Dynamical Mean Field Theory equations on nearly real frequency axis

M. B. FATHI\textsuperscript{a} S. A. JAFARI\textsuperscript{b}

\textsuperscript{a}Department of Physics, Sharif University of Technology, Tehran 14588-89694, Iran
\textsuperscript{b}Department of Physics, Isfahan University of Technology, Isfahan 84156, Iran

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 can not be captured by conventional methods for solving DMFT-IPT equations on Matsubara frequencies. Our method suggests that at finite temperatures, there is an abrupt decrease in the height of the quasiparticle (Kondo) peak at a critical value of $U_c$, to a non-zero, but small bump, which gradually suppresses as one moves deeper into the bad insulator regime. In contrast to Vollhardt & coworkers [J. Phys. Soc. Jpn. 74, 136, 2005] down to $T=0.01$ of the half-bandwidth we find no $T^*$ separating bad insulator from a true Mott insulator.

PACS: 71.30.+h

Key words: diagrammatic for nearly real frequencies, DMFT, bad insulator.

1 Introduction

Feynman introduced a graphical representation of various perturbation schemes in the field theory which bears his name\cite{1}. Feynman diagrams. In condensed matter physics, the natural high momentum cut-off provided by the lattice dimensions prevents ultraviolet divergences. But yet remains the practical task of calculating them and interpreting the results.

Email addresses: mb.fathi@gmail.com (M. B. FATHI), sa.jafari@cc.iut.ac.ir (S. A. JAFARI).
Matsubara on the other hand introduced a very clever mathematical trick, which not only combines the thermal and quantum mechanical averaging required in calculations of the correlation functions in a neat way and treats them on the same footing, but also provides a very convenient method for numerical calculations of the diagrams. 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 in imaginary time, which are very convenient for putting on computer and convergence is particularly fast in iterative or self-consisted formulations of perturbation theory. However, the price will be payed when one has to undo the Wick rotation at the end of calculation to obtain dynamical quantities by replacing $i \omega_n \rightarrow \omega + i\eta$, where $\eta$ is an infinitesimal positive constant.

The hurdle one faces in undoing the Wick rotation is that, if using the Padé approximation one 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 $z \rightarrow \omega + i\eta$ in the resulting function, the calculated spectral weight 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.

People have been worried about this question from time to time, and there has been some proposals for reliable way of using the Padé approximation in analytic continuation of numerical data: Beach and coworkers [2] 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 qualitative measure of the reliability of continued data. Mishchenko and collaborators [3,4] proposed an stochastic optimization method which allows one to handle both broad and sharp features of the spectrum on equal footing.

On the other hands, Schmalian and colleagues proposed an alternative method which is quite intuitive and general[5]: Instead of solving the diagrammatic equations for Matsubara frequencies $i \omega_n$, solve them for frequencies $\omega + i\gamma$, where $\gamma$ is a finite constant. The finite value of $\gamma$ (usually taken to be less than the first nonzero Matsubara frequency) is important, and provides the damping required for convergence of the iterative solutions. At the same time analytic continuation from $\omega + i\gamma$ to $\omega + i\eta$, where $\eta = 0^+$, not only is stable, but also sustains fine features of the spectral function, such as shadow bands of the high temperature superconductors[6], as they found by applying this method to solve the diagrammatic equations of the fluctuation exchange approximation[7].

Dynamical mean field theory approximation has been successful in addressing
the issue of metal-insulator transitions in correlated electron systems at zero temperature\cite{8}. Keeping the aforementioned concerns about the reliability of the Padé analytic continuation procedure in mind, in this paper we use the method of Schmalian \textit{et. al.}\cite{5} to re-examine the nature of MIT in the half-filled Hubbard model at finite temperatures. We find that paying the price at the beginning and solving slightly more difficult equations for $\omega + i\gamma$ pays off and in addition to providing reliable Padé analytic continuation with absolutely no negative spectral weights, 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 can not be captured by Padé analytical continuation of the solutions of DMFT equations for Matsubara frequencies.

