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Dynamical mean field theory equations on nearly real frequency axis

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ABSTRACT

The iterated perturbation theory (IPT) equations of the dynamical mean field theory (DMFT) for the half-filled Hubbard model are solved on nearly real frequencies at various values of the Hubbard parameters, U, to investigate the nature of metal–insulator transition (MIT) at finite temperatures. This method avoids the instabilities associated with the infamous Padé analytic continuation and reveals fine structures across the MIT at finite temperatures, which cannot be captured by conventional methods for solving DMFT-IPT equations on Matsubara frequencies. Our method suggests that at finite temperatures, there is a crossover from a *bad* metal to a *bad* insulator in which the height of the quasi-particle (Kondo) peak decreases to a non-zero small bump, which gradually suppresses as one moves deeper into the *bad* insulating regime.

1. Introduction

Dynamical mean field theory (DMFT) approximation which is based on a mapping of lattice models onto a single quantum impurity subject to a self-consistency condition has been successful in addressing the issue of metal–insulator transitions (MIT) in correlated electron systems at zero temperature [1,2]. It is realized experimentally that MIT in three-dimensional homogeneous systems of transition metal oxides is driven by the strength of electron–electron interactions [3]. DMFT predicts a zero-temperature metal insulator transition as the local interaction U (the Hubbard parameter) exceeds a critical strength U_c [1,4]. At finite temperature there is no qualitative distinction between the insulating and metallic states and a first order MIT is occurred in the Hubbard model [5,6]. However, As in any approximation theory, the complete determination of the physics of MIT in the DMFT method involves the computational solving of the equations and so we need for development of new reliable methods to overcome the non-analytic errors produced in the process of numerical calculation.

Beginning with DMFT equations, one has to calculate the Feynman diagrams at non-zero temperature and analytically continue the equations to real frequency axis to interpret the results. The practical task of calculating the Feynman diagrams is performed with Matsubara method that provides a very convenient and neat way for numerical calculations of the diagrams [7]. The essential ingredient is that the Wick rotation $\tau = it$ replaces the oscillatory $e^{-i\xi_k t}$ factors by decaying $e^{-\xi_k \tau}$ factors at imaginary time, which makes it convenient for putting on computer and so the convergence in iterative or self-consisted formulations of perturbation theory is particularly achieved fast. However, the computational price will be payed when one attempts to undo the Wick rotation at the end of calculation to obtain dynamical quantities by analytical continuing $i\omega_n \to \omega + i\eta$, where η is an infinitesimal positive constant, $\eta = 0^+$.

The hurdle one faces in undoing the Wick rotation is that, if one uses the Padé approximation [8], and fits a quotient of two polynomials $f_N(z)$ and $g_M(z)$ to the table of data obtained for Matsubara frequencies $i\omega_n$, and then replaces $z \to \omega + i\eta$ in the resulting function, the calculated spectral weights are not always stable with respect to variations in parameters N, M. Even if for some parameter regime, or for some particular problem one obtains relatively stable results, the aforementioned disrepute of the Padé approximation warns us about the reliability and/or the quality of the dynamical quantities obtained in this way.

There has been some proposals for reliable way of using the Padé approximation in analytic continuation of numerical data: Beach et al. [8] proposed a symbolic computer aided algebra with arbitrary precision (typically 100–200 decimal places, which lack in single or double precision arithmetics of standard programming languages like `C++` or `Fortran`). They also proposed a quantitative measure for the reliability of continued data. Mishchenko et al. [9,10] proposed an stochastic optimization method which allows one to handle both broad and sharp features of the spectrum on equal footing.

On the other hand, Schmalian et al. proposed an alternative method which is quite intuitive and general [11]: Instead of

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solving the diagrammatic equations for Matsubara frequencies $i\omega_n$, solve them for frequencies $\omega+i\gamma$, where γ is a finite constant. The *finite* value of γ (usually taken to be less than the first nonzero Matsubara frequency) provides the damping required for convergence of the iterative solutions. The analytic continuation from $\omega+i\gamma$ to $\omega+i\eta$, where $\eta=0^+$, is stable and also sustains fine features of the spectral function, such as shadow bands of the high temperature superconductors. Schmalian et al. found this feature by applying this method to solve the diagrammatic equations of the fluctuation exchange approximation [12].

