Kernel polynomial representation of imaginary-time Green’s functions

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Inspired by the recent proposed Legendre orthogonal polynomial representation of imaginary-time Green’s functions, we develop an alternate representation for the Green’s functions of quantum impurity models and combine it with the hybridization expansion continuous-time quantum Monte Carlo impurity solver. This representation is based on the kernel polynomial method, which introduces various integral kernels to filter fluctuations caused by the explicit truncations of polynomial expansion series and improve the computational precision significantly. As an illustration of the new representation, we reexamine the imaginary-time Green’s functions of single-band Hubbard model in the framework of dynamical mean-field theory. The calculated results suggest that with carefully chosen integral kernels the Gibbs oscillations found in previous orthogonal polynomial representation have been suppressed vastly and remarkable corrections to the measured Green’s functions have been obtained.

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I. INTRODUCTION

The rapid development of efficient numerical and analytical methods for solving quantum impurity models has been driven in recent years by the great success of dynamical mean-field theory (DMFT)\cite{Georges1996, Nersesyan2014} and its non-local extensions.\cite{Mougel2007, Gull2013} In the framework of DMFT, the momentum dependence of self-energy is neglected, then the solution of general lattice model may be obtained from the solution of an appropriately defined quantum impurity model plus a self-consistency condition. To solve the quantum impurity models numerous quantum impurity solvers have been developed in the last decades.\cite{Eckstein2002, Dagotto2005} In particular, continuous-time quantum Monte Carlo impurity solvers\cite{Jarrell1996, Bo路径henke2007} have become a very important tool for studying quantum impurity models, due to their accuracy, efficiency and ability to treat extreme low temperature and arbitrary interaction terms (for a recent review, see Ref.\textsuperscript{12}).

Among various continuous-time quantum Monte Carlo algorithms, the hybridization expansion version (abbreviated CT-HYB)\cite{Bo路径henke2007, Bo路径henke2009} is the most powerful and reliable impurity solver up to now and is widely used. In practice, as for the CT-HYB quantum impurity solver several severe technical limits still remain. One well-known problem is the high frequency noises commonly observed in the Matsubara Green’s function and the self-energy.\cite{Bo路径henke2007, Bo路径henke2009} Similar problems also arise in the calculations of imaginary-time Green’s functions and vertex functions, which are less emphasized in the literatures. In order to cure these problems, intuitive idea is to run more statistics in the Monte Carlo simulations to suppress the data fluctuations as far as possible. This strategy should mitigate the problems, but it will not avert them and will deteriorate the efficiency of CT-HYB quantum impurity solver rapidly. Recently, Lewin Boehnke et al.\cite{Bo路径henke2010} have suggested to measure the single-particle and two-particle Green’s function in the basis of Legendre orthogonal polynomials. The orthogonal polynomial method (OPM) provides a more compact representation of Green’s functions than standard Matsubara frequencies, and therefore significantly reduces the memory storage size of these quantities. Moreover, it can be used as an efficient noise filter for various physical quantities within the CT-HYB quantum impurity solver: the statistical noise is mostly carried by high-order Legendre coefficients which should be truncated, while the physical properties are determined by low-order coefficients which should be retained. By and by the OPM is used for the computations of single-particle Green’s function and lattice susceptibilities in the context of realistic DMFT calculations in combination with the local density approximation to the density functional theory (LDA+DMFT).\cite{Jezouin2008, Jezouin2011} By using the Legendre orthogonal polynomial representation, the accuracy of CT-HYB impurity solver is greatly improved. But according to careful examinations, the so-called Gibbs oscillations can be easily found in the resulting Green’s functions and other physical quantities, which may be mainly due to the rough truncation of Legendre basis. The sign of Gibbs oscillations is that the resulting physical quantities are smooth but oscillating periodically with the scattered direct measurements. The situation is even worse in the insulating state where the Gibbs oscillations will cause the reconstructed single-particle Green’s function to break the causality. Noted that a common procedure to damp these oscillations relies on an appropriate modification of the expansion coefficients by some integral kernels, which is the well-known kernel polynomial representation.\cite{Chen2012} Thus we adopt the kernel polynomial method (KPM) to improve the measurement of single-particle and two-particle quantities within CT-HYB quantum impurity solver and expect to...
obtain significant improvements.

