Quantitative Description of $V_2O_3$ by the Hubbard Model in Infinite Dimensions

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Abstract

We show that the analytic single-particle density of states and the optical conductivity for the half-filled Hubbard model on the Bethe lattice in infinite dimensions describe quantitatively the behavior of the gap and the kinetic energy ratio of the correlated insulator $V_2O_3$. The form of the optical conductivity shows $\omega^{3/2}$ rising and is quite similar to the experimental data, and the density of states shows $\omega^{1/2}$ behavior near the band edges.

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It has been an interesting question that how well does the Hubbard model describe a real strongly correlated system. To answer this question, appropriate experiments are required. Recently, Thomas, et. al. [1] have measured optical conductivity for the insulating state of $V_2O_3$ whose magnetic phase has been known as antiferromagnetic [2]. They observed some interesting features for the properties of the insulating phase of $V_2O_3$ from the measurement of optical conductivity. They found that the insulator gap is not the Slater gap come from antiferromagnetic ordering [3] but the correlation gap resulted from strong on-site repulsion [4]. In other words, the optical conductivity rises as $(\omega - 2\Delta)^{3/2}$, where $2\Delta$ is the gap width, instead of $\omega^{1/2}$ expected from a Slater antiferromagnet. This $\omega^{3/2}$ rising is expected from the $\omega^{1/2}$ behavior of the single-particle density of states (DOS) near the band edges. They compared their experimental data with various theories [5–8]. The best fitting one was the paramagnetic solution of the dynamical mean-field theory [7,8] which is valid in infinite dimensions. They explained that the reason why paramagnetic solution describes the insulating state of $V_2O_3$ quite well was caused by the spin frustration. The spin structure of $V_2O_3$ is substantially frustrated, i.e., there are both ferromagnetic and antiferromagnetic nearest neighbors. In addition, it is known that a theory in infinite dimensions is well-applicable to a bulk system. [4] They also argued that their results are representative of the zero-temperature limit.

In this Letter, we report that the behaviors of $\omega^{3/2}$ in optical conductivity and $\omega^{1/2}$ in single-particle DOS can be seen in the Hubbard model on the Bethe lattice in infinite dimensions and our results in infinite dimensions fit experiments over all the insulator regime of $V_2O_3$, while the dynamical mean-field theory shown in Ref. 1 does not cover full insulator regime, especially near the metal-insulator transition. We show explicitly that the form of the optical conductivity is quite similar to that of experiment. In addition, the area under the curve of optical conductivity which gives the average kinetic energy has been compared with experiment by using the ratios of the averaged kinetic energy to its noninteracting value. The agreement between our theoretical values and experimental data is quantitatively good.

We now show our theoretical works and comparison with experiment. Before we go
further, we first consider spin frustration in the Bethe lattice since $V_2O_3$ is considered as a spin frustrated system [1]. We include next nearest neighbor hopping to take the frustration into account, since the Bethe lattice is a bipartite lattice which does not have frustration in lattice arrangement. For the Bethe lattice, however, the number of next nearest neighbor is $q(q-1)$, where $q$ is the coordination number. Therefore, $t_2$ representing next nearest neighbor hopping integral must be scaled as $t_2 = t_*/q$ to make the kinetic energy finite in infinite dimensions. The $t_2$, however, is $1/\sqrt{q}$ times less than $t_1$ which represents nearest neighbor hopping and scales as $t_1 = t_*/\sqrt{2q}$ [10]. Thus the effect of next nearest neighbor hopping can be neglected in calculating the DOS on the Bethe lattice in infinite dimensions. Therefore, the result obtained in the previous work [11] can be used without any change for the present analysis.

We briefly introduce the dynamical Lanczos method [9,12,13] used in this work. The single-particle DOS can be obtained by calculating the one-particle Green’s function of the fermion operator at the same site, i.e., $\langle \Psi_0|\{c^+_{j\sigma}(t), c_{j\sigma}\}|\Psi_0\rangle$ where $c^+_{j\sigma}$ and $c_{j\sigma}$ are the fermion creation and annihilation operators with spin $\sigma$ at site $j$, the curly brackets mean anticommutator, and $|\Psi_0\rangle$ denotes ground state. The single-particle DOS $\rho_\sigma(\omega)$ is given by [4]

$$\rho_\sigma(\omega) = -\frac{2}{N} \lim_{\epsilon \to 0^+} \sum_j \text{Im} G^{(+)}_{jj}(\omega + i\epsilon), \quad (1)$$

where

$$G^{(+)}_{jj}(\omega + i\epsilon) = -\frac{i}{2\pi} \int_0^\infty \langle \Psi_0|\{c^+_{j\sigma}(t), c_{j\sigma}\}|\Psi_0\rangle e^{i\omega t - \epsilon t} dt$$

