Convergence of continued-fraction representation for the Green's function in the Hubbard model

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Using the operator algebra technique with a set of projection operators generated from the primary operator defined by Wilson's group [S. K. Kim and R. S. Wilson, Phys. Rev. A 7, 1396 (1973)], we set up a continued-fraction representation for the single-particle Green's function in the Hubbard model. We find that, in a simple one-dimensional system with five lattice points, at least one cutoff stage appears in the representation.

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One of the most popular ways to investigate transport phenomena in condensed matter systems is the following technique. The transport coefficients are expressed in terms of the relaxation functions which are the Laplace transform (LT) of time-correlation functions or Green's functions of dynamical variables.

Among the several approaches to this problem reported so far, the continued-fraction representation (CFR) developed by some authors [1–5] has drawn the attention of the present authors. We, however, encounter frequently the question of whether the CFR is convergent or has any cutoff stage in order that any numerical result can be obtained.

The purpose of this paper is to show that the CFR for the single-particle Green's functions (SPGF) may have at least one cutoff stage. We choose the Hubbard model [6] as our example, since this model is one of the typical models adopted in the present time condensed matter physics [7].

The SPGF, in the ω space, is defined in the unit system in which $\hbar=1$ as

$$\tilde{G}_{ij\sigma}(\omega)=\langle\{a_{i\sigma},a_{j\sigma}^{\dagger}(\bar{\omega})\}\rangle\ , \tag{1}$$

where $a_{j\sigma}^{\dagger}(\bar{\omega})$ is the LT of $a_{j\sigma}^{\dagger}(t)\equiv\exp(iLt)a_{j\sigma}^{\dagger}$. Here $a_{j\sigma}^{\dagger}$ ($a_{j\sigma}$) is the fermion creation (annihilation) operator for the Wannier state at lattice site $\vec{R}_j$ and the spin state $|\sigma\rangle$; $\{A,B\}$ is the anticommutator; $\langle A\rangle$ means the grand canonical average of any operator A; $\bar{\omega}=\omega-i\varepsilon(\varepsilon\to 0^{+})$ for the frequency ω; and L is the Liouville operator corresponding to the Hubbard Hamiltonian defined by

$$H=\frac{I}{2}\sum_{j\sigma}n_{j-\sigma}n_{j\sigma}-\mu\sum_{j\sigma}n_{j\sigma}+\sum_{\langle ij\rangle\sigma}(t_{ij}a_{i\sigma}^{\dagger}a_{j\sigma}+\text{H.c.})\ , \tag{2}$$

where $n_{j\sigma}\equiv a_{j\sigma}^{\dagger}a_{j\sigma}$, I is the intra-atomic Coulomb repulsion factor, μ the chemical potential, and t_{ij} the matrix element for the hopping from site j to nearest neighbor site i. Hereafter we will drop the subscripts ij on t, assuming that the hopping intensity is constant throughout the system.

Now, in order to obtain the Dyson equation in the CFR, we set up a Hilbert space with the basis vectors $a_{i\sigma}^{n}(\bar{\omega})$ $(n=1,2,3,\ldots)$ as

$$a_{i\sigma}^{n}(\bar{\omega})\equiv(\bar{\omega}-L_n)^{-1}a_{i\sigma}^{n}\ , \tag{3}$$

where $a_{i\sigma}^{n}\equiv L_n a_{i\sigma}^{n-1}$ and $a_{i\sigma}^{0}\equiv a_{i\sigma}$. Here the nth Liouville operator L_n is defined as $L_n\equiv(1-P_{n-1})L_{n-1}$ and $L_0\equiv L$ where the projection operators P_n are defined as

$$P_0X\equiv\sum_j a_{j\sigma}^{\dagger}\langle\{a_{j\sigma},X\}\rangle \tag{4}$$

for $n=0$ following Kim and Wilson [8] and

$$P_nX\equiv a_{j\sigma}^{n\dagger}\frac{\langle\{a_{i\sigma}^{n},X\}\rangle}{\langle\{a_{i\sigma}^{n},a_{j\sigma}^{n\dagger}\}\rangle} \tag{5}$$

for $n\neq 0$. We then obtain the Dyson equation in the CFR as

$$\sum_l\left[\bar{\omega}\frac{\delta_{il}}{\delta_{ij}}-\omega_0+\cfrac{\Delta_1}{\bar{\omega}-\omega_1+\cfrac{\Delta_2}{\bar{\omega}-\omega_2+\cfrac{\Delta_3}{\bar{\omega}-\omega_3+\cdots}}}\right]\tilde{G}_{lj\sigma}(\bar{\omega})=1\ , \tag{6}$$

where the modified frequency factor ω_0, the characteristic frequency ω_n, and the reciprocal decay time $(\Delta_n)^{1/2}$ are given as

$$\omega_0\equiv\frac{\langle\{a_{i\sigma},La_{j\sigma}^{\dagger}\}\rangle}{\delta_{ij}}\ , \tag{7}$$

$$\omega_n\equiv\frac{\langle\{a_{i\sigma}^{n},L_na_{l\sigma}^{n\dagger}\}\rangle}{\langle\{a_{i\sigma}^{n},a_{l\sigma}^{n\dagger}\}\rangle}\quad(n\neq 0)\ , \tag{8}$$

$$\Delta_n\equiv\frac{\langle\{a_{i\sigma}^{n},a_{l\sigma}^{n\dagger}\}\rangle}{\langle\{a_{i\sigma}^{n-1},a_{l\sigma}^{n-1\dagger}\}\rangle}\ . \tag{9}$$

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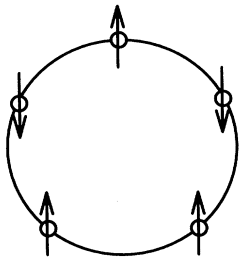

FIG. 1. One-dimensional spin system with five lattice sites; three spin-up and two spin-down electrons.