Keeping the aforementioned concerns about the reliability of the Padé analytic continuation procedure in mind, in this paper we use the method of Schmalian et al. [11] to re-examine the nature of MIT in the half-filled Hubbard model at finite temperatures within the DMFT approximation scheme. We find that paying manipulation price at the beginning, for solving slightly more difficult equations for $\omega+i\gamma$ and then providing reliable Padé analytic continuation with absolutely no negative spectral weights, pays off and also reveals fine structure in the insulating side of the MIT. A small bump in the spectral weight which persists in the insulating phase is stably produced in our approach and cannot be captured by Padé analytical continuation of the solutions of DMFT equations for Matsubara frequencies. The asymptotic behaviors at $T\to 0$ limit in our approach agree with other methods of solving the DMFT equations.

The paper is organized as follows: First we analytically continue the iterated perturbation theory (IPT) [13–15] equations of DMFT to $\omega+i\gamma$ line above the real frequency axis. Then we present the numerical solutions of the resulting equations for various values of the Hubbard parameters, U, at half-filling, and elevated temperatures. Finally we present our conclusions.

2. Formulation

Within DMFT approximation, the problem of interacting electrons on a lattice can be mapped onto an effective impurity problem surrounded by a self-consistent bath. The impurity Green's function, $\mathcal{G}$, is related to its bare counterpart via the Dyson equation [1],

$$\mathcal{G}_0^{-1}=\Sigma+\frac{1}{\tilde{D}}(i\omega_n+\mu-\Sigma) \tag{1}$$

where

$$\tilde{D}(i\omega_n+\mu-\Sigma)=\int_{-\infty}^{\infty}d\varepsilon\frac{D(\varepsilon)}{i\omega_n+\mu-\Sigma-\varepsilon} \tag{2}$$

is the Hilbert transform of density of states (DOS). In (2), $\tilde{D}(i\omega_n+\mu-\Sigma)$ is the on-site full Green's function for site o, i.e. G_{oo} and its imaginary part gives the interacting DOS,

$$G(i\omega_n)=\tilde{D}(i\omega_n+\mu-\Sigma(i\omega_n)) \tag{3}$$

In IPT approximation, the self-energy is given by the second order perturbation theory [1] as

$$\Sigma(i\omega_n)\simeq U^2\int_0^{\beta}d\tau\, e^{i\omega_n\tau}\hat{\mathcal{G}}_0(\tau)\hat{\mathcal{G}}_0(\tau)\hat{\mathcal{G}}_0(-\tau) \tag{4}$$

DMFT equations written in Matsubara form yield no dynamical quantities, until the analytical continuation to real frequency axis is done, $i\omega_n\to\omega+i\eta$. To see where lies the root of numerical problems, one notes that the real-frequency and imaginary time Green's functions are connected by [17]

$$G(\tau)=\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega\frac{e^{-\tau\omega}}{1+e^{-\omega/T}}\,\mathrm{Im}\,G(\omega+i0^+) \tag{5}$$

where $G(\tau)=T\sum_n e^{i\omega_n\tau}G(i\omega_n)$ is the Fourier transform of Matsubara function. Due to exponential factors, the small changes in $G(\tau)$ (equivalently in $G(i\omega_n)$) are associated with large changes in $G(\omega+i\eta)$.

Now we turn our attention to the question of analytic continuation of DMFT equations in IPT approximation, parallel to the work of Schmalian et al. [11]. We rewrite the equation to be solved for nearly real frequencies $\omega+i\gamma$, with a finite γ. Then, we go to the limit $\gamma\to 0^+$ via Padé approximation. Padé approximation at this stage turns out to be stable. The finite parameter γ is chosen to provide the attenuation factors (as will be seen below) needed for convergence of the self-consistent equations.

