Efficient calculation of imaginary-time-displaced correlation functions in the projector auxiliary-field quantum Monte Carlo algorithm

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The calculation of imaginary-time-displaced correlation functions with the auxiliary-field projector quantum Monte Carlo algorithm provides valuable insight (such as spin and charge gaps) into the model under consideration. One of the authors and M. Imada proposed a numerically stable method to compute those quantities [J. Phys. Soc. Jpn. **65**, 189 (1996)]. Although precise, this method is expensive in CPU time. Here we present an alternative approach which is an order of magnitude quicker, just as precise, and very simple to implement. The method is based on the observation that for a given auxiliary field the equal-time Green-function matrix G is a projector: $G^2=G$.

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For a given Hamiltonian $H=\Sigma_{x,y}c_x^\dagger T_{x,y}c_y+H_I$ and its ground state $|\Psi_0\rangle$, our aim is to calculate

$$G_{x,y}^{<}(\tau)=\frac{\langle\Psi_0|c_y^\dagger(\tau)c_x|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle},\quad \tau\geqslant 0. \tag{1}$$

Here $c_x^\dagger$ creates an electron with quantum numbers x, $c_x(\tau)=e^{\tau(H-\mu N)}c_x e^{-\tau(H-\mu N)}$, and the chemical potential $\mu=E_0^{N+1}-E_0^N$. H_I corresponds to the interaction. Within the projector quantum Monte Carlo (PQMC) algorithm, this quantity is obtained by propagating a trial wave $|\Psi_T\rangle$ function along the imaginary time axis:[2–4]

$$\frac{\langle\Psi_0|c_y^\dagger(\tau)c_x|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}=\lim_{\Theta\to\infty}\frac{\langle\Psi_T|e^{-\Theta H}c_y^\dagger(\tau)c_x e^{-\Theta H}|\Psi_T\rangle}{\langle\Psi_T|e^{-2\Theta H}|\Psi_T\rangle}\equiv\lim_{\Theta\to\infty}G^{<}(\Theta,\Theta+\tau). \tag{2}$$

The above is valid provided that $\langle\Psi_0|\Psi_T\rangle\neq 0$.

To fix the notation, we will briefly summarize the essential steps required for a calculation of the right hand side of the above equation at fixed values of the projection parameter Θ. A detailed review may be found in Ref. 5. The formalism—without numerical stabilization—to compute time-displaced correlation functions follows Ref. 6. The first step is to carry out a Trotter decomposition of the imaginary-time propagation:

$$e^{-2\Theta H}=(e^{-\Delta\tau H_t/2}e^{-\Delta\tau H_I}e^{-\Delta\tau H_t/2})^m+O[(\Delta\tau)^2]. \tag{3}$$

Here H_t (H_I) denotes the kinetic (interaction) term of the model, and $m\Delta\tau=2\Theta$. Having isolated the interaction term H_I, one may carry out a Hubbard-Stratonovitch (HS) transformation to obtain

$$e^{-\Delta\tau H_I}=\sum_{\vec{s}}\exp\left(\sum_{x,y}c_x^\dagger D_{x,y}(\vec{s})c_y\right), \tag{4}$$

where $\vec{s}$ denotes a vector of HS fields. For a Hubbard interaction, one can, for example, use various forms of Hirsch's discrete HS decomposition.[7,8] For interactions taking the form of a perfect square, decompositions presented in Ref. 9 are useful.

The imaginary-time propagation may now be written as

$$e^{-2\Theta H}=\sum_{\vec{s}}U_{\vec{s}}(2\Theta,0)+O[(\Delta\tau)^2], \tag{5}$$

where

$$U_{\vec{s}}(2\Theta,0)=\prod_{n=1}^{m}e^{-\Delta\tau H_t/2}e^{\sum_{x,y}c_x^\dagger D_{x,y}(\vec{s}_n)c_y}e^{-\Delta\tau H_t/2}.$$

The HS field has acquired an additional imaginary-time index, since we need independent fields for each time increment.

