A Nonperturbative Approach to One-Particle Green’s Function

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A nonperturbative method to obtain on- and off-site one-particle Green’s function is introduced and applied to noninteracting Hubbard model with next nearest neighbor hopping and interacting Hubbard model in large dimensions, for example. The former gives some lessons on the method and shows the advantage of the method compared with continued fraction formalism. The latter is treated by selecting important dynamic processes contributing to the Green’s function when correlation is strong. We consider the model in the Bethe lattice with large connectivity. The dynamic processes describing on-site spin fluctuation clearly shows metal-insulator transition in the paramagnetic ground state at half filling.

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One of recent interesting subjects in condensed matter physics is the phenomena of the strongly correlated systems. A typical characteristic of the strongly correlated system is the hardness of getting reasonable solution in terms of the traditional perturbative method. The Hubbard model, for instance, is one of typical strongly correlated systems and is recently revisited with great interest as a possible model for high temperature superconductor. This model has not been solved exactly except some of statics in one dimension via Bethe ansatz even though it looks simple. Recently, however, the statics and dynamics of the Hubbard model have been treated exactly in large dimensions, where mean-field approximation is valid, with help of numerical techniques. These exact solutions show interesting behaviors such as band collapsing and quasiparticle mass enhancement near Mott-Hubbard transition, which usual perturbative method cannot show. In finite dimensions, however, only numerical methods such as exact diagonalization and quantum Monte Carlo method have shown some meaningful results even though they have severe limitations. Therefore, an effective nonperturbative method is badly required.

This Letter reports a novel method to calculate one-particle Green’s function nonperturbatively. The Green’s function is usually obtained by summing Feynman diagrams or truncating equation of motion for the Green’s function. The former is well-known and solid in its foundation, but it is perturbative in principle and the latter suggested by Zubarev needs truncation at very low level. The famous works of Hubbard have been done using the latter method. But the results are only partly acceptable. The method we present here is very simple in its form and has never been used before as far as we know. We test the effectiveness of the method by solving finite-size noninteracting Hubbard model and interacting Hubbard model in large dimensions.

In this work, we treat the retarded Green’s function which is related to other types of Green’s functions such as time-ordered and thermal Green’s function and to physical quantities such as single-particle density of states (DOS) and internal energy directly. The well-known one-particle retarded Green’s function in real space is

$$G_{jk}(t) = -i\theta(t)\langle\{c_{j\sigma}(t), c_{k\sigma}^{\dagger}(t)\}\rangle \quad (1)$$

and its Fourier transform is

$$G_{jk}(\omega + i\epsilon) = -\frac{i}{2\pi} \int_{0}^{\infty} \langle\{c_{j\sigma}(t), c_{k\sigma}^{\dagger}(t)\}\rangle \exp^{i\omega t - \epsilon t} dt, \quad (2)$$

where the superscript R denotes the notation of the retarded Green’s function. Let’s notice that the main part of Eq. (1) is the projection of the time evolution $c_{j\sigma}(t)$ onto $c_{k\sigma}$ in the Liouville space whose inner product is defined as

$$(f, g) \equiv \langle\{f, g\}\rangle, \quad (3)$$

where $f$ and $g$ are vectors of the Liouville space and the angular brackets mean ensemble average, and Eq. (2) is the Laplace transform of $\langle\{c_{j\sigma}(t), c_{k\sigma}^{\dagger}(t)\}\rangle$. Thus our interest to get the Green’s function (1) or (2) is in the projection $\langle\{c_{j\sigma}(t), c_{k\sigma}^{\dagger}(t)\}\rangle$. Let us assume that we have a complete set of orthogonal bases $\{\epsilon_{\nu}\} = 1, 2, \cdots, \infty$ where $\epsilon_{1} = c_{j\sigma}$, which spans the Liouville space describing the dynamics of $c_{j\sigma}(t)$. Thus the time evolution $\epsilon_{1}(t) = c_{j\sigma}(t)$ can be described in terms of these bases,

$$\epsilon_{1}(t) = \sum_{\nu=1}^{\infty} A_{\nu}(t) \epsilon_{\nu}. \quad (4)$$

Here $A_{1}(t) = (\epsilon_{1}(t), \epsilon_{1})/(\epsilon_{1}, \epsilon_{1}) = \langle\{c_{j\sigma}(t), c_{j\sigma}^{\dagger}(t)\}\rangle$ is just the projection we are interested in Eqs. (1) and (2). To get $A_{1}(t)$, we apply the operator identity $\partial/\partial t = i\hbar L$ to Eq. (4), where $L$ is the Liouville operator and we set $\hbar = 1$. Then one obtains

