AN ANALYTICAL STRONG COUPLING APPROACH IN DYNAMICAL MEAN-FIELD THEORY*

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In the limit of infinite spatial dimensions a thermodynamically consistent theory of the strongly correlated electron systems, which is valid for arbitrary value of the Coulombic interaction ($U < \infty$), is built. For the Hubbard model the total auxiliary single-site problem exactly splits into four subspaces, which describe Fermi and non-Fermi liquid components. Such analytical approach allows to construct different thermodynamically consistent approximations: alloy-analogy approximation, Hartree–Fock approximation, and further, that which describes the self-consistent renormalization of the bosonic excitations (magnons and doublons).

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In the last decade a lot of the rigorous results in the theory of strongly correlated electron systems are connected with the development of the Dynamical Mean-Field Theory (DMFT) proposed by Metzner and Vollhardt [1] for the Hubbard model (see also [2] and references therein). It maps lattice problem on the effective single impurity Anderson model with the generalized partition function

$$\hat{\rho} = \mathrm{e}^{-\beta\hat{H}_0} T \exp\left\{ -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma \zeta_\sigma(\tau-\tau') a_\sigma^\dagger(\tau) a_\sigma(\tau') \right\}, \qquad (1)$$

where $\zeta_\sigma(\tau-\tau')$ is an auxiliary Kadanoff–Baym field (single-site hopping) and for the Hubbard model

$$\hat{H}_0 = U n_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow) - h(n_\uparrow - n_\downarrow) = U n_\uparrow n_\downarrow - \sum_\sigma \mu_\sigma n_\sigma = \sum_p \lambda_p \hat{X}^{pp}, \quad (2)$$

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and there are no restrictions on the U value within this theory. Moreover, some classes of binary-alloy-type models (*e.g.*, the Falicov–Kimball model) can be studied exactly within DMFT [3]. But in the case of the Hubbard model, the treatment of the effective single impurity Anderson model is very complicated and mainly computer simulations are used, which calls for the development of the analytical approaches [4]. For the partition function (1) such approach can be build within a perturbation theory expansion in terms of the electron hopping using a diagrammatic technique for Hubbard operators [5], which is based on the corresponding Wick theorem [6]. In present article we supplement such strong-coupling approach by the consideration of the bosonic fluctuations.

Consecutive pairing of all off-diagonal Hubbard operators X^{pq} is performed until we get the product of the diagonal operators only. For the single impurity problem (1) and (2) all diagonal operators act at the same site, their products can be reduced to the single operators and for the Hubbard model our problem exactly splits into four subspaces with "vacuum states" $|p\rangle = |0\rangle$, $|2\rangle$, $|\uparrow\rangle$ and $|\downarrow\rangle$ and only excitations, as fermionic, as bosonic, around these "vacuum states" are allowed. Finally, for the grand canonical potential we get [5]

$$\Omega_a = -\frac{1}{\beta} \ln \sum_p \mathrm{e}^{-\beta \Omega_{(p)}}, \tag{3}$$

where $\Omega_{(p)}$ are the "grand canonical potentials" for the subspaces. Now we can find the single-electron Green functions by

$$G_\sigma^{(a)}(\tau - \tau') = \frac{\delta \Omega_a}{\delta \zeta_\sigma(\tau - \tau')} = \sum_p w_p G_{\sigma(p)}(\tau - \tau'), \tag{4}$$

where $G_{\sigma(p)}(\tau - \tau')$ are single-electron Green functions for the subspaces characterized by the "statistical weights"

$$w_p = \frac{\mathrm{e}^{-\beta \Omega_{(p)}}}{\sum_q \mathrm{e}^{-\beta \Omega_{(q)}}}. \tag{5}$$

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

$$G^{-1}_{\sigma(p)}(\omega_\nu) = \Xi^{-1}_{\sigma(p)}(\omega_\nu) - \zeta_\sigma(\omega_\nu) \tag{6}$$

and self-energies in subspaces $\Sigma_{\sigma(p)}$ (Dyson equation for the irreducible parts)

$$\Xi^{-1}_{\sigma(p)}(\omega_\nu) = i\omega_\nu + \mu_\sigma - U n^{(0)}_{\bar{\sigma}(p)} - \Sigma_{\sigma(p)}(\omega_\nu), \tag{7}$$

where $n^{(0)}_{\sigma(p)} = -\frac{d\lambda_p}{d\mu_\sigma} = 0$ for $p = 0, \bar{\sigma}$ and 1 for $p = 2, \sigma$. Here, self-energy $\Sigma_{\sigma(p)}(\omega_\nu)$ depends on the hopping integral $\zeta_{\sigma'}(\omega_{\nu'})$ only through quantities

$$\Psi_{\sigma'(p)}(\omega_{\nu'}) = G_{\sigma'(p)}(\omega_{\nu'}) - \Xi_{\sigma'(p)}(\omega_{\nu'}) \,. \tag{8}$$