The damping part, the third term in Eq. (6), is expressed in the CFR and is our major concern.

Now we would like to see whether the CFR given in Eq. (6) is convergent or has any cutoff stage. For that purpose we choose a very simple one-dimensional system which has only five lattice sites (see Fig. 1), since any larger size system requires a great amount of computer calculation. We expect that the demonstration for this simple system may give a clue for convergence of the CFR in general systems. For our computer simulation, we choose the initial states as the array in Fig. 1; three spin-up and two spin-down electrons with the periodic boundary condition. Note that this is one of the 12 possible arrangements.

We now calculate Δ_n and the characteristic frequencies ω_n in the damping factor, using Lanczo's recursion method [9] and the diagonalization method [10] and keeping the exclusion principle in mind. Here we choose $\mu=I/2$, considering the electron-hole symmetry in the half-filled system. Figures 2 and 3 show the values of Δ_n and ω_n $(n=1,2,3,\ldots,15)$ for different values of I/t $(I/t=0.2,1.5,10,50,100,500)$, respectively. We see that the patterns of Δ_n and ω_n vs n are randomly oscillatory without any periodicity. Both Δ_n and ω_n increase with I/t. The crucial difference is that ω_n has both positive and negative values, while Δ_n has only positive values. For all the I/t values given, Δ_{13} becomes zero, which implies that we can ignore the degrees $n \geq 13$ unless the denominator of the CFR stage with $n=13$ approaches zero. This feature agrees qualitatively with the reports of some other authors including Li, Callaway, and Tan [10] that the factor corresponding to our Δ_n disappears at some stage. We guess that the disappearance of Δ_{13} in our model results from the separation of eigenfunction by dint of the projection operators. With a close look at the philosophy of the CFR technique, we expect that the disappearance of Δ_n at some stage will be a general feature for all systems, regardless of the size and dimension.

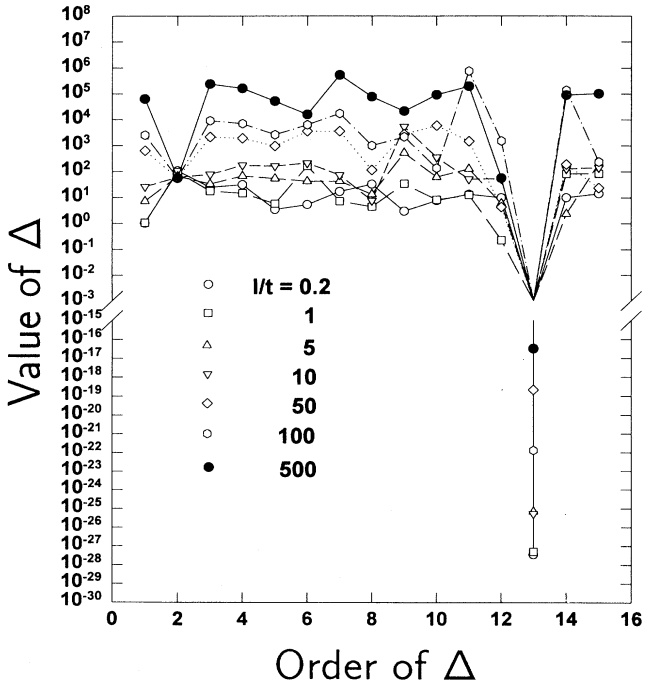

FIG. 2. Variation of Δ's: The pattern is oscillatory, but Δ_{13} becomes zero.

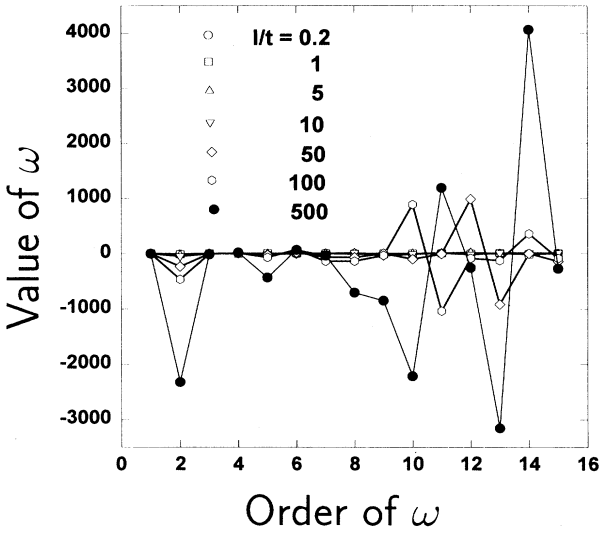

FIG. 3. Variation of ω's: The pattern is oscillatory.

So far we have demonstrated that the CFR for SPGF may have at least one cutoff stage in the Hubbard model. For the CFR, we have followed the standard projection scheme, in which the nth projection operators are generated from the primary one defined by Kim and Wilson. Through the computer experiment on our one-dimensional system with five lattice sites, we have seen that there appears a cutoff stage in the CFR. This result may be compared to the report of Li, Callaway, and Tan that the convergence may appear in the spectral function for a two-dimensional system. But in the present situation, whether this feature is general or only within the limit of the Hubbard model is uncertain. However, we may claim that, if we define a set of proper projection operators, we will be able to meet this kind of feature.

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