$$\sum_{\nu=1}^{\infty} \dot{A}_{\nu}(t) \epsilon_{\nu} = \sum_{\nu=1}^{\infty} A_{\nu}(t) i\hbar \epsilon_{\nu}. \quad (5)$$
Taking inner product in both sides of Eq. (3) with $e_\mu$, one gets a system of linear equations for $A_\nu(t)$ such that
\[
A_\mu(t) = \sum_{\nu=1}^{\infty} M_{\mu \nu} A_\nu(t) \quad (6)
\]
for $\mu = 1, 2, \cdots, \infty$, where $M_{\mu \nu} = \frac{(iLe_\mu e_\nu)}{\langle c_{\nu}^\dagger c_{\nu} \rangle}$. Laplace transform of Eq. (3) is written as $z A_1(z) - 1 = \sum_{\nu=1}^{\infty} M_{\mu \nu} A_\nu(z)$ for $\mu = 1$ and $z A_\nu(z) = \sum_{\nu=1}^{\infty} M_{\mu \nu} A_\nu(z)$ for $\mu \geq 2$. Use of the boundary conditions $A_1(t = 0) = 1$ and $A_\nu(t = 0) = 0$ for $\nu \geq 2$ has been made. These equations can be represented in a matrix form
\[
(zI - M) A_c = B_c, \quad (7)
\]
where $I$ is unit matrix and $A_c$ and $B_c$ are column matrices with elements $A_1(z), A_2(z), A_3(z), \cdots$ and 1, 0, 0, $\cdots$, respectively. Using Cramer’s rule, one gets
\[
A_1(z) = \frac{\text{cofactor of } (zI - M)_{11}}{\det(zI - M)} \quad (8)
\]
and
\[
A_\nu(z) = \frac{\text{cofactor of } (zI - M)_{1\nu}}{\det(zI - M)} \quad (9)
\]
for $\nu \geq 2$, where numerators are cofactors of the elements in $\det(zI - M)$.

It is well-known that the single-particle DOS $\rho_\sigma(\omega)$ is given by the one-particle retarded Green’s function at the same site $[12]$, i.e.
\[
\rho_\sigma(\omega) = -\frac{2}{N} \lim_{\epsilon \to 0^+} \sum_j \text{Im} G_{j j}^R(\omega + i\epsilon) \quad (10)
\]
\[
= \frac{1}{\pi} \lim_{\epsilon \to 0^+} \text{Re} A_1(z)|_{z = -i\omega + \epsilon}. \quad (11)
\]

On the other hand, the off-site retarded Green’s function $G_{j j}^R(\omega + i\epsilon)$ is given by $A_\nu(z)$ of Eq. (9) when $e_\nu = c_{k\sigma}$. Therefore, our task is to get one-particle retarded Green’s function to construct orthogonal bases describing the dynamics of the fermion operator, $c_{j \sigma}(t)$, first and calculate the matrix elements $M_{\mu \nu}$ of Eq. (3).

This is a right place to give a remark on this formalism. One may consider the operators $(iL)^\nu c_1$ as a complete set of linearly independent bases and construct orthogonal bases in terms of Gram-Schmidt process. Then we have the following recurrence relation $[14] - [16]$
\[
e_{\nu+1} = iLe_\nu - \alpha_\nu e_\nu + \Delta_\nu e_{\nu-1}, \quad (12)
\]
where $e_0 \equiv 0$, $\alpha_\nu = \frac{(iLe_\nu e_\nu)}{\langle c_{\nu}^\dagger c_{\nu} \rangle}$ and $\Delta_\nu = \frac{\langle c_{\nu+1} c_{\nu+1} \rangle}{\langle c_{\nu}^\dagger c_{\nu} \rangle}$, when the inner product satisfies the relation $(iLe_\nu, e_\nu) = -(e_\nu, iLe_\mu)$ which implies the time-reversal symmetry of the inner product. Therefore, when inner product contains equilibrium average such as Eq. (3), this relation is always satisfied.

