Two-scale analysis of the Hubbard model

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Abstract

An energy-scale dependent approach, developed within the framework of the Composite Operator Method (COM), for the Hubbard model is proposed. The dynamics is derived from the equations of motion of fermionic composite operators whose high- and low- energy components are treated separately. A fully self-consistent solution which exactly conserves the first spectral moments is found.

Key words: Hubbard model; COM.

The main problem we have to face in describing highly correlated systems is to establish a connection between the high and low scales of energy. The very strong interactions present in these systems generate composite fields with a quite complex dynamics. Methods based on the use of the equations of motion and of the spectral moment conservation usually give a rather reliable description of the high-energy features, but do not reproduce the low-energy physics accurately enough. The choice of an effective expansion basis is the real problem. Recently, a new efficient approach was developed [1], within the framework of the COM, for the investigation of the Kondo and the Anderson models which has permitted to resolve their low-frequency features correctly. The central idea of this approach is to pick up and split the relevant composite fields in two components describing the dynamics at low and high energy, respectively. In the present manuscript we report a proposal regarding the application of this method to the single-band d-dimensional Hubbard model:

$$H = \sum_{\boldsymbol{i},\boldsymbol{j}} (t_{\boldsymbol{ij}} - \mu\delta_{\boldsymbol{ij}}) c^\dagger(i) c(j) + U \sum_{\boldsymbol{i}} n_\uparrow(i) n_\downarrow(i), \quad (1)$$

where $c(i)$ is the annihilation electron operator in spinorial notation, $n_\sigma(i) = c^\dagger_\sigma(i) c_\sigma(i)$, $i = (\boldsymbol{i}, t)$, $\boldsymbol{i}$ is a lattice vector, μ is the chemical potential, $t_{\boldsymbol{ij}} = -2dt\alpha_{\boldsymbol{ij}}$, $\alpha_{\boldsymbol{ij}}$ is the projector on the nearest neighbor sites. $c(i)$ satisfies the Heisenberg equation

$$\mathrm{i}\frac{\partial}{\partial t} c(i) = -\mu c(i) - 2dt c^\alpha(i) + U\eta(i), \quad (2)$$

where $c^\alpha(\boldsymbol{i}, t) = \sum_{\boldsymbol{j}} \alpha_{\boldsymbol{ij}} c(\boldsymbol{j}, t)$ and $\eta(i) = n(i)c(i)$. This latter field satisfies the following equation of motion

$$\mathrm{i}\frac{\partial}{\partial t} \eta(i) = -(\mu - U)\eta(i) + 2dt\pi(i), \quad (3)$$

where $\pi(i) = \sigma^\mu n_\mu c^\alpha(i)/2 + c^{\alpha\dagger}(i)c(i)c(i)$, $n_\mu(i) = c^\dagger(i)\sigma_\mu c(i)$ is the charge ($\mu = 0$) and spin ($\mu = 1, 2, 3$) density operator, $\sigma^\mu = (-\mathbf{1}, \sigma)$ and $\sigma_\mu = (\mathbf{1}, \sigma)$, σ are the Pauli matrices.

Let us introduce the basic composite field

$$\psi^\dagger(i) = (c^\dagger(i), \eta^\dagger(i)) = (\psi_1^\dagger(i), \psi_2^\dagger(i)), \quad (4)$$

and consider the thermal retarded Green's function $G(i,j) = \langle \mathcal{R}\left[\psi(i)\psi^\dagger(j)\right]\rangle$. After Eqs. (2) and (3) we have in the reciprocal space

$$\left[\omega - \varepsilon(\boldsymbol{k})\right] G_{1\nu}(\boldsymbol{k}, \omega) = I_{1\nu}(\boldsymbol{k}) + U G_{2\nu}(\boldsymbol{k}, \omega), \quad (5)$$

where $\nu = 1, 2$, $\varepsilon(\boldsymbol{k}) = -\mu - 2dt\alpha(\boldsymbol{k})$ with $\alpha(\boldsymbol{k}) = \mathcal{F}\left[\alpha_{\boldsymbol{ij}}\right]$ and $I(\boldsymbol{k}) = \mathcal{F}\left[\langle\{\psi(\boldsymbol{i}, t), \psi^\dagger(\boldsymbol{j}, t)\}\rangle\right]$ is the normalization matrix. $\mathcal{F}$ is the Fourier transform.

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In the paramagnetic state we have $I_{11}(\boldsymbol{k}) = 1$ and $I_{12}(\boldsymbol{k}) = I_{21}(\boldsymbol{k}) = I_{22}(\boldsymbol{k}) = n/2$, where n is the electron density.

