STUDY OF MOTT-HUBBARD TRANSITION IN THE HALH-FILLED HUBBARD MODEL IN LARGE DIMENSIONS

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A dynamical theory treating the strongly correlated system such as those described by the Hubbard model is introduced. Our analytic results describe the Mott-Hubbard transition and some experiments even quantitatively.

I. Introduction

The Hubbard model may be applicable to describing the metal-insulator transition in the materials like V_2O_3 [1,2] and $Ca_{1-x}Sr_xVO_3$ [3]. Mott-Hubbard transitions showing band collapsing and mass enhancement due to strong correlation and magnetic ordering are common phenomena of the Mott-Hubbard systems. These bring renewed interest in the Mott-Hubbard system recently. Working in large dimensions [4] makes it possible to treat the Hubbard model analytically, since spatial correlations do not play an important role in the limit of large dimensions. [5–7]

We introduce an extremely simple approach to studying the dynamics of Mott- Hubbard system by calculating the single-particle density of states through a continued fraction formalism for the one-particle Green's function. For the infinite dimensions, it is possible to obtain the optical conductivity from the single-particle density of states, because the self-energy can be expressed in terms of the on-site Green's function in infinite dimensions. [8] The optical conductivity has been measured recently [1], therefore, we can compare our theory with experiment.

Our result shows the Hubbard feature of band collapsing and the Brinkman-Rice feature of mass enhancement for the metal-insulator transition in one theoretical scheme. We have a sharp delta-function peak at chemical potential as an indication of the Fermi-liquid quasi-particle. We also obtain optical conductivity. Our result can describe recent experiment on V_2O_3 quantitatively.

II. Formalism

The single-particle DOS $\rho_\sigma(\omega)$ is given by

$$\rho_\sigma(\omega) = -\frac{2}{N}\lim_{\eta\to 0^+}\sum_j \mathrm{Im}G_{jj}^{(+)}(\omega + i\eta), \tag{1}$$

where the one-particle retarded on-site Green's function $G_{jj}^{(+)}(\omega+i\eta)$ is written as

$$G_{jj}^{(+)}(\omega+i\eta) = -\frac{i}{2\pi}\int_0^\infty \langle\{c_{j\sigma}(t), c_{j\sigma}^\dagger\}\rangle e^{i\omega t-\eta t}dt \equiv -\frac{i}{2\pi}\Xi_{jj}(z)|_{z=-i\omega+\eta}, \tag{2}$$

where $\Xi_{jj}(z)$ is the Laplace transform of the dynamics $\langle\{c_{j\sigma}(t), c_{j\sigma}^\dagger\}\rangle$.

Let us consider the dynamics of $c_{j\sigma}(t)$ in a Liouville space (operator Hilbert space) with inner product $(A,B) = \langle\{A, B^\dagger\}\rangle$. Then, the Green's function (2) is the projection of $c_{j\sigma}(t)$ onto $c_{j\sigma}$. The projection is most easily obtained in the orthogonalized Liouville space which can be constructed by choosing the first vector as $f_0 = c_{j\sigma}$ and using the recurrence relation

$$f_{\nu+1} = iLf_\nu - \alpha_\nu f_\nu + \Delta_\nu f_{\nu-1}, \tag{3}$$

where $\alpha_\nu = \frac{(iLf_\nu, f_\nu)}{(f_\nu, f_\nu)}$, $\Delta_\nu = \frac{(f_\nu, f_\nu)}{(f_{\nu-1}, f_{\nu-1})}$.

The projection in the Laplace transformed space, is written as

$$(c_{j\sigma}(z), c_{j\sigma}) = \cfrac{1}{z-\alpha_0+\cfrac{\Delta_1}{z-\alpha_1+\cfrac{\Delta_2}{z-\alpha_2+\ddots}}} \equiv \Xi_{jj}(z) \tag{4}$$

and the retarded Green's function and the single-particle DOS are given by $G_{jj}^{(+)}(\omega+i\eta) = -\frac{i}{2\pi}\Xi_{jj}(z)|_{z=-i\omega+\eta}$ and $\rho_\sigma(\omega) = \frac{1}{N\pi}\lim_{\eta\to 0^+}\sum_j \mathrm{Re}\Xi_{jj}(z)|_{z=-i\omega+\eta}$, respectively.

III. Dynamics of the Hubbard Model at Half-Filling

Now we obtain the dynamics of $c_{j\sigma}(t)$ for the Hubbard model

$$H = -\sum_{<jl>\sigma} t_{jl}c_{j\sigma}^\dagger c_{l\sigma} + \frac{U}{2}\sum_{j\sigma} n_{j\sigma}n_{j,-\sigma}, \tag{5}$$

where $< jl >$ means nearest neighbor sites. We consider the paramagnetic state of the half-filled Hubbard model on a Bethe lattice. The model shows interesting physics such as band collapsing [9] (Hubbard feature) and quasiparticle mass enhancement [10] (Brinkman-Rice feature) in the process of metal-insulator transition at a finite U.