The recurrence relation (12) makes the matrix elements $M_{\mu \nu}$ vanish for $|\nu - \mu| \geq 2$, since inner products $(iLe_\nu, e_\nu)$ vanish, and this reduces the determinants of Eq. (8) to tridiagonal forms. Then $A_1(z)$ can be written as a well-known infinite continued fraction $[14] - [16]$
\[
A_1(z) = \frac{1}{z - \alpha_1 + \frac{\Delta_1}{z - \alpha_2 + \frac{\Delta_2}{z - \alpha_3 + \cdots}}}. \quad (13)
\]

However, it is practically hard to construct orthogonal bases using $(iL)^\nu c_1$ and impossible to get off-site Green’s function. More recommendable way is to find linearly independent bases intuitively with help of $(iL)^\nu c_1$ which generates all kinds of linearly independent operators.

The author and Kee [7] have studied the Hubbard model using recurrence relation (12) and continued fraction (13) in terms of the bases obtained by large-$U/t$ expansion. Even though the bases were orthogonal, they did not satisfy the recurrence relation for whole region of $U/t$. Therefore, the continued fraction formalism cannot describe the physics of intermediate and low $U/t$ regime. For this reason, the experiment for insulating $V_2O_3$ [13] has been explained very well. [13] Similar method has been applied to doped Hubbard model with large-$U/t$ and shown characteristic features of La- and Nd-based doped cuprates quite well. [20] To describe the transition regime well one must use present formalism instead of continued fraction (13).

We present here a tutorial example of our formalism using noninteracting Hubbard model on 4-site lattice with next nearest neighbor hopping, i.e.
\[
H_0 = -t(c_1^\dagger c_2 + c_2^\dagger c_3 + c_3^\dagger c_4 + c_4^\dagger c_1 + h.c.)
+ t'(c_1^\dagger c_3 + c_2^\dagger c_4 + h.c.). \quad (14)
\]

We first consider $t' = 0$ case. One naturally selects $c_1, c_2, c_3, c_4$ as 4-orthogonal bases $c_1, c_2, c_3, c_4$. Using these bases Eq. (8) gives $A_1(z) = (\frac{2}{t} + 2t^2)/[z^2 + 4t^2]$ and $\rho(\omega) = \frac{1}{\pi} \frac{1}{2} \delta(\omega) + \frac{1}{\pi} \frac{1}{2} \delta(\omega - 2t) + \frac{1}{\pi} \frac{1}{2} \delta(\omega + 2t)$. On the other hand, $A_2(z)$ and $A_3(z)$ give off-site Green’s functions as $G_{12}^R(z) = \frac{1}{z + \frac{2t}{t}}$ and $G_{13}^R(z) = \frac{\Delta_1}{z^2 + 4t^2}$, respectively. One can also easily construct orthogonal bases using $(iL)^\nu c_1$, i.e., Eq. (12). If we choose $c_1 = c_3$, then Eq. (14) gives $e_2 = it(c_2 + c_4)$, $e_3 = -2t^2 c_3$, and $e_4 = 0$. $(iL)^\nu c_1$ for $\nu \geq 3$ are no longer linear independent vectors. Eq. (13) and Eq. (14) give rise to the same $A_1(z)$ and $\rho(\omega)$ as above. However, this does not give off-site Green’s function.
Including next nearest hopping discriminates two methods. The first approach raises no difficulty in treating next nearest hopping, while the second raises big complexity in constructing orthogonal bases. The first method easily gives $A_1(z) = \frac{z^3 + (2t^2 + t^2)z + 2it^4t^z}{z^3 + (4t^2 + 2t^2)z^2 + 8it^4t^z - 4t^4t^2 + t^4}$ from Eq. (8).

This trivial example gives us some lessons about this method. First, the bases represent possible independent ways of annihilating fermion at a particular site. Second, the bases obtained intuitively also give the same result as one obtained by using recurrence relation and continued fraction, while this does not give off-site Green’s function and meets great complexity when next nearest neighbor hopping is included. Third, one can figure out the meaning of bases, e.g. $t^2c_3$ means annihilation at site 1 after twice hopping from site 3. Therefore, one can construct bases describing $c_j(t)$ by considering the roles of bases intuitively. It is safe to be guided by Eq. (12) when one constructs independent bases intuitively.

As a meaningful example of constructing bases by considering their roles, we treat the half-filled Hubbard model in large dimensions. In describing $c_{j,\sigma}(t)$, where $\sigma$ denotes up-spin, one must consider all possible processes while an up-spin electron at site $k$, which represents all lattice sites including $j$, hops, arrives at site $j$, and annihilates. For the strongly correlated case ($U > t$), where $U$ and $t$ are on-site Coulomb interaction and hopping integral, respectively, the down-spin number fluctuation (on-site spin fluctuation) when up-spin exists at the same site is the most effective part in a basis representing the process of the same order of energy, because it yields $U$ for each fluctuation.