$$= \frac{1}{2\pi} \langle \Psi_0|\{c_{j\sigma}, (\omega + i\epsilon)^{-1}c^+_{j\sigma}\}|\Psi_0\rangle$$

$$\equiv -\frac{i}{2\pi} \Xi_{jj}(z)|_{z=-i\omega+\epsilon}, \quad (2)$$

where $L$ is the Liouville operator. The superscript $(+)$ denotes the usual notation of the retarded Green’s function [4]. The on-site Green’s function $\Xi_{jj}(z)$ can be represented by an infinite continued fraction [12,13].
\[ \Xi_{jj}(z) = \frac{1}{z - \alpha_0 + \frac{\Delta_1}{z - \alpha_1 + \Delta_2}} , \]  

(3)

where \( \alpha_\nu = (iL_f, f_\nu) / (f_\nu, f_\nu) \), \( \Delta_\nu = (f_\nu, f_\nu) / (f_{\nu-1}, f_{\nu-1}) \). The inner product is defined by \( (A, B) = \langle \Psi_0 | \{ A, B \} | \Psi_0 \rangle \), where \( A \) and \( B \) are operators of the Liouville space, \( B^\dagger \) is the adjoint of \( B \). These \( \alpha_\nu \) and \( \Delta_\nu \) are obtained using a recurrence relation \( f_{\nu+1} = iL_f - \alpha_\nu f_\nu + \Delta_\nu f_{\nu-1} \). [13]

The Hubbard model which we study here is written as

\[ H = -\sum_{j,l,\sigma} t_{jl} c_{j\sigma}^\dagger c_{l\sigma} + \frac{U}{2} \sum_{j,\sigma} n_{j\sigma} n_{j,-\sigma} . \]  

(4)

By choosing \( f_0 = c_{j,\sigma}^\dagger \), we have obtain the on-site Green’s function \( \Xi_{jj}(z) \) for the half-filled Hubbard model on the Bethe lattice in infinite dimensions whose ground state is assumed as paramagnetic, [11]

\[ \Xi_{jj}(\tilde{z}) = \frac{\tilde{z} + \Delta_1}{\tilde{z}^2 + \frac{\Delta_2}{2b} [(b - a) - \tilde{z}^2 \pm \sqrt{(\tilde{z}^2 + a - b)^2 + 4b\tilde{z}^2}]} + \Delta_1 \]  

(5)

where \( \Delta_1 = \frac{U^2}{4} + \frac{t^2}{2} \), \( \Delta_2 = \frac{U^2 + t_\ast^2}{4\Delta_1} \), \( a = \frac{t^2}{4} \), \( b = 1t_\ast^2 \), and \( \tilde{z} = z - i\frac{U}{2} \).

If we set the chemical potential at \( \mu = \frac{U}{2} \), Eq. (5) gives the single-particle DOS for the insulating phase \( (a > b) \) as follows:

\[ \rho_\sigma(\omega) = \frac{1}{\pi} \text{Re} \Xi_{jj}(z) |_{z = -i\omega + 0^+} = \frac{\Delta_1 \Delta_2}{2\pi |\omega| \sqrt{W}} \]  

\[ \frac{\Delta_1 \Delta_2}{2\pi |\omega| \sqrt{W}} \left[ \left( \frac{\Delta_1}{2b} (b - a) + \Delta_1 + (\frac{\Delta_2}{2b} - 1) \omega^2 \right)^2 + \frac{\Delta_1^2}{4b^2} \right] \]  

(6)

where \( W = \{ \omega^2 - (\sqrt{a} - \sqrt{b})^2 \} \{ (\sqrt{a} + \sqrt{b})^2 - \omega^2 \} \). We take \((-)\) sign for \( \omega > 0 \) and \((+)\) for \( \omega < 0 \) to satisfy the boundary condition \( \Xi_{jj}(t = 0) = 1 \) given in Eq. (2). The lower and upper Hubbard bands exist \(- (\sqrt{a} + \sqrt{b}) \leq \omega \leq -\sqrt{a} + \sqrt{b} \) and \( \sqrt{a} - \sqrt{b} \leq \omega \leq \sqrt{a} + \sqrt{b} \), respectively. One can observe \( \omega^{1/2} \) behavior near band edges from Eq. (6).

One can observe that this single-particle DOS has band width \( 2D = 2\sqrt{b} = 2t_\ast \) and band gap \( 2\Delta = 2(\sqrt{a} - \sqrt{b}) = U - 2D \). Thus we get the following relation.
\[
\frac{2\Delta}{D} = \frac{U}{D} - 2 \tag{7}
\]

We draw Eq. (7) with experimental data in Fig. 1. A remarkable agreement is seen over all insulator regime.