Now, one can reconstruct expressions for the grand canonical potentials $\Omega_{(p)}$ in subspaces from the known structure of Green functions:

$$\begin{aligned} \Omega_{(p)} = \lambda_p \; &- \; \frac{1}{\beta} \sum_{\nu\sigma} \ln \left[1 - \zeta_\sigma(\omega_\nu) \, \Xi_{\sigma(p)}(\omega_\nu) \right] \\ &- \; \frac{1}{\beta} \sum_{\nu\sigma} \Sigma_{\sigma(p)}(\omega_\nu) \, \Psi_{\sigma(p)}(\omega_\nu) + \Phi_{(p)} \,, \end{aligned} \tag{9}$$

where $\Phi_{(p)}$ is some functional, such that its functional derivative with respect to Ψ produces the self-energy:

$$\beta \frac{\delta \, \Phi_{(p)}}{\delta \, \Psi_{\sigma(p)}(\omega_\nu)} = \Sigma_{\sigma(p)}(\omega_\nu) \,. \tag{10}$$

The second term in (9) corresponds to the sum of the fermionic single loop contributions whereas the next ones describe different scattering processes.

From the grand canonical potential (3) and (9) we get for mean values

$$\begin{aligned} n_\sigma \; &= \; -\frac{d\Omega_a}{d\mu_\sigma} = \sum_p w_p n_{\sigma(p)} \,, \\ n_{\sigma(p)} \; &= \; n^{(0)}_{\sigma(p)} + \frac{1}{\beta} \sum_\nu \Psi_{\sigma(p)}(\omega_\nu) - \frac{\partial \, \Phi_{(p)}}{\partial \mu_\sigma} \,, \end{aligned} \tag{11}$$

where in the last term the partial derivative is taken over μ_σ not in quantities Ψ (8).

Falicov–Kimball model corresponds to the case of $\zeta_\downarrow(\omega_\nu) \equiv 0$ and, as a result, $\Phi_{(p)} \equiv 0$ and $\Sigma_{\uparrow(p)}(\omega_\nu) \equiv 0$ which immediately gives results of [3] (see also [7]).

Presented above equations allow one to construct different thermodynamically consistent approximations.

The simplest *alloy-analogy approximation*, which is a zero-order approximation within the considered approach, is to put $\Phi_{(p)} = 0$, $\Sigma_{\sigma(p)}(\omega_\nu) = 0$ and for the Green's function for the single impurity problem one can obtain a two-pole expression ($\lambda_{pq} = \lambda_p - \lambda_q$)

$$G^{(a)}_\sigma(\omega_\nu) = \frac{w_0 + w_\sigma}{i\omega_\nu - \lambda_{\sigma 0} - \zeta_\sigma(\omega_\nu)} + \frac{w_2 + w_{\bar{\sigma}}}{i\omega_\nu - \lambda_{2\bar{\sigma}} - \zeta_\sigma(\omega_\nu)} \,. \tag{12}$$

Strong coupling Hartree–Fock approximation takes into account the first corrections into the self energy in the form

$$\begin{aligned} \Sigma_{\sigma(p)}(\omega_\nu) &= U\left(n_{\sigma(p)} - n^{(0)}_{\sigma(p)}\right), \\ n_{\sigma(p)} &= n^{(0)}_{\sigma(p)} + \frac{1}{\beta}\sum_\nu \Psi_{\sigma(p)}(\omega_\nu) \end{aligned} \tag{13}$$

which gives for the Green's function a four-pole expression:

$$G^{(a)}_\sigma(\omega_\nu) = \sum_p \frac{w_p}{i\omega_\nu + \mu_\sigma - U n_{\bar\sigma(p)} - \zeta_\sigma(\omega_\nu)}. \tag{14}$$

Now, grand canonical potentials in the subspaces (9) are determined by functional

$$\Phi_{(p)} = U\left(n_{\sigma(p)} - n^{(0)}_{\sigma(p)}\right)\left(n_{\bar\sigma(p)} - n^{(0)}_{\bar\sigma(p)}\right). \tag{15}$$

Expression (14) possesses the correct Hartree–Fock limit for the small Coulombic interaction U and electron or hole concentrations. 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 [5, 8] it was shown that the main contributions come from the subspaces $p = 0$ or 2, that describe the Fermi-liquid component, for the low electron ($n \ll 1$) or hole ($2 - n \ll 1$) concentrations, respectively, ("overdoped regime" of high-T_c's) and $p = \uparrow, \downarrow$, that describe the non-Fermi-liquid component, close to half filling ($n \sim 1$) ("underdoped regime"). At low temperatures the Fermi-liquid component is in the ferromagnetic (Stoner) state, while the non-Fermi-liquid one is antiferromagnetic close to half-filling.