Finally, we only need to compute the propagator $G_{22}(\boldsymbol{k},\omega)$ in Eq. (5). Without loss of generality we can always decompose the field ψ_2 into its high (ψ_2^H) and low (ψ_2^L) energy components $\psi_2(i) = \psi_2^H(i) + \psi_2^L(i)$ where $\psi_2^L(i)$ satisfies the following dynamics

$$\mathrm{i}\frac{\partial}{\partial t}\psi_2^L(\boldsymbol{k},t) = \gamma_L(\boldsymbol{k})\psi_1(\boldsymbol{k},t). \tag{6}$$

According to this decomposition, we have the following representation of the propagators

$$\begin{aligned} G_{12}(\boldsymbol{k},\omega) &= \sum_a G_{12}^a(\boldsymbol{k},\omega) \\ G_{22}(\boldsymbol{k},\omega) &= \sum_{ab} G_{22}^{ab}(\boldsymbol{k},\omega) \end{aligned} \tag{7}$$

where $a, b = L$, H and

$$\begin{aligned} G_{12}^a(\boldsymbol{k},\omega) &= \mathcal{F}\left\langle \mathcal{R}\left[\psi_1(i)\psi_2^{a\dagger}(j)\right]\right\rangle, \\ G_{22}^{ab}(\boldsymbol{k},\omega) &= \mathcal{F}\left\langle \mathcal{R}\left[\psi_2^a(i)\psi_2^{b\dagger}(j)\right]\right\rangle. \end{aligned} \tag{8}$$

By means of Eqs. (5-8), we can express all Green's functions through $G_{22}^{HH}(\boldsymbol{k},\omega)$ and the four parameters I_{12}^H, I_{12}^L, I_{22}^{LH}, I_{22}^{LL} where

$$\begin{aligned} I_{12}^a(\boldsymbol{k}) &= \mathcal{F}\left[\left\langle\left\{\psi_1(\boldsymbol{i},t), \psi_2^{a\dagger}(\boldsymbol{j},t)\right\}\right\rangle\right] \\ I_{22}^{ab}(\boldsymbol{k}) &= \mathcal{F}\left[\left\langle\left\{\psi_2^a(\boldsymbol{i},t), \psi_2^{b\dagger}(\boldsymbol{j},t)\right\}\right\rangle\right] \end{aligned} \tag{9}$$

To determine $G_{22}^{HH}(\boldsymbol{k},\omega)$ we will set an equation of motion for $\psi_2^H(i)$. In the high energy limit we can safely project Eq. (3) on the basis (4) and obtain:

$$\mathrm{i}\frac{\partial}{\partial t}\psi_2^H(\boldsymbol{k}) = a_1(\boldsymbol{k})\psi_1(\boldsymbol{k}) + a_2(\boldsymbol{k})\psi_2^H(\boldsymbol{k}) \tag{10}$$

where $a_1(\boldsymbol{k}) = 2dt\left[\Delta + \alpha(\boldsymbol{k})\left(p - I_{22}\right)\right]/\left(1 - I_{22}\right)$ and $a_2(\boldsymbol{k}) = -a_1(\boldsymbol{k})/I_{22} + \varepsilon(\boldsymbol{k}) + U$ with $\Delta = \left\langle c^\alpha(i)c^\dagger(i)\right\rangle - 2\left\langle c^\alpha(i)\eta^\dagger(i)\right\rangle$ and $p = \frac{1}{4}\left\langle n_\mu^\alpha(i)n_\mu(i)\right\rangle - \left\langle [c_\uparrow(i)c_\downarrow(i)]^\alpha\, c_\downarrow^\dagger(i)c_\uparrow^\dagger(i)\right\rangle$.

By means of the Eq. (10) we obtain the following relation

$$\left[\omega - a_2(\boldsymbol{k})\right] G_{22}^{HH}(\boldsymbol{k},\omega) = I_{22}^{HH}(\boldsymbol{k}) + a_1(\boldsymbol{k})G_{12}^H(\boldsymbol{k},\omega) \tag{11}$$

which permits to close the system of linear equations for the Green's functions and get

$$G_{11}(\boldsymbol{k},\omega) = \frac{\sigma_{11}^{(0)}(\boldsymbol{k})}{\omega - \varepsilon(\boldsymbol{k}) + \mathrm{i}\delta} + \sum_{n=1}^{5}\frac{\sigma_{11}^{(n)}(\boldsymbol{k})}{\omega - E_n(\boldsymbol{k}) + \mathrm{i}\delta} \tag{12}$$