The trial wave function is required to be a Slater determinant:

$$|\Psi_T\rangle=\prod_{n=1}^{N_p}\left(\sum_x c_x^\dagger P_{x,n}\right)|0\rangle. \tag{6}$$

Here N_p denotes the number of particles, and P is an $N_s\times N_p$ rectangular matrix where N_s is the number of single-particle states. Since $U_{\vec{s}}(2\Theta,0)$ describes the propagation of noninteracting electrons in an external HS field, one may integrate out the fermionic degrees of freedom to obtain

$$G^{<}(\Theta,\Theta+\tau)=\sum_{\vec{s}}W_{\vec{s}}G_{\vec{s}}^{<}(\Theta,\Theta)B_{\vec{s}}(\Theta,\Theta+\tau), \tag{7}$$

where we have omitted the $(\Delta\tau)^2$ systematic error produced by the Trotter decomposition. In the above equation,

$$B_{\vec{s}}(\Theta_2,\Theta_1)=\begin{cases}\displaystyle\prod_{n=n_1+1}^{n_2}e^{-\Delta\tau T/2}e^{D(\vec{s}_n)}e^{-\Delta\tau T/2} & \text{if } \Theta_2>\Theta_1\\ B_{\vec{s}}^{-1}(\Theta_1,\Theta_2) & \text{if } \Theta_1>\Theta_2,\end{cases}$$

where $n_1\Delta\tau=\Theta_1$, and $n_2\Delta\tau=\Theta_2$,

$$M_{\vec{s}}=P^T B_{\vec{s}}(2\Theta,0)P, \quad W_{\vec{s}}=\frac{\det(M_{\vec{s}})}{\sum_{\vec{s}}\det(M_{\vec{s}})},$$

and

$$G_{\vec{s}}^{<}(\Theta,\Theta)=R_{\vec{s}}(\Theta)[L_{\vec{s}}(\Theta)R_{\vec{s}}(\Theta)]^{-1}L_{\vec{s}}(\Theta),$$

$$R_{\vec{s}}(\Theta)=B_{\vec{s}}(\Theta,0)P, \quad L_{\vec{s}}(\Theta)=P^T B_{\vec{s}}(2\Theta,\Theta).$$

Restricting ourselves to models where W_s is positive definite (such as the half-filled Hubbard, half-filled Kondo lattice, or attractive Hubbard models) we can sample the probability distribution with Monte Carlo methods. For each auxiliary-field configuration we then have to evaluate the quantity $G_{\vec{s}}^{<}(\Theta,\Theta)B_{\vec{s}}(\Theta,\Theta+\tau)$ in a numerically stable and efficient way. This corresponds to the subject of the paper.

At first glance it is clear that the evaluation of $G_{\vec{s}}^{<}(\Theta,\Theta)B_{\vec{s}}(\Theta,\Theta+\tau)$ is a numerically ill-posed problem. We illustrate this by considering free electrons on a two-dimensional square lattice:

$$H=-t\sum_{\langle\vec{i},\vec{j}\rangle} c_{\vec{i}}^{\dagger}c_{\vec{j}}. \tag{8}$$

Here the sum runs over nearest neighbors. For this Hamiltonian one has

$$\langle\Psi_0|c_{\vec{k}}^{\dagger}(\tau)c_{\vec{k}}|\Psi_0\rangle=\langle\Psi_0|c_{\vec{k}}^{\dagger}c_{\vec{k}}|\Psi_0\rangle\exp[\tau(\epsilon_{\vec{k}}-\mu)], \tag{9}$$