The only difficulty with this method is that with conventional double precision numeric accuracy at lower temperatures it is hard to achieve convergence. But the asymptotic behaviors at $T \rightarrow 0$ limit in our approach agree with other methods of solving the DMFT equations.

The paper is organized as follows: First we analytically continue the IPT 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 it’s bare counterpart via the Dyson equation\cite{8},

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

where,

$$\tilde{D}(i\omega_n + \mu - \Sigma) = \int_{-\infty}^{\infty} d\varepsilon \frac{D(\varepsilon)}{i\omega_n + \mu - \Sigma - \varepsilon}$$ \hspace{1cm} \text{(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 \textit{o} \textit{i.e.} $G_{oo}$ and it’s imaginary part...
gives the interacting DOS,

\[ G(i\omega_n) = \tilde{D}(i\omega_n + \mu - \Sigma(i\omega_n)) \]  

(3)

In IPT approximation, the self-energy is given by the second order perturbation theory\[8\] as,

\[ \Sigma(i\omega_n) \simeq U^2 \int_0^\beta e^{i\omega_n\tau} \hat{\mathcal{G}}_0(\tau)^3. \]  

(4)

DMFT equations written in Matsubara form yield no dynamical quantities, until the analytical continuation to real frequency axis is done,

\[ i\omega_n \rightarrow \omega + i\eta \]

To see where lies the root of numerical problems, one notes that the real-frequency and imaginary time Green’s functions are connected by\[9\]

\[ G(\tau) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{e^{-\tau\omega}}{1 + e^{-\omega/T}} Im G(\omega + i0^+) \]  

(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 and coworkers\[5\]. We rewrite the equation to be solved for nearly real frequencies \( \omega + i\gamma \), with a finite \( \gamma \). Then, we go to the limit \( \gamma \rightarrow 0^+ \) via Padé approximation. Padé approximation at this stage turns out to be stable. The finite parameter \( \gamma \) 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,

\[ G(\omega + i\gamma) = \tilde{D}(\omega + i\gamma + \mu - \Sigma(\omega + i\gamma)). \]  

(6)
The next equation to be continued to nearly real-frequency axis is (1), which again simply reads

$$ G_0^{-1}(\omega + i\gamma) = \Sigma(\omega + i\gamma) + \frac{1}{\tilde{D}(\omega + i\gamma + \mu - \Sigma(\omega + i\gamma))} \quad (7) $$

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 the Green’s function $G_0(\tau)$. In this case, analytical continuation must be performed through the change of integral to it’s retarded form. Here the difficulty arises from the fact that we’ve solved the action equation (for a detailed review see Georges et al. [8], 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 [10,11] made an ansatz for self-energy on the real frequency axis of the form

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

where, $\Sigma^{(2)}$ is the second order contribution to self-energy from (4). Of course, this equation alone doesn’t solve the problem, since there are other functions written in Matsubara form. Fortunately there is another way to overcome the problem. Equation (4) can be written as

$$ \Sigma(i\omega_n) \simeq U^2 \int_0^\beta d\tau e^{i\omega_n \tau} \hat{G}_0(\tau)\hat{G}_0(\tau)\hat{G}_0(-\tau). \quad (9) $$

Using the Fourier transformation

$$ G_0(\tau) = \sum_{n=-\infty}^\infty e^{i\omega_n \tau} G_0(i\omega_n), \quad (10) $$

it can be written as

$$ \int_0^\beta d\tau e^{i\omega_n \tau} G_0(\tau)G_0(\tau)G_0(-\tau) = \sum_k G_0(i\omega_k)\chi^0(i(\omega_n + \omega_k)), \quad (11) $$

where,
\[ \chi^0(i(\omega_n + \omega_k)) = \sum_l G_0(i\omega_l) G_0(i(\omega_n + \omega_l + \omega_k)) \] (12)

is the particle-hole bubble.