where $E_n(\boldsymbol{k})$ are the poles of the following equations: $\omega^3 + M_2(\boldsymbol{k})\omega^2 + M_1(\boldsymbol{k})\omega + M_0(\boldsymbol{k}) = 0$ and $\omega^2 - \varepsilon(\boldsymbol{k})\omega - U\gamma_L(\boldsymbol{k}) = 0$ where $M_2(\boldsymbol{k}) = -a_2(\boldsymbol{k}) - \varepsilon(\boldsymbol{k})$, $M_1(\boldsymbol{k}) = -\varepsilon(\boldsymbol{k})a_2(\boldsymbol{k}) - U(\gamma_L(\boldsymbol{k}) + a_1(\boldsymbol{k}))$ and $M_0(\boldsymbol{k}) = U\gamma_L(\boldsymbol{k})a_2(\boldsymbol{k})$. For the sake of brevity, the expressions of the spectral weights will be given elsewhere. It is worth noticing that this solution conserves exactly the first three spectral moments for both fields in the basis.

The Green's functions depend on the following sets of parameters: (i) external: U, T, n ; (ii) internal: $I_{12}^a(\boldsymbol{k})$, $I_{22}^{ab}(\boldsymbol{k})$, $\gamma_L(\boldsymbol{k})$; (iii) internal: μ, Δ, p. We fix the parameters (iii) by means of the following set of the self-consistent equations:

$$\begin{aligned} &n = 2(1 - C_{11}) \\ &\Delta = C_{11}^\alpha - 2C_{12}^\alpha \\ &C_{12} = C_{22} \end{aligned} \tag{13}$$

where $C = \left\langle\psi(i)\psi^\dagger(i)\right\rangle$ and $C^\alpha = \left\langle\psi^\alpha(i)\psi^\dagger(i)\right\rangle$ are correlation functions. The first two equations are dictated by the definitions of the parameters, the third by the Pauli principle and they are all necessary in order to fix the representation of the Green's functions [2].

Exploiting the time-translation invariance of the normalization matrix and the relations among the high- and low- energy components of its entries we get:

$$\begin{aligned} &I_{12}^L(\boldsymbol{k}) = I_{22} - I_{12}^H(\boldsymbol{k}), \\ &\gamma_L(\boldsymbol{k}) = -a_1(\boldsymbol{k}) + b(\boldsymbol{k}), \\ &I_{22}^{LH}(\boldsymbol{k}) = \left[-a_1(\boldsymbol{k})I_{22} + I_{12}^H(\boldsymbol{k})b(\boldsymbol{k})\right]/a_2(\boldsymbol{k}), \\ &I_{22}^{LL}(\boldsymbol{k}) = d(\boldsymbol{k}) + I_{22} - 2a_1(\boldsymbol{k})/U - g(\boldsymbol{k}), \\ &I_{22}^{HH}(\boldsymbol{k}) = d(\boldsymbol{k}) + g(\boldsymbol{k}), \end{aligned} \tag{14}$$

where $b(\boldsymbol{k}) = I_{22}\left[\varepsilon(\boldsymbol{k}) + U\right] - a_2(\boldsymbol{k})I_{12}^H(\boldsymbol{k})$, $d(\boldsymbol{k}) = a_1(\boldsymbol{k})\left[I_{22}/a_2(\boldsymbol{k}) + 1/U\right]$ and $g(\boldsymbol{k}) = I_{12}^H(\boldsymbol{k})\left[(a_2(\boldsymbol{k}) - \varepsilon(\boldsymbol{k}))/U - b(\boldsymbol{k})/a_2(\boldsymbol{k})\right]$. As a result, Eqs. (14) establish the dependence of all the other parameters (ii) on $I_{12}^H(\boldsymbol{k})$. The last self-consistent equation, the one setting $I_{12}^H(\boldsymbol{k}) = a_1(\boldsymbol{k})/a_2(\boldsymbol{k})$, can be obtained from the requirement that the Green's function $G_{11}(\boldsymbol{k},\omega)$ does not have a pole at $\omega = \varepsilon(\boldsymbol{k})$ (i.e., by setting $\sigma_{11}^{(0)}(\boldsymbol{k}) = 0$).

In conclusion, we have proposed a fully self-consistent formulation, derived from the COM and positively tested on impurity systems [1], to study the coexistence of high- and low- energy scales in the d-dimensional Hubbard model. The computational implementation is still in progress.

References

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