{t}}_{\boldsymbol{k}}(i\omega_\nu)$ and irreducible part $\boldsymbol{\Xi}_{\boldsymbol{k}}(i\omega_\nu)$. Such formal analogy allows to build the Φ-derivatible theory starting from the functional (7) in the same way as it was done by Baym and Kadanoff.

First of all, for the electron concentration we have

$$n_1 = -\frac{1}{N}\frac{d\Omega_{\rm lat}}{d\mu_1} = -\left.\frac{d\Omega_{\rm imp}}{d\mu_1}\right|_{\boldsymbol{J}=\mathrm{const}} = -\frac{1}{N}\frac{\partial\tilde{\Phi}}{\partial\mu_1}, \tag{11}$$

where the partial derivative is taken over μ not in chains $\tilde{\boldsymbol{t}}_{\boldsymbol{k}}(i\omega_\nu)$ (8). Next, for the correlation function (dynamical susceptibility) we get an expression that can be presented diagrammatically as [7]

$$\chi_{12} = -\frac{1}{N}\frac{d^2\Omega_{\rm lat}}{d\mu_1 d\mu_2} =$$



, (12)

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

(13)

Here the thick wavy lines represent the renormalized hopping $\tilde{\boldsymbol{t}}_{\boldsymbol{k}}(i\omega_\nu)$ and

$$
\begin{aligned}
\boxed{1 \quad 2} &= -\frac{1}{N}\frac{\partial^2\tilde{\Phi}_{\rm lat}}{\partial\mu_1\partial\mu_2} = \frac{\partial n_1}{\partial\mu_2} = \frac{\partial n_2}{\partial\mu_1},\\
1\triangleleft^{2}_{3} &= \beta\frac{\partial}{\partial\mu_1}\frac{\delta\tilde{\Phi}_{\rm lat}}{\delta\tilde{t}_{32}} = \frac{\partial\Xi_{23}}{\partial\mu_1} = \frac{\delta n_1}{\delta\tilde{t}_{32}},\\
\begin{matrix}1 & & 4\\ 2 & & 3\end{matrix}\!\!\square &= -\beta\frac{\delta^2\tilde{\Phi}_{\rm lat}}{\delta\tilde{t}_{21}\delta\tilde{t}_{43}} = -\frac{\delta\Xi_{12}}{\delta\tilde{t}_{43}} = -\frac{\delta\Xi_{34}}{\delta\tilde{t}_{21}}
\end{aligned}
\qquad (14)
$$

are irreducible vertices that can not be divided into parts by cutting two hopping lines. In the $D \to \infty$ limit all irreducible vertices become local [7].

In this article we presented the general DMFT approach to the description of correlated hopping. It is based on the Larkin equation (expansion over electron hopping) that considers all hopping terms in a same manner. Another starting point is the local character of the irreducible parts (cumulants) of the Green's functions in the $D \to \infty$ limit that is a more general statement than the local character of the self-energy. Such approach keeps the DMFT local ideology and allows to calculate the thermodynamical functions. To do this a new grand canonical potential functional of the Baym–Kadanoff-type that allows to build a Φ-derivatible theory without introducing the self-energy is proposed.

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