We now obtain the optical conductivity \(\sigma(\omega)\) using a formula valid in infinite dimensions \[14\],

\[
\sigma(\omega) = \sigma_0 \int d\omega' \int d\epsilon \rho^{(0)}(\epsilon) \rho(\epsilon, \omega') \frac{f(\omega') - f(\omega' + \omega)}{\omega}, \tag{8}
\]

where \(f(\omega)\) is the Fermi distribution function and \(\sigma_0 = \frac{\pi^2 e^2 a^2 N}{2\hbar V}\) where \(a, N, V\) are lattice constant, number of lattice sites, volume, respectively. In Eq. (8), \(\rho^{(0)}(\epsilon) = \frac{1}{\pi} \sqrt{2t^2 - \epsilon^2}\) which is the single-particle DOS for \(U = 0\), and \(\rho(\epsilon, \omega) = -\frac{1}{\pi} \text{Im}G(\epsilon, \omega) = -\frac{1}{\pi} \text{Im}[\omega + i\eta - \epsilon - \Sigma(\omega)]^{-1}\). Use of the momentum-independence of the self-energy in infinite dimensions has been made. This property make it possible to express the self-energy in terms of the on-site Green’s function \(G(\omega) = -i\Xi_{jj}(-i\omega)\).

If we set \(\zeta = \omega - \Sigma(\omega)\), the one-particle Green’s function is mapped into the frequency renormalized noninteracting one which describes the noninteracting system under effective field, i.e., \(G^{(0)}(\zeta, \epsilon) = [\zeta - \epsilon]^{-1}\). Since we obtain \(\alpha_\nu = iU/2, \Delta_\nu = \frac{t^2}{2}\) for all \(\nu\) for the noninteracting Hubbard model on the Bethe lattice in the paramagnetic state, Eq. (3) gives

\[
\Xi^{(0)}_{jj}(\tilde{z}) = -\frac{\tilde{z}}{t^2} + \frac{\sqrt{\tilde{z}^2 + 2t^2}}{t^2} \bigg|_{\tilde{z} = -i\zeta + 0^+} = iG^{(0)}(\zeta) = iG(\omega). \tag{9}
\]

Solving Eq. (9) for \(\zeta\) gives the self-energy as

\[
\Sigma(\omega) = \omega - \frac{t^2}{2} G(\omega) - \frac{1}{G(\omega)}. \tag{10}
\]

This relation has been obtained by Georges and Krauth \[7\] in terms of the effective action theory.

Using Eqs. (5) and (10), we get \(\rho(\epsilon, \omega)\) and finally the optical conductivity \(\sigma(\omega)\) from Eq. (8). Fig. 2 shows theoretical \(\sigma(\omega/t_*)\) in units of \(\sigma_0\) for various \(U/t_*=\). We use approximation \(\Delta_1 \approx a\) and \(\Delta_2 \approx b\) in drawing \(\sigma(\omega/t_*)\). We choose \(U/D = 2.1\) and \(U/D = 4\) to compare
with experiment. To make the comparison appropriate, we need to adjust \( \omega/t_\ast \) for each sample, since each sample has different band width \( D \) which is equal to \( t_\ast \) in our theory. Therefore, for the horizontal scale, we set one unit of \( \omega/t_\ast \) to 0.31eV for \( U/D = 4 \) and 1.21eV for \( U/D = 2.1 \). The former gives \( 2\Delta = 0.62\text{eV} \) and the latter 0.12eV. Both gap widths are within experimental error bounds. For the vertical scale, however, we multiply each \( \sigma(\omega) \) by the corresponding \( D_m^2 \) \( (D_m = 0.47\text{eV} \) and 0.31eV for \( U/D = 2.1 \) and 4) in Ref. 1 to take \( \sigma_0 \) which is proportional to \( t_\ast^2 \) into account. Since the vertical scale itself is arbitrary, only relative height is meaningful. The optical conductivities represented by experimental scale are shown in Fig. 3 with \( \omega^{3/2} \) rising expressed by the dashed line.

Even though the theoretical value of the optical conductivity at a particular frequency is not quite close to that of experiment, overall structure is quite similar each other. An additional test for our theory related to optical conductivity can be performed by comparing the ratio of the average kinetic energy \( \langle \hat{T} \rangle \) to its noninteracting counterpart \( \langle \hat{T}_0 \rangle \) with experimental data. Since the conductivity sum rule

\[
\int_0^\infty \sigma(\omega)d\omega = -\xi \langle \hat{T} \rangle
\]  

(11)
gives rise to the average kinetic energy, one can immediately obtain the average kinetic energy by performing the integration. The explicit form of the constant \( \xi \) has been given by \( \xi = \frac{\pi e^2}{2\hbar c} \) \[|13\]. However, we do not need the explicit expression, because it is cancelled in getting the kinetic energy ratio.