Taking the first vector as $f_0 = c_{j\sigma}$, and using the method of section II, one gets the orthogonal basis f_ν such as $f_0 = c_{i\sigma}, f_1 = -iU\delta n_{i,-\sigma}c_{i\sigma} - i\Sigma_l' t_{il}c_{l,\sigma}, f_2 = -U\Sigma_l'(\delta n_{l,-\sigma} + \delta n_{i,-\sigma})t_{il}c_{l\sigma} - \Sigma_l'\Sigma_k' t_{il}t_{lk}c_{k\sigma}, f_3 = iU^2\Sigma_l'(\delta n_{i,-\sigma}\delta n_{l,-\sigma} + \frac{1}{4})t_{il}c_{l\sigma}, f_4 = U^2\Sigma_l'\Sigma_k'(\delta n_{i,-\sigma}\delta n_{l,-\sigma} +$

$\delta n_{i,-\sigma}\delta n_{k,-\sigma} + \delta n_{l,-\sigma}\delta n_{k,-\sigma} + \frac{1}{4})t_{il}t_{lk}c_{k\sigma}, f_5 = -iU^3\Sigma_l'\Sigma_k'\{\delta n_{i,-\sigma}\delta n_{l,-\sigma}\delta n_{k,-\sigma} + \frac{1}{4}(\delta n_{i,-\sigma} + \delta n_{l,-\sigma} + \delta n_{k,-\sigma})\}t_{il}t_{lk}c_{k\sigma}$. We used large-$U$ expansion. A further approximation $(q-1) \approx q$ valid at higher dimensions has been made.

One can see that only the leading terms in f_ν above preserve the orthogonality. Constructing orthogonal space with these vectors, we obtain $\alpha_\nu = -iU/2, \Delta_{2\nu+1} = U^2/4 \equiv a$, and $\Delta_{2\nu+2} = 2qt^2 \equiv b$, for $\nu \geq 0$. Then the infinite continued fraction (4) can be calculated as follows:

$$\Xi_{jj}(\tilde{z}) = \frac{(b-a) - \tilde{z}^2 \pm \sqrt{(\tilde{z}^2 + a - b)^2 + 4b\tilde{z}^2}}{2b\tilde{z}} \tag{6}$$

where $\tilde{z} = z + i\frac{U}{2}$. We take $(-)$ sign for $\omega > 0$ and $(+)$ for $\omega < 0$ to satisfy the boundary condition $\Xi_{jj}(t=0) = 1$.

If we set the chemical potential at $\mu = \frac{U}{2}$, Eq. (6) gives the single-particle DOS for the insulating phase $(a > b)$ as

$$\rho_\sigma(\omega) = \frac{\sqrt{\{\omega^2 - (\sqrt{a} - \sqrt{b})^2\}\{(\sqrt{a} + \sqrt{b})^2 - \omega^2\}}}{2b\pi|\omega|} \tag{7}$$

and

$$\rho_\sigma(\omega) = \left(1 - \frac{a}{b}\right)\frac{1}{\pi}\frac{\eta}{\omega^2 + \eta^2} + \frac{\sqrt{\{\omega^2 - (\sqrt{a} - \sqrt{b})^2\}\{(\sqrt{a} + \sqrt{b})^2 - \omega^2\}}}{2b\pi|\omega|} \tag{8}$$

for the metallic phase $(a < b)$. The key approximation used in this work is the Hartree-Fock type decoupling approximation.

We now obtain the optical conductivity $\sigma(\omega)$ using a formula valid in infinite dimensions, [8]

$$\sigma(\omega) = \sigma_0 \int d\omega' \int d\epsilon \rho^{(0)}(\epsilon)\rho(\epsilon,\omega')\rho(\epsilon,\omega'+\omega)\frac{f(\omega') - f(\omega'+\omega)}{\omega}. \tag{9}$$

The momentum-independence of the self-energy in infinite dimensions make it possible to express the self-energy in terms of the on-site Green's function. For the Bethe lattice in the paramagnetic state, there is a self-consistent relation for the self-energy such as [5,7] $\Sigma(\omega) = \omega - \frac{t_*^2}{2}G(\omega) - \frac{1}{G(\omega)}$ and the on-site Green's function is $G(\omega) = -i\Xi_{jj}(z)|_{z=-i\omega+\eta}$. We show the results of the optical conductivity compared with experiment [1] in Fig.1.

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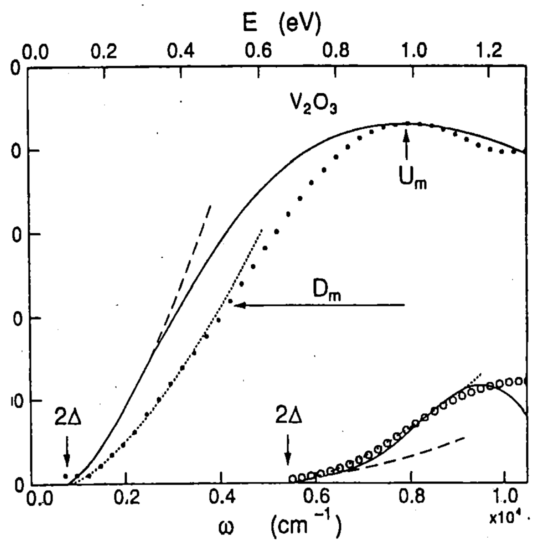

Fig. 1 : Comparison of optical conductivities for $U/D = 2.1$ and 4 with experimental data (solid points for $U/D \approx 2.1$ and open circles for $U/D \approx 4$) shown in Ref. 1. The solid lines are theoretical values and the dashed and the dotted lines denote $\omega^{3/2}$ rising in theory and experiment, 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.