where $\epsilon_{\vec{k}}=-2t[\cos(\vec{k}\vec{a}_x)+\cos(\vec{k}\vec{a}_y)]$, $\vec{a}_x$, and $\vec{a}_y$ being the lattice constants. We will assume $|\Psi_0\rangle$ to be nondegenerate. In a numerical calculation the eigenvalues and eigenvectors of the above Hamiltonian will be known up to machine precision ϵ. In the case $\epsilon_{\vec{k}}-\mu>0$ and $\langle\Psi_0|c_{\vec{k}}^{\dagger}c_{\vec{k}}|\Psi_0\rangle\equiv 0$. However, on a finite precision machine the latter quantity will take a value of the order of ϵ. When calculating $\langle\Psi_0|c_{\vec{k}}^{\dagger}(\tau)c_{\vec{k}}|\Psi_0\rangle$, this roundoff error will be blown up exponentially, and the result for large values of τ will be unreliable.

In the PQMC approach and since, for a given HS configuration, we have independent electrons in an external field, a similar form is obtained for the time-displaced Green function. The $B_{\vec{s}}$ matrix plays the role of the exponential factors, and contains exponentially large and small scales, whereas $G_{\vec{s}}^{<}(\Theta,\Theta)$ contains scales bounded by order unity. Since we equally expect the result $G_{\vec{s}}^{<}(\Theta,\Theta+\tau)$ to be bounded by order unity, we will eventually run into numerical problems when τ becomes *large*.

In order to circumvent this problem, Assaad and Imada[1] proposed doing the calculation at finite temperatures, and then taking the limit to vanishingly small temperatures. For the example of free electrons, this amounts to performing calculation via

$$\langle\Psi_0|c_{\vec{k}}^{\dagger}(\tau)c_{\vec{k}}|\Psi_0\rangle=\lim_{\beta\to\infty}\frac{\exp[\tau(\epsilon_{\vec{k}}-\mu)]}{1+\exp[\beta(\epsilon_{\vec{k}}-\mu)]}. \tag{10}$$

Even if the eigenvalues are known only up to machine precision, the right-hand side of the above equation for large but finite values of β is a numerically stable operation. To implement this idea in the QMC method, Assaad and Imada considered a single-particle Hamilton H_0 which has the trial wave function $|\Psi_T\rangle$ as a nondegenerate ground state, and then compute

$$G_{\vec{s}}^{<}(\Theta,\Theta+\tau)\equiv\lim_{\beta\to\infty}\frac{\mathrm{Tr}[e^{-\beta H_0}U_{\vec{s}}(2\Theta,\Theta)c_y^{\dagger}(\tau)c_x U_s(\Theta,0)]}{\mathrm{Tr}[e^{-\beta H_0}U_s(2\Theta,0)]}. \tag{11}$$

Although the right-hand side of the above equation may be computed in a numerically stable way, the approach is cumbersome and numerically expensive. In particular, for each measurement, all quantities have to be computed from scratch since the *ad hoc* inverse temperature β has to be taken into account.

Here we propose an alternative method. We will again start with the example of free electrons. Since $\langle\Psi_0|c_{\vec{k}}^{\dagger}(\tau)c_{\vec{k}}|\Psi_0\rangle=1$ and 0, we can rewrite Eq. (9) as

$$\langle\Psi_0|c_{\vec{k}}^{\dagger}(\tau)c_{\vec{k}}|\Psi_0\rangle=\{\langle\Psi_0|c_{\vec{k}}^{\dagger}c_{\vec{k}}|\Psi_0\rangle\exp[(\epsilon_{\vec{k}}-\mu)]\}^{\tau}, \tag{12}$$

which involves only well-defined numerical manipulations even in the large-τ limit.