The rest of this paper is organized as follows: In Sec.[11] a brief introduction to the orthogonal polynomial representation is provided. The original implementation is based on Legendre polynomials only, and a straightforward generalization to Chebyshev polynomials is proposed. In Sec.[11] the kernel polynomial representation is presented in details. Then in Sec.[11] we benchmark the KPM by reexamining the imaginary-time Green’s function of single-band half-filled Hubbard model, and the characteristics of different integral kernel functions which are used to alter the expansion coefficients are discussed. Section [IV] serves as a conclusion and outlook. Finally in Appendix [A] concise introductions for the Chebyshev and Legendre orthogonal polynomial series are available as well.

II. METHOD

A. Orthogonal polynomial representation

In the OPM, the imaginary-time Green’s function $G(\tau)$ where $\tau \in [0, \beta]$ can be expanded in terms of Legendre orthogonal polynomials $P_n(x)$ defined on the interval $[-1, 1]$,

$$G(\tau) = \frac{1}{\beta} \sum_{n=0}^{n_{\text{max}}} \sqrt{2n + 1} P_n(\tau) G_n,$$  \hspace{1cm} (1)

$$G_n = \sqrt{2n + 1} \int_0^\beta d\tau P_n(\tau) G(\tau),$$  \hspace{1cm} (2)

where $\beta$ is inverse temperature, $x(\tau) = \frac{2\tau}{\beta} - 1$ and $G_n$ denotes the expansion coefficients of $G(\tau)$ in the Legendre orthogonal polynomials basis.\[12] Since the expansion coefficients generally show a very fast decay with $n$, the expansion in Legendre polynomials can be truncated at a maximum order $n_{\text{max}}$. In the CT-HYB quantum impurity solver, the formula for measuring imaginary-time Green’s function $G(\tau)$\[12] is

$$G(\tau) = -\frac{1}{\beta} \left\langle \sum_{i=1}^{k} \sum_{j=1}^{k} M_{ij} \Delta(\tau, \tau_i^s - \tau_j^s) \right\rangle,$$  \hspace{1cm} (3)

$$\Delta(\tau, \tau') = \begin{cases} \delta(\tau - \tau'), & \tau' > 0 \\ -\delta(\tau - \tau' - \beta), & \tau' < 0 \end{cases},$$  \hspace{1cm} (4)

where $k$ is the order of diagrammatic perturbation expansion series, matrix element $(M^{-1})_{ij} = F(\tau_i^s - \tau_j^s)$ where $F(\tau)$ is the hybridization function, $\tau_i^s$ and $\tau_j^s$ are the coordinates in imaginary-time axis for create and destroy operators, respectively. By utilizing Eq.(3) and Eq.(4), the Legendre coefficients for $G(\tau)$ finally become

$$G_n = -\frac{\sqrt{2n + 1}}{\beta} \left\langle \sum_{i=1}^{k} \sum_{j=1}^{k} M_{ij} \tilde{P}_n(\tau_i^s - \tau_j^s) \right\rangle,$$  \hspace{1cm} (5)

$$\tilde{P}_n(\tau) = \begin{cases} P_n[\tau(\tau)], & \tau > 0 \\ -P_n[\tau(\tau + \beta)], & \tau < 0 \end{cases}.$$  \hspace{1cm} (6)

Lewin Boehmke et al.\[12] have chosen the Legendre orthogonal polynomials as their preferred basis to expand single-particle and two-particle Green’s functions. But it should be stressed that a priori different orthogonal polynomial bases may be used as well. Thus we try to generalize the OPM to use Chebyshev orthogonal polynomials as an optional basis. It is well-known that there exist two kinds of Chebyshev polynomials.\[19] By using the Chebyshev polynomials of second kind $U_n(x)$ as basis, the imaginary-time Green’s functions $G(\tau)$ can be expressed by the following equations,

$$G(\tau) = \frac{2}{\beta} \sum_{n=0}^{n_{\text{max}}} U_n[\tau(\tau)] G_n,$$  \hspace{1cm} (7)

$$G_n = \frac{2}{\pi\beta} \int_{0}^{\beta} d\tau U_n[\tau(\tau)] \sqrt{1 - x(\tau)^2} G(\tau).$$  \hspace{1cm} (8)