With the aid of contour integration and employing the complex forms of Fermi and Bose functions,

\[ f(z) = \frac{1}{e^{\beta z} + 1}, \quad n(z) = \frac{1}{e^{\beta z} - 1} \] (13)

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,

\[ \chi^0(i\nu_k) = \sum_l G_0(i(\nu_n + \omega_l)) G_0(i\omega_l) \]
\[ = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} \]
\[ \{ f(\epsilon + i\gamma') G_0(i\nu_k + \epsilon + i\gamma') G_0(\epsilon + i\gamma') \]
\[ - f(\epsilon - i\gamma') G_0(i\nu_k + \epsilon - i\gamma') G_0(\epsilon + i\gamma') \]
\[ + f(\epsilon + i\gamma') G_0(\epsilon + i\gamma') G_0(\epsilon + i\gamma' - i\nu_k) \]
\[ - f(\epsilon - i\gamma') G_0(\epsilon - i\gamma') G_0(\epsilon - i\gamma' - i\nu_k) \}. \]

Now, performing the analytical continuation \( i\nu_k \rightarrow \omega + i\gamma \), and making use of Kramers-Kronig transformation for the green function, along with the Laplace transformation

\[ \frac{1}{\omega + i\gamma} = -i \int_0^\infty dt \ e^{i(\omega + i\gamma)t} \] (15)

the particle-hole bubble reduces to

\[ \chi^0(\omega + i\gamma) = \int_0^\infty dt \ \chi^0(t) e^{i(\omega + i\gamma)t}, \] (16)

where,

\[ \chi(t) = -i(2\pi)^2 \left( \rho(t) \left[ A^*(t) + A(-t)e^{2\gamma t} \right] \right. \]
\[ - \rho^*(t) \left[ A(t) + A^*(-t)e^{2\gamma t} \right] \) (17)
In the above formula the spectral densities are given by,
\[ \rho(t) = -\frac{1}{2\pi} \frac{1}{\pi} \int_{-\infty}^{\infty} d\epsilon \ ImG_0(\epsilon + i\gamma)e^{-i\epsilon t}, \] (18)
and,
\[ A(t) = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\epsilon \ f^*(\epsilon + i\gamma)G_0^*(\epsilon + i\gamma)e^{-i\epsilon t}. \] (19)

In an analogous manner, the Laplace transform of self-energy can be written as:
\[ \Sigma(t) = -i2\pi T U^2 Re\chi^0(0 + i0^+) e^{\gamma t} \rho(t) \\
+ i(2\pi)^2 U^2 \times \left( v^0(t)[A(t) + A^*(-t)e^{2\gamma t}] \\
- \rho(t)[B^*(t) + B(-t)e^{2\gamma t}] \right) \] (20)
where,
\[ v^0(t) = -\frac{1}{2\pi} \frac{1}{\pi} \int_{-\infty}^{\infty} d\epsilon \ Im\chi^0(\epsilon + i\gamma)e^{-i\epsilon t}, \] (21)
and
\[ B(t) = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\epsilon \ n^*(\epsilon + i\gamma)\chi^0(\epsilon + i\gamma)e^{-i\epsilon t}. \] (22)

3 Numerical Results

The numerical results are given in units of the half bandwidth $W/2 = 1$. The temperature $T = 0.048$ and the Hubbard parameter $U$ varies from $U = 0$ through 7.5.

To perform the Fourier transforms we used the FFT routines. To overcome the alias effects arising from the $1/\omega$ tail, we chose the energy mesh large enough to ensure that the function vanishes at the boundaries. We have used $N = 2^{15}$ frequency points in an energy range of $2\omega_{max} = 250$. Also we have taken $\gamma = \pi T/4$. The finite value of $\gamma$ provides necessary damping factors in
the convergence of the iteration process. Therefore at lower temperatures it becomes harder to achieve convergence. Convergence at lower temperatures requires smaller values of $\gamma$ and hence higher accuracy than conventional double precision [2].