The noninteracting counterpart \( \langle \hat{T}_0 \rangle \) can easily be obtained from Eq. (8) by using \( \rho^{(0)}(\epsilon, \omega) = \delta(\omega - \epsilon) \). Then we get \( \langle \hat{T}_0 \rangle = \frac{-\sqrt{2\pi\sigma_0}}{\xi} \). Using this and performing the integration in Eq. (11) for the optical conductivities shown in Fig. 2, we obtain the ratios as follows: \( \langle \hat{T} \rangle / \langle \hat{T}_0 \rangle = 0.349, 0.205, 0.147, \) and 0.116 for \( U/D = 2.1, 3, 4, \) and 5, respectively. We put these values with experimental data and other theoretical work in Fig. 4. Our theoretical values are quite close to the result of dynamical mean field theory and its extension to the metastable branch where both insulating and metallic solutions coexist \[7,8\].

In conclusion, we argue that the paramagnetic solution obtained by the dynamical Lanc-
zos method for the Hubbard model on a Bethe lattice in infinite dimensions may describe
the insulating phase of the three-dimensional strongly correlated system like $V_2O_3$ quantita-
tively well. The spin frustration effect which makes the system paramagnetic-like has been
treated by considering next nearest neighbor hoppings in the Bethe lattice. The behavior of
the insulating gap and the average kinetic energy ratio according to the change of $U/D$ is
quite well agreed with experiment quantitatively, while the optical conductivities showing
$(\omega - 2\Delta)^{3/2}$ rising are agreed qualitatively. Finally we expect that the metallic regime of
$V_2O_3$ can also be explained quantitatively in terms of our result for metallic phase. This
will be a forthcoming work.

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REFERENCES

[1] G.A. Thomas et al., Phys. Rev. Lett. 73, 1529 (1994).

[2] D.B. McWhan, A. Menth, J.P. Remeika, W.F. Brinkman, and T.M. Rice, Phys. Rev. B 7, 1920 (1973).

[3] J.C. Slater, Phys. Rev. 82, 538 (1951).

[4] J. Hubbard, Pro. R. Soc. London A 276, 238 (1963); ibid. 281, 401 (1964).

[5] C. Castellani, C.R. Natoli, and J. Ranninger, Phys. Rev. B 18, 4967 (1978).

[6] R. Raimondi and C. Castellani, Phys. Rev. B 48, 11453 (1993).

[7] A. Georges and W. Krauth, Phys. Rev. B 48, 7167 (1993).

[8] M.J. Rozenberg, G. Kotliar, and X.Y. Zhang, Phys. Rev. B 49, 10181 (1994).

[9] See, e.g., P. Fulde, Electron Correlations in Molecules and Solids, Solid-State Sciences Vol. 100, 2nd edn. (Springer-Verlag, Berlin, 1993) p. 293.

[10] W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989); E. Müller-Hartmann, Z. Physik B 74, 507 (1989).

[11] J. Hong and H-Y. Kee, to be published in Phys. Rev. B (1995).

[12] E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).

[13] J. Hong, J. Kor. Phys. Soc. 20, 174 (1987).

[14] Th. Pruschke, D.L. Cox, and M. Jarrell, Phys. Rev. B 47, 3553 (1993); and Europhys. Lett. 21, 5 (1993).

[15] G. Kotliar and M.J. Rozenberg, Lecture Note, SMR. 758-33 (I.C.T.P., Trieste, 1994).
Figure Captions

Fig. 1: Comparison of Eq. (7) with experimental data (solid circles for optical measurements, open circles and diamonds for dc measurements) of Ref. 1. The dashed line is the present theory and the solid line is the stable solution of the dynamical mean field theory.

Fig. 2: Theoretical optical conductivities for $U/D = 2.1, 3, 4, \text{ and } 5$ obtained by using Eq. (8). We express $\sigma(\omega/t_\ast)$ in units of $\sigma_0$.

Fig. 3: Comparison of optical conductivities for $U/D = 2.1$ and 4 with experimental data (solid points for $U/D \approx 2.1$ and open circles for $U/D \approx 4$) shown in Ref. 1. The solid lines are theoretical values and the dashed and the dotted lines denote $\omega^{3/2}$ rising in theory and experiment, respectively. The horizontal scale for theoretical curves is reexpressed by the energy scale used in experiment. Arbitrary units are used for the vertical scale for theoretical values. Details are explained in the text.

Fig. 4: Comparison of average kinetic energy ratios $\langle \hat{T} \rangle / \langle \hat{T} \rangle_0$ for $U/D = 2.1, 3, 4, \text{ and } 5$ with experiment (solid circles) and theory. Present theoretical values are expressed by solid triangles. The solid, dashed, and dash-dot line denote dynamical mean field theory given in Ref. 1. The region covered by dashed line is the metastable regime suggested in Refs. 7 and 8.