The first equation to be continued analytically to nearly real axis is (3), which bears no difficulty,

$$G(\omega+i\gamma)=\tilde{D}(\omega+i\gamma+\mu-\Sigma(\omega+i\gamma)) \tag{6}$$

The next equation to be continued to nearly real-frequency axis is (1), which again simply reads

$$\mathcal{G}_0^{-1}(\omega+i\gamma)=\Sigma(\omega+i\gamma)+\frac{1}{\tilde{D}}(\omega+i\gamma+\mu-\Sigma(\omega+i\gamma)) \tag{7}$$

The main problem relies on analytically continuing the IPT approximation, Eq. (4) to nearly real frequency axis. This equation depends on the frequency not only through the Fourier factor $e^{i\omega_n\tau}$, but also through Green's function $\mathcal{G}_0(\tau)$. In this case, analytical continuation must be performed through the change of integral to its retarded form. Here the difficulty arises from the fact that we have solved the action equation (for a detailed review see Georges et al. [1, Section III.A]), on the imaginary axis to yield Matsubara function, so if one wishes to gain the physical quantities (such as retarded Green's function) one must either solve the problem originally on real frequency axis or analytically continue it. Kajueter and Kotliar [18,4] made an ansatz for self-energy on the real frequency axis of the form

$$\Sigma(\omega)=U+\frac{A\Sigma^{(2)}(\omega)}{1-B\Sigma^{(2)}(\omega)} \tag{8}$$

where $\Sigma^{(2)}$ is the second order contribution to self-energy from (4). Of course, this equation alone does not solve the problem, since there are other functions written in Matsubara form. Fortunately there is another way to overcome the problem. Using the Fourier transformation

$$\mathcal{G}_0(\tau)=\sum_{n=-\infty}^{\infty}e^{i\omega_n\tau}\mathcal{G}_0(i\omega_n) \tag{9}$$

Eq. (4) can be written as

$$\int_0^{\beta}d\tau\, e^{i\omega_n\tau}\mathcal{G}_0(\tau)\mathcal{G}_0(\tau)\mathcal{G}_0(-\tau)=\sum_k\mathcal{G}_0(i\omega_k)\chi^0(i(\omega_n+\omega_k)) \tag{10}$$

where

$$\chi^0(i(\omega_n+\omega_k))=\sum_l\mathcal{G}_0(i\omega_l)\mathcal{G}_0(i(\omega_n+\omega_l+\omega_k)) \tag{11}$$

is the particle–hole bubble. With the aid of contour integration and employing the complex forms of Fermi and Bose functions,

$$f(z)=\frac{1}{e^{\beta z}+1},\quad n(z)=\frac{1}{e^{\beta z}-1} \tag{12}$$

which have their poles exactly at Matsubara frequencies $z=i\omega_n=i(2n+1)\pi/\beta$ and $z=i\omega_n'=i(2n)\pi/\beta$, respectively, the summation over imaginary frequencies can be done,

$$\begin{aligned}\chi^0(iv_k)&=\sum_l\mathcal{G}_0(i(v_k+\omega_l))\mathcal{G}_0(i\omega_l)\\&=\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi i}\{f(\varepsilon+i\gamma')\mathcal{G}_0(iv_k+\varepsilon+i\gamma')\mathcal{G}_0(\varepsilon+i\gamma')-f(\varepsilon-i\gamma')\mathcal{G}_0(iv_k\\&\quad+\varepsilon-i\gamma')\mathcal{G}_0(\varepsilon+i\gamma')+f(\varepsilon+i\gamma')\mathcal{G}_0(\varepsilon+i\gamma')\mathcal{G}_0(\varepsilon+i\gamma'-iv_k)\\&\quad-f(\varepsilon-i\gamma')\mathcal{G}_0(\varepsilon-i\gamma')\mathcal{G}_0(\varepsilon-i\gamma'-iv_k)\}\end{aligned} \tag{13}$$