There are many lattices examined by the DMFT method, some of which is mentioned in the review paper by Georges et al. [8]. We work with Bethé lattice with semicircular DOS [12].

We begin with an initial guess for the green function, $G_0(\omega + i\gamma)$. Using Eqs. (18,19) we calculate $\rho(t)$ and $A(t)$ which are used to evaluate $\chi^0(t)$ in Eq. (17). Then we calculate $v^0(t)$ and $B(t)$, Eqs. (21,22), through which the self-energy $\Sigma(t)$, Eq. (20), and hence its Laplace transform, $\Sigma(\omega + i\gamma)$, can be evaluated. To close the iteration loop, $\Sigma(\omega + i\gamma)$ is inserted in the self-consistency equation (1) to update the initial Greens’ function and iteration is performed until convergence is achieved.

We have obtained converged solutions for $U$ in the range $[0, 7.5]$ for $T = 0.048$. At this temperature the transition occurs at critical value $U_c \approx 3.0^+$, in agreement with the results of Zhang and coworkers [13], and Vollhardt et al. [14].

3.1 The spectral density before the transition

![Fig. 1. DOS at $T = 0.048$ and values of $U < U_c$ in the metallic side. When the Hubbard parameter is increased the weight of fine peak is transferred to it’s neighbors. unlike the zero temperature case, the height of the central Kondo peak is not constant.](image)

Before the transition in the metallic regime, as one increases $U$ the DOS tends to split, leaving a central Kondo peak corresponding to quasiparticle at the Fermi level (Fig. 1) in agreement with the conventional methods of solving the DMFT equations [8]. In our computer code we have not forced the height of the Kondo peak to be constant. In our finite $T$ solution unlike the zero
temperature case the height of the Kondo resonance is not constant during the transition [15]. The height of the quasiparticle peak at Fermi energy is instead gradually redistributed and shifted to the upper(lower) edge of the lower(upper) Hubbard band.

3.2 The spectral density near the transition

The transition occurs at a critical Hubbard parameter $U_c$. We find the value for this critical Hubbard parameter in the range $2.99 \leq U_c \leq 3.01$. At the transition the height of peak falls off suddenly to a very small, but nonzero value, Fig. 2.

![Fig. 2. The evolution of DOS when the transition occurs. The results is shown for two representative values $U = 2.9$ and $U = 3.1$ at temperature $T = 0.048$.](image)

3.3 The spectral density after the transition

The evolution of the spectral function after the transition is shown in Fig. 3. In our solution increasing $U$ results in depletion of the spectral weight but does not give a clean gap at finite temperatures. For larger values of $U$ the spectral density at Fermi level is still finite and vanishes only in the limit $U \to \infty$, so that there is no real transition but a crossover from a metallic-like to an insulating-like solution. Vollhardt et al. [14] named this state as a bad insulator.

The finite temperature analogue of the Mott-Hubbard gap can be thought of as the peak-to-peak distance between the upper and lower Hubbard bands in Fig. 3. As can be seen this distance increases proportional to $U$. With increasing $U$ the "gap" tends to expand and the spectral weight in this region tends to decrease, but as we mentioned the gap is not clean at $T = 0.048$. At
Fig. 3. DOS after the transition, at temperature $T = 0.048$. Increasing $U$ tends to push upper and lower Hubbard bands far apart, but the little peak resists and remains there at even much larger values of $U$.

$U \rightarrow \infty$ one expects to obtain a clean gap around the Fermi level. In order to obtain clean gap at finite large $U$ one has to go to $T \rightarrow 0$ limit.