After a straightforward substitute, the Chebyshev coefficients for $G(\tau)$ finally become

$$G_n = \frac{-2}{\pi\beta} \left( \sum_{i=1}^{k} \sum_{j=1}^{k} M_{ij} U_n(\tau_i^s - \tau_j^s) \sqrt{1 - \tilde{x}(\tau_i^s - \tau_j^s)^2} \right),$$ \hspace{1cm} (9)

where

$$\tilde{U}_n(\tau) = \begin{cases} U_n[\tau(\tau)], & \tau > 0 \\ -U_n[\tau(\tau + \beta)], & \tau < 0 \end{cases},$$ \hspace{1cm} (10)

and

$$\tilde{x}(\tau) = \begin{cases} x(\tau), & \tau > 0 \\ x(\tau + \beta), & \tau < 0 \end{cases}.$$ \hspace{1cm} (11)

The CT-HYB quantum impurity solver can directly accumulate the Legendre or Chebyshev coefficients $G_n$ instead of original Green’s functions $G(\tau)$. Once the Monte Carlo sampling has been finished, $G(\tau)$ can be reconstructed analytically by using the expansion coefficients. Since the coefficients decay very quickly, the orthogonal polynomial bases are much more compact and are particularly interesting for storing and manipulating the two-particle quantities, like vertex function etc. Furthermore, the Monte Carlo noises are mainly concentrated in the high-order expansion coefficients, and the numerical values of them are usually very small. So a rough truncation method can be developed to filter out the noises and obtain more smooth and accurate results.
TABLE I. Summary of different integral kernel functions $f_n$ that can be used to improve the quality of an order $N$ Chebyshev or Legendre series

| name       | $f_n$                                                                 | parameters positive |
|------------|----------------------------------------------------------------------|---------------------|
| Jackson    | $\frac{1}{N} \left( (N - n + 1) \cos(\frac{n\pi}{N + 1}) + \sin(\frac{n\pi}{N + 1}) \cot(\frac{n\pi}{N + 1}) \right)$ | none yes            |
| Lorentz    | $\sinh[\lambda(1 - n/N)]/\sinh(\lambda)$                           | $\lambda \in \mathbb{R}$ yes |
| Fejér      | $1 - n/N$                                                             | none yes            |
| Wang-Zunger| $\exp\left[ -\left( \frac{\alpha}{N} \right)^\beta \right]$        | $\alpha, \beta \in \mathbb{R}$ no |
| Dirichlet  | 1                                                                    | none no             |

FIG. 1. (Color online) Classic integral kernels $f_n$ used to improve the quality of polynomial expansion series. In this figure, the order of expansion series is $N = 64$. The Dirichlet, Jackson, and Fejér kernels take no parameters. For Lorentz kernel, the $\lambda$ parameter is fixed to be 1.0. And for Wang-Zunger kernel, the $\alpha$ and $\beta$ parameters are 1.0 and 4.0, respectively.

B. Kernel polynomial representation

The basic idea of OPM is to expand single-particle Green’s functions $G(\tau)$ in infinite series of Chebyshev or Legendre polynomials, and then Monte Carlo algorithm to sample the expansion coefficients $G_n$ directly. As expected for a numerical approach, however, the expansion series will remain finite actually, and we thus arrive at a classical problem of approximation theory. In our case the problem is equivalent to find the best approximation to $G(\tau)$ given a finite number of $G_n$. Experience shows that a simple truncation of the infinite series leads to poor precision and fluctuations, which also known as Gibbs oscillations.\[18\] For examples, as for the reconstructed Green’s function $G(\tau)$ in insulating state, almost periodic Gibbs oscillations are clearly identified in a wide $\tau$ range.

A common procedure to damp the Gibbs oscillations is to introduce some kind of integral kernel function $f_n$ and change the expansion coefficients from $G_n$ to $G_nf_n$.\[18\] Obviously, the simplest integral kernel function, which is usually attributed to Dirichlet, is obtained by setting $f_n = 1$. By using the Dirichlet kernel, the KPM is equivalent to previous OPM. In addition to the Dirichlet kernel, other classic integral kernel functions, like Jackson, Lorentz, Fejér, and Wang-Zunger etc., are collected in Tab. I and plotted in Fig. I respectively. Note that for all the kernels $f_0$ must be equal to 1 and $f_1$ must approach 1 as $n \to \infty$. The optimal integral kernel function partially depends on the considered application. According to the literature, the Jackson kernel may be the best for most applications, the Lorentz kernel may be the best for Green’s function, while the Fejér kernel is mainly of academic interest.