The implementation of this idea in the QMC algorithm is as follows. First one has to notice that the Green function $G_{\vec{s}}^{<}(\Theta,\Theta)$ is a projector:

$$G_{\vec{s}}^{<}(\Theta,\Theta)^2=G_{\vec{s}}^{<}(\Theta,\Theta). \tag{13}$$

This is simply shown by carrying out a singular value decomposition of the $N_s\times N_p$ $R_{\vec{s}}(\Theta)$ and $L_{\vec{s}}(\Theta)$ matrices

$$R_{\vec{s}}(\Theta)=U_{r,\vec{s}}D_{r,\vec{s}}V_{r,\vec{s}},$$

$$L_{\vec{s}}(\Theta)=V_{l,\vec{s}}D_{l,\vec{s}}U_{l,\vec{s}}.$$

Here $U_r(U_l)$ is a $N_s\times N_p(N_p\times N_s)$ and column (row) orthogonal matrix, $D_{l,r}$ are diagonal $N_p\times N_p$ matrices, and $V_{l,r}$ unit upper triangular $N_p\times N_p$ matrices. For the equal-time Green function, only $U_{r,\vec{s}}$ and $U_{l,\vec{s}}$ are important:

$$G_{\vec{s}}^{<}(\Theta,\Theta)=U_{r,\vec{s}}[U_{l,\vec{s}}U_{r,\vec{s}}]^{-1}U_{l,\vec{s}}.$$

Equation (13) then follows from

$$[G_{\vec{s}}^{<}(\Theta,\Theta)]^2 = U_{r,\vec{s}}[U_{l,\vec{s}}U_{r,\vec{s}}]^{-1}[U_{l,\vec{s}}U_{r,\vec{s}}][U_{l,\vec{s}}U_{r,\vec{s}}]^{-1}U_{l,\vec{s}} = G_{\vec{s}}^{<}(\Theta,\Theta).$$

This in turn implies that $G_{\vec{s}}^{<}(\Theta_1,\Theta_3)$ obeys a simple composition identity

$$G_{\vec{s}}^{<}(\Theta_1,\Theta_2)G_{\vec{s}}^{<}(\Theta_2,\Theta_3) = G_{\vec{s}}^{<}(\Theta_1,\Theta_3), \tag{14}$$

since

$$\begin{aligned} G_{\vec{s}}^{<}(\Theta_1,\Theta_3) &= G_{\vec{s}}^{<},(\Theta_1,\Theta_1), \quad B_{\vec{s}}(\Theta_1,\Theta_3) \\ &= [G_{\vec{s}}^{<}(\Theta_1,\Theta_1)]^2 B_{\vec{s}}(\Theta_1,\Theta_3) \\ &= G_{\vec{s}}^{<}(\Theta_1,\Theta_1)G_{\vec{s}}^{<}(\Theta_1,\Theta_3) \\ &= G_{\vec{s}}^{<}(\Theta_1,\Theta_2)G_{\vec{s}}^{<}(\Theta_2,\Theta_3). \end{aligned}$$

Using composition property (14) we can break up a large τ interval into a set of smaller intervals of length $\tau = N\tau_1$, so that

$$G_{\vec{s}}^{<}(\Theta,\Theta+\tau) = \prod_{n=0}^{N-1} G_{\vec{s}}^{<}(\Theta+[n+1]\tau_1,\Theta+n\tau_1). \tag{15}$$

The above equation is the generalization of Eq. (12). If τ_1 is *small* enough, each Green function in the above product is accurate, and has matrix elements bounded by order unity. The matrix multiplication is then numerically well defined.

We illustrate the efficiency of the method for the Kondo lattice model:

$$H_{KLM} = -t\sum_{\langle\vec{i},\vec{j}\rangle,\sigma} c_{\vec{i},\sigma}^{\dagger}c_{\vec{j},\sigma} + J\sum_{\vec{i}} \vec{S}_{\vec{i}}^{c}\vec{S}_{\vec{i}}^{f}. \tag{16}$$

Here $\vec{i}$ runs over the L^2 sites of a square lattice, $\langle\vec{i},\vec{j}\rangle$ corresponds to nearest neighbors, $c_{\vec{i},\sigma}^{\dagger}$ creates a conduction electron with z component of spin σ on site $\vec{i}$, and periodic boundary conditions are imposed. $\vec{S}_{\vec{i}}^{f} = (1/2)\Sigma_{\sigma,\sigma'} f_{\vec{i},\sigma}^{\dagger}\vec{\sigma}_{\sigma,\sigma'}f_{\vec{i},\sigma'}$, with $\vec{\sigma}$ the Pauli matrices. An equivalent form holds for the conduction electrons. A constraint of one fermion per f site is enforced. As shown in Ref. 10 at half-filling, the PQMC method may be used to carry out sign-free simulations of the model.