In the solution obtained by Vollhardt et al. [14] they introduce a temperature $T^*$ below which the bad insulator becomes a true insulator. Down to $T = 0.01$ where we have obtained converged solution in our method we do not find such a $T^*$. The trend of the lower $T$ data in Fig. 4 shows that at $T \rightarrow 0$ limit the gap starts to become cleaner and develops sharp edge characteristic of IPT method [8]. The small central peak in the bad insulating side gradually suppresses with decreasing $T$ but does not vanish at any finite $U$ (Fig. 4). The filling of the Mott-Hubbard gap by spectral weight transfer with increasing temperature has recently been detected experimentally by photoemission experiments [16].

An important aspect of insulating phase obtained in the present method is
the presence of a small bump at the Fermi level which is clearly seen in the Figs. 3 and 4. This little peak has a height about 10% of neighboring bands and does not vanish after the transition at any $U$.

4 Summary and conclusions

We employed a new method for solving diagrammatic equations to solve IPT equations of DMFT. We first analytically continued the equations to nearly real frequencies. Solving the continued equations is slightly harder, but seems to capture fine features of the spectral weight not previously reported.

We found that the height of Kondo peak does not remain constant before transition which is in contrast to the zero temperature result of Müller-Hartmann [15], which states that the height of the Kondo peak must remain constant before the transition occurs. The transition is first order and the Kondo peak suddenly falls off to a very small but non-zero value. For larger values of $U$ this small spectral density at Fermi level will persist and vanishes only in the limit $U \rightarrow \infty$ or $T \rightarrow 0$. In this limit the gap also becomes cleaner and we obtain a true insulator only in $T \rightarrow 0$ limit. Hence we do not find a $T^*$ [14].

Acknowledgement

M.B.F. would likes to thank Prof. M.A. Vesaghi for his many suggestions and constant support during this research. S.A.J. was supported by ALAVI Group Ltd.

References

[1] H. Bruus, and K. Flensberg: *Many-body Quantum Theory in Condensed Matter Physics*, Oxford University Press, (2004).

[2] K.S.D. Beach, R.J. Gooding and F. Marsiglio: Phys. Rev. B 61 (2000) 5147.

[3] A.S. Mishchenko, N.V. Prokofev, A. Sakamoto, and B.V. Svistunov: Phys. Rev. B 62 (2000) 6317.

[4] A.S. Mishchenko, N. Nagaosa, N.V. Prokofev, A. Sakamoto, and B.V. Svistunov: Phys. Rev. B 66 (2002) 020301.

[5] J. Schmalian, M. Langer, S. Grabowski, K. H. Bennemann: Computer Physics Communications 93 (1996) 141.
[6] M. Langer, J. Schmalian, S. Garbowski, K.H. Bennemann: Phys. Rev. Lett. 75 (1995) 4508.

[7] N.E. Bickers, D.J. Scalapino: Ann. Phys. (NY) 193 (1989) 206.

[8] Georges and G. Kotliar and W. Krauth and M. J. Rozenberg: Rev. Mod. Phys. 68 (1996) 13.

[9] G. Dopf et al.: Helv. Phys. Acta 65 (1992) 257.

[10] H. Kajueter and G. Kotliar: Int. J. Mod. Phys. 11 (1997) 729.

[11] K. Held: arXiv:cond-mat/0511293 (2005).

[12] E. N. Economou: Green’s Function in Quantum Physics (1983) 2nd Ed.

[13] X.Y. Zhang, M.J. Rozenberg, and G. Kotliar: Phys. Rev. Lett. 70 (1993) 1666.

[14] D. Vollhardt, K. Held, G. Keller, R. Bulla, Th. Pruschke, I. A. Nekrasov and V. I. Anisimov: J. Phys. Soc. Jpn. 74, 136, 2005

[15] E. Müller-Hartmann: Int. J. Mod. Phys. B 3 (1989) 2169.

[16] S. K. Mo, H. D. Kim, J. W. Allen, G.-H. Gweon, J. D. Denlinger, J. H. Park, A. Sekiyama, A. Yamasaki, S. Suga, P. Metcalf, and K. Held: Phys. Rev. Lett. 93 (2004) 076404.