Finally, we note that the integral kernel functions $f_n$ can be evaluated and stored in advance, so the KPM has not effect on the computational efficiency of CT-HYB quantum impurity solver. The implementation of KPM is very simple, only small modifications are needed for the OPM’s version of CT-HYB, i.e., replacing $G_n$ by $G_nf_n$. Since the kernel polynomial and orthogonal polynomial representations are only alternate bases for single-particle and two-particle quantities, so both methods can be implemented in segment picture\[7\] and general matrix\[8\] formulations of CT-HYB impurity solvers to improve the accuracy and efficiency.

III. BENCHMARK

In this section, we try to benchmark the kernel polynomial representation and compare the calculated results with those obtained by orthogonal polynomial representation and conventionally direct measurements. For the sake of simplicity, a single-band Hubbard model on Bethe lattice is used as a toy model to examine our implementations of OPM and KPM. Here $U = 4.0$ and $\beta = 10.0$ for metallic case, and $U = 6.0$ and $\beta = 50.0$ for insulating case. The band is with bandwidth 2.0, and a semicircular density of states is chosen. The chemical potential $\mu$ is fixed to be $U/2$ to keep the model under half-filling. Unless it is specifically stated, this model is used throughout this section. This toy model is studied in the framework of single site DMFT\[1, 2\] and the segment picture version of CT-HYB\[7\] is used as quantum impurity solver. In each DMFT iterations, typically $4 \times 10^8$ Monte Carlo sweeps have been performed to reach sufficient numerical precision.
Let’s first concentrate our attentions to the metallic state. In figure 2 the “bare” expansion coefficients $\beta|G_n|$ of Chebyshev and Legendre orthogonal polynomials are shown. As is pointed out by Lewin Boehnke et al.\textsuperscript{[15]}, due to the constraint of particle-hole symmetry the expansion coefficients for odd order $n$ should be zero. Indeed, the coefficients in our data for odd $n$’s all take on a very small value, compatible with a vanishing value within their error bars. The even $n$ coefficients instead show a very fast decay. As is shown in this figure, $n_{\text{max}} = 15 \sim 25$ is enough for both Chebyshev and Legendre polynomial representations to obtain converged and accurate results. In our simulations, $n_{\text{max}}$ is fixed to be 24.

Figure 3 shows the calculated imaginary-time Green’s function $G(\tau)$ by using KPM with different orthogonal polynomials and integral kernel functions. It is apparent that the directly measured $G(\tau)$ is full of noises and fluctuations, which are negative for the later analytical continuation procedure.\textsuperscript{[20]} Once the OPM is used (i.e., Dirichlet kernel $f_n = 1$ is adopted), $G(\tau)$ turns smooth but obvious undulations still exist. If the Lorentz, Fejér, and Wang-Zunger kernels are applied one by one, the Green’s functions are smooth and without obvious undulations, but deviate systematically from the scattered data. As a general view, the Jackson kernel function is the optimal choice. The resulting $G(\tau)$ evaluated by Jackson kernel function is smooth and nicely interpolates the directly measured data. As is expected, the type of orthogonal polynomials has little impact to the interpolated $G(\tau)$. It seems that the Chebyshev polynomials do a bit better than Legendre polynomials.

A. Metallic state

Now let’s turn to the insulating state. When $U = 6.0$ and $\beta = 50$ an definitely insulating solution is obtained within DMFT. The “bare” Chebyshev and Legendre coefficients $\beta|G_n|$ of $G(\tau)$ are shown in Fig.4. Just similar to the metallic state, $G_n$ takes very small value for odd $n$ and can be ignored safely, and for even $n$, $G_n$ converges to zero very quickly. For Chebyshev and Legendre polynomials, $n_{\text{max}} = 35 \sim 45$ or $n_{\text{max}} = 40 \sim 50$, respectively. Thus the Chebyshev polynomials is more compact and efficient than Legendre polynomials. In current simulations, $n_{\text{max}}$ is fixed to be 64 uniformly.