We consider the Bethe lattice with arbitrarily large connectivity, which is rather easy since the mean-field approximation is valid. We show the metal-insulator transition in the paramagnetic ground state for the half-filled Hubbard model by calculating the single-particle density of states [1]. This is the well-known phenomenon studied by Hubbard [2] and Brinkman and Rice [21] long time ago. Recently the infinite dimensional model has been studied exactly by several authors. [3, 4, 5]

The interacting Hubbard model is written as

$$H = -t \sum_{j,k,\sigma} c_{j,\sigma}^\dagger c_{k,\sigma} + \frac{U}{2} \sum_{j,\sigma} n_{j,\sigma} n_{j,-\sigma}. \quad (15)$$

We consider only nearest neighbor hopping. To construct bases, we choose $c_1 = c_{j,\sigma}$ as before and consider down-spin fluctuation at each site where up-spin electron hops. We collect the dominant processes describing down-spin number fluctuation and neglect hopping dominant processes such as hopping without down-spin number fluctuation. The bases are written as

$$e_{2\nu-1} = (-U)^{\nu-1} \prod_{k}^{\nu-2} \prod_{pq}^{\nu-1} t_{jk} \cdots t_{pq}.$$

We use $\nu = 1, 2, \ldots$ for the bases obtained intuitively also give the same result as

$$\nu = 1, 2, \ldots$$

for $\nu \geq 1$, where $\delta n_{j,\sigma} = n_{j,\sigma} - \langle n_{j,\sigma} \rangle$, $\nu$ above the overlbrace denotes the number of the same symbols, and the prime means that all site indices under summation sign are different each other. The orthogonality of above bases is retained by site-difference and the prime means annihilation at site 1 after

$$t_{jk} \cdots t_{pq}$$

with large connectivity. Once matrix elements $M_{\nu,\nu}$ are obtained as follows in terms of the definition of inner product [3] and the mean-field approximation neglecting spatial correlations, e.g. $\langle n_{j,\sigma}n_{k,\sigma} \rangle = \langle n_{j,\sigma} \rangle \langle n_{k,\sigma} \rangle$ for $j \neq k$, which is valid in the limit of large connectivity:

$$M_{\nu,\nu} = \frac{-iU}{2}, \quad M_{2\nu-1,2\nu} = \frac{-U^2}{4}, \quad M_{2\nu,2\nu-1} = 1,$$

$$M_{2\nu,2\nu+1} = \frac{-t^2}{2}, \quad M_{2\nu+1,2\nu} = \frac{1}{2},$$

$$M_{2\nu-1,2\nu+2} = \frac{U^2t^2}{8}, \quad M_{2\nu+2,2\nu-1} = \frac{-2}{U^2} \quad (18)$$

for $\nu \geq 1$, where we scale $t$ as $t \equiv \sqrt{\nu}$. The energy finite for large coordination. All other matrix elements vanish because electron leaving $j$ site cannot come back to the original site via nearest neighbor hopping. In calculating the matrix elements, use of the approximation $q - 1 \approx q$ in addition to mean-field approximation has been made, which is good enough for a system with large connectivity. Once matrix elements $M_{\nu,\nu}$ are obtained, the single-particle DOS can be given by Eq. (11).

Fig. 1 shows the results of the single-particle DOS for various $U/t_s$. The rank of the matrix $M$ is 101. The metal-insulator transition is clearly shown at $U_c = 2t_s$, by showing band collapsing from insulating side and quasiparticle mass enhancement via disappearance of Fermi liquid quasiparticle band from metallic side.

As a conclusion, we introduced a nonperturbative method calculating the one-particle Green’s function and applied it to a simple tutorial model and the half-filled Hubbard model on a Bethe lattice with large connectivity. The former provides some lessons on this new method and shows advantages compared with continued fraction formalism, while the latter shows interesting
Mott-Hubbard transition by collecting orthogonal bases describing important dynamical processes of strong correlation.

The most crucial part of this method is the construction of orthogonal bases which describe the various situation of electron annihilation processes. These processes are obviously very complicated. However, as an approximation, one can select some important processes which play a major role in a particular parameter regime. The second example shows this well. Therefore, this formalism may provide a possibility to treat the strongly correlated systems in lower dimensions, which is a great challenging problem in current condensed matter physics. More applications of this formalism will follow.

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