Figure 1 plots the on-site time-displaced spin-spin correlation functions as well as the on-site Green function for a 6×6 lattice at $J/t=1.2$ and half-band filling. Here, we consider the total spin: $\vec{S}_{\vec{i}} = \vec{S}_{\vec{i}}^{f} + \vec{S}_{\vec{i}}^{c}$. Both methods based on Eqs. (15) and (11) produce identical results within the error bars.

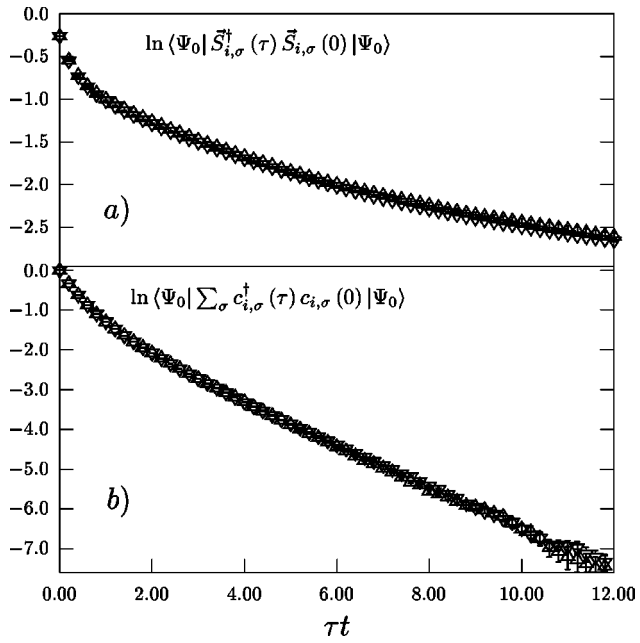

FIG. 1. Imaginary-time-displaced on-site spin-spin (a) and Green-function (b) correlation function. We consider a 6×6 lattice at half-filling, and $J/t=1.2$. In both (a) and (b) results obtained from Eqs. (15) ($\triangle$) and (11) ($\triangledown$) are plotted.

(Had we used the same series of random numbers, we would have obtained exactly the same values up to roundoff errors which are of the order 10^{-8}.)

The important point however, is that the method based on Eq. (15), for this special case, more than an order of magnitude quicker in CPU time than the calculation based on Eq. (11). A calculation following Eq. (15) involves matrix inversions (multiplications) of size $N_p\times N_p$ $[(N_p\times N)(N\times N)]$. Here N denotes the number of sites. To this we add that many quantities required for the calculation are at hand during the simulation, and do not have to be recalculated. On the other hand, the method based on Eq. (11) involves matrix inversions and multiplications of size up to $2N\times2N$.[1] In this approach, and for a given set of HS fields all quantities have to be computed from scratch.

In summary, we have described an efficient method for the calculation of imaginary-time-displaced correlation functions in the framework of the PQMC algorithm. The method is elegant and easy to implement in a standard PQMC code, and is an order of magnitude quicker than previously used methods. We have demonstrated the efficiency of the method in the special case of the two-dimensional Kondo lattice model. Given the ability of efficiently calculating time-displaced correlation functions at arbitrarily large imaginary times enables us to pin down charge and spin gaps[10] as well as quasiparticle weights.[11] Dynamical properties may equally well be obtained after continuation to real time via the maximum entropy method.[12]

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