B. Insulating state
is very close to zero in this region. The scattered data obtained by direct measurement exhibit periodical undulations. The reconstructed $G(\tau)$ by OPM (with Dirichlet kernel) displays stronger periodical oscillations and violates the causality at the same time, which means that the results will be even deteriorated by using orthogonal polynomial representation. The results obtained by Wang-Zunger kernel fit original data very well and obvious improvement is not observed. As for the Lorentz and Fejér kernels, the calculated results deviate the scattered data systematically. Again, the Jackson kernel is the optimal choice. The calculated results are very smooth, perfectly interpolate the scattered data, and obey the causality.

IV. CONCLUSIONS

It is suggested that the OPM based on Legendre orthogonal polynomials can be used to improve the accuracy and computational efficiency of CT-HYB quantum impurity solver. In this paper, we develop a better representation to calculate the single-particle and two-particle quantities. Firstly, we generalize the OPM to Chebyshev orthogonal polynomial basis. Secondly, the KPM based on various integral kernel functions is proposed to damp the Gibbs oscillations observed in the single-particle and two-particle Green’s functions obtained with OPM and improve the accuracy of them further. According to the benchmark results for single-band half-filled Hubbard model, it is demonstrated that the Jackson kernel is the optimal choice for imaginary-time Green’s function $G(\tau)$ and other quantities. Though the KPM presented in this paper is mainly developed for the CT-HYB quantum impurity solver, it can be easily generalized to other continuous-time quantum Monte Carlo impurity solvers.

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Appendix A: Chebyshev and Legendre polynomials

In this appendix, we summarize for convenience some basic properties of the Chebyshev and Legendre polynomials, and the first few Chebyshev and Legendre polynomials are illustrated in Fig. 6. Further reference can be found in Ref. 19. The Chebyshev polynomials are a sequence of orthogonal polynomials which can be defined recursively. One usually distinguishes between Chebyshev polynomials of the first kind which are denoted by $T_n$ and Chebyshev
FIG. 6. (Color online) Chebyshev and Legendre orthogonal polynomials. Upper panel: The first few Chebyshev polynomials of the second kind $U_n$ in the domain $1 < x < 1$. Lower panel: The first few Legendre polynomials $P_n$ in the domain $1 < x < 1$.

Polynomials of the second kind which are denoted by $U_n$. The Chebyshev polynomials $T_n$ or $U_n$ are polynomials of degree $n$. $T_n$ and $U_n$ are defined by the following recurrence relations:

$$T_0(x) = 1, \quad (A1)$$

$$T_1(x) = x, \quad (A2)$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x). \quad (A3)$$

and

$$U_0(x) = 1, \quad (A4)$$

$$U_{n+1}(x) = 2xU_n(x) - U_{n-1}(x). \quad (A5)$$

The Chebyshev polynomials of the first and second kind are closely related by the following equations:

$$T_{n+1}(x) = xT_n(x) - (1 - x^2)U_{n-1}(x), \quad (A7)$$

and

$$T_n(x) = U_n(x) - xU_{n-1}(x). \quad (A8)$$

The Chebyshev polynomials of the first kind are orthogonal with respect to the weight $\frac{1}{\sqrt{1-x^2}}$ on the interval $[-1, 1]$, i.e. we have:

$$\int_{-1}^{1} T_n(x)T_m(x) \frac{dx}{\sqrt{1-x^2}} = \begin{cases} 
0 & : n \neq m, \\
\pi & : n = m = 0, \\
\pi/2 & : n = m \neq 0. 
\end{cases} \quad (A9)$$

Similarly, the Chebyshev polynomials of the second kind are orthogonal with respect to the weight $\sqrt{1-x^2}$ on the interval $[-1, 1]$, i.e. we have:

$$\int_{-1}^{1} U_n(x)U_m(x)\sqrt{1-x^2} dx = \begin{cases} 
0 & : n \neq m, \\
\pi/2 & : n = m. 
\end{cases} \quad (A10)$$

Similar to the Chebyshev polynomials, Legendre polynomials $P_n$ are orthogonal polynomials of degree $n$, which can be defined by the following recurrence relations:

$$P_0(x) = 1, \quad (A11)$$

$$P_1(x) = x, \quad (A12)$$

$$(n + 1)P_{n+1}(x) = (2n + 1)xP_n(x) - nP_{n-1}(x). \quad (A13)$$

The orthogonality of Legendre polynomials on the interval [-1,1] reads:

$$\int_{-1}^{1} P_m(x)P_n(x) dx = \frac{2}{2n+1} \delta_{mn}. \quad (A14)$$

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