In order to go *beyond the Hartree–Fock approximation* one has to consider, besides the fermionic excitations, also the bosonic ones [5] which correspond to the creation and annihilation of the doublons (pairs of electrons), described by the $\hat X^{20}$ and $\hat X^{02}$ operators, for subspaces $p = 0, 2$ and magnons, described by the $\hat X^{\uparrow\downarrow}$ and $\hat X^{\downarrow\uparrow}$ operators, for $p = \uparrow, \downarrow$. The single loop contributions of such bosonic excitations can be summed up and one can obtain

$$\Phi_{(p)} = \frac{1}{\beta}\sum_m \ln\left[1 - U\left(1 \pm U\tilde D_{\sigma\bar\sigma(p)}(\omega_m)\right)\tilde\chi_{\sigma\bar\sigma(p)}(\omega_m)\right], \tag{16}$$

where

$$\tilde D_{\sigma\bar\sigma(p)}(\omega_m) = \frac{1}{i\omega_m - \lambda_{20} - U\frac{1}{\beta}\sum_\nu\left[\Psi_{\sigma(p)}(\omega_\nu) + \Psi_{\bar\sigma(p)}(\omega_\nu)\right]}, \tag{17}$$

$$\tilde\chi_{\sigma\bar\sigma(p)}(\omega_m) = -\frac{1}{\beta}\sum_\nu \Psi_{\sigma(p)}(\omega_\nu)\,\Psi_{\bar\sigma(p)}(\omega_{m-\nu}) \tag{18}$$

for subspaces $p = 0, 2$ and

$$\tilde{D}_{\sigma\bar{\sigma}(p)}(\omega_m) = \frac{1}{i\omega_m - \lambda_{\sigma\bar{\sigma}} - U\frac{1}{\beta}\sum_\nu \left[\Psi_{\bar{\sigma}(p)}(\omega_\nu) - \Psi_{\sigma(p)}(\omega_\nu)\right]}, \quad (19)$$

$$\tilde{\chi}_{\sigma\bar{\sigma}(p)}(\omega_m) = -\frac{1}{\beta}\sum_\nu \Psi_{\sigma(p)}(\omega_\nu)\,\Psi_{\bar{\sigma}(p)}(\omega_{\nu-m}) \quad (20)$$

for subspaces $p = \sigma, \bar{\sigma}$, which give for mean values the following expression

$$n_{\sigma(p)} = n^{(0)}_{\sigma(p)} + \frac{1}{\beta}\sum_\nu \Psi_{\sigma(p)}(\omega_\nu) \mp \frac{1}{\beta}\sum_m \frac{U^2\tilde{D}^2_{\sigma\bar{\sigma}(p)}(\omega_m)\tilde{\chi}_{\sigma\bar{\sigma}(p)}(\omega_m)}{1 - U\left(1 \pm U\tilde{D}_{\sigma\bar{\sigma}(p)}(\omega_m)\right)\tilde{\chi}_{\sigma\bar{\sigma}(p)}(\omega_m)}. \quad (21)$$

Now the self-energy contains the frequency dependent part

$$\Sigma_{\sigma(p)}(\omega_\nu) = U\left(n_{\bar{\sigma}(p)} - n^{(0)}_{\bar{\sigma}(p)}\right) + \tilde{\Sigma}_{\sigma(p)}(\omega_\nu), \quad (22)$$

$$\tilde{\Sigma}_{\sigma(p)}(\omega_\nu) = U^2\frac{1}{\beta}\sum_m \frac{\left(1 \pm U\tilde{D}_{\sigma\bar{\sigma}(p)}(\omega_m)\right)\tilde{\chi}_{\sigma\bar{\sigma}(p)}(\omega_m) \pm \tilde{D}_{\sigma\bar{\sigma}(p)}(\omega_m)}{1 - U\left(1 \pm U\tilde{D}_{\sigma\bar{\sigma}(p)}(\omega_m)\right)\tilde{\chi}_{\sigma\bar{\sigma}(p)}(\omega_m)} \times \begin{cases} \Psi_{\bar{\sigma}(p)}(\omega_{m-\nu}), & \text{for } p = 0, 2 \\ \Psi_{\bar{\sigma}(p)}(\omega_{\nu-m}), & \text{for } p = \sigma, \bar{\sigma} \end{cases}, \quad (23)$$

that describes the contributions from the doublons for the Fermi liquid component ($p = 0, 2$) and magnons for the non-Fermi liquid one ($p = \uparrow, \downarrow$) with the renormalized spectrum determined by the zeros of denominator in (23).

Expression (16) for functional $\Phi_{(p)}$ has the same form as the correction to free energy in the theory of the Self-Consistent Renormalization (SCR) of spin fluctuations by Moriya [9]. But in our case it describes contributions from the single-site bosonic (magnon or doublon) fluctuations with specific renormalization functions different for different subspaces. Spin fluctuations give the main contribution close to half filling in the non-Fermi liquid regime but for small electron ($n \ll 1$) or hole ($2 - n \ll 1$) concentrations the contributions from the doublon (charge) fluctuations must be taken into account.

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