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<th>STUDY OF MOTT-HUBBARD TRANSITION IN THE HALH-FILLED HUBBARD MODEL IN LARGE DIMENSIONS (Session I: Cross-Disciplinary Physics, The 1st Tohwa University International Meeting on Statistical Physics Theories, Experiments and Computer Simulations)</th>
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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 quasiparticle. We also obtain optical conductivity. Our result can describe recent experiment on $V_2O_3$ quantitatively.

II. Formalism
The single-particle DOS $\rho_\omega(\omega)$ is given by
\[ \rho_\omega(\omega) = \frac{2}{N} \lim_{\eta \to 0^+} \sum_j \text{Im} G_{jj}^{(+)}(\omega + i\eta), \] (1)
where the one-particle retarded on-site Green's function $G_{jj}^{(+)}(\omega + i\eta)$ is written as
\[ G_{jj}^{(+)}(\omega + i\eta) = -i \frac{1}{2\pi} \int_0^{\infty} \langle \{ c_{j\sigma}(t), c_{j\sigma}^\dagger \} \rangle e^{i\omega t - \eta t} dt \equiv \frac{-i}{2\pi} \Xi_{jj}(z)|_{z = -i\omega + \eta}, \] (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 $\langle A, B \rangle = \langle \{ A, B^\dagger \} \rangle$. 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
\[ f_{\nu+1} = iLf_\nu - \alpha_\nu f_\nu + \Delta_\nu f_{\nu-1}, \] (3)
where $\alpha_\nu = \frac{(i\nu f_\nu f_\nu)}{(i\nu f_\nu)}$, $\Delta_\nu = \frac{(f_\nu f_\nu)}{(f_{\nu-1}, f_{\nu-1})}$.

The projection in the Laplace transformed space, is written as
\[ (c_{j\sigma}(z), c_{j\sigma}) = \frac{1}{z - \alpha_0 + \frac{\Delta_1}{z - \alpha_1 + \frac{\Delta_2}{z - \alpha_2 + \cdots}} \equiv \Xi_{jj}(z) \] (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 $\rho_\omega(\omega) = \frac{1}{N\pi} \lim_{\eta \to 0^+} \sum_j \text{Re} \Xi_{jj}(z)|_{z = -i\omega + \eta}$, respectively.

### III. Dynamics of the Hubbard Model at Half-Filling

Now we obtain the dynamics of $c_{j\sigma}(t)$ for the Hubbard model
\[ H = -\sum_{<jl>\sigma} t_{jl} c_{j\sigma}^\dagger c_{l\sigma} + \frac{U}{2} \sum_{j\sigma} n_{j\sigma} n_{j,-\sigma}, \] (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 $f_\nu$ such as $f_0 = c_{j\sigma}$, $f_1 = -iU\delta n_{i,-\sigma} c_{i\sigma} - i\Sigma^t t_{il} c_{l\sigma}$, $f_2 = -U\Sigma^t (\delta n_{i,-\sigma} + \delta n_{i,-\sigma}) t_{il} c_{l\sigma} - \Sigma^t \Sigma_h t_{il} t_{lk} c_{l\sigma}$, $f_3 = iU^2 \Sigma^t (\delta n_{i,-\sigma} \delta n_{l,-\sigma} + \frac{1}{4}) t_{il} c_{l\sigma}$, $f_4 = U^2 \Sigma^t \Sigma_h (\delta n_{i,-\sigma} \delta n_{l,-\sigma} + \frac{1}{4}) t_{il} c_{l\sigma}$,

\[ \cdots \]
δn_{i,-σ}δn_{k,-σ} + δn_{i,-σ}δn_{k,-σ} + \frac{1}{4}t_ilt_kc_{kσ}, f_5 = -iU^3\Sigma'_k(S\delta n_{i,-σ}δn_{i,-σ} + \frac{1}{4}(δn_{i,-σ} + δn_{i,-σ} + δn_{k,-σ})t_ilt_kc_{kσ}. We used large-U expansion. A further approximation (q - 1) ≈ 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 $α_ν = -iU/2, Δ_{2ν+1} = U^2/4 \equiv a$, and $Δ_{2ν+2} = 2qt^2 \equiv b, for ν > 0$. Then the infinite continued fraction (4) can be calculated as follows:

$$\Xi_{ij}(z) = \frac{(b - a) - z^2 \pm \sqrt{(z^2 + a - b)^2 + 4b^2}}{2b^2}$$

(6)

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

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

$$ρ_σ(ω) = \frac{\sqrt{ω^2 - (\sqrt{a} - \sqrt{b})^2}((\sqrt{a} + \sqrt{b})^2 - ω^2)}{2bπ|ω|}$$

(7)

and

$$ρ_σ(ω) = \left(1 - \frac{a}{b}\right)\frac{1}{\pi ω^2 + \eta^2}$$

$$+ \frac{\sqrt{ω^2 - (\sqrt{a} - \sqrt{b})^2}((\sqrt{a} + \sqrt{b})^2 - ω^2)}{2bπ|ω|}$$

(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 $σ(ω)$ using a formula valid in infinite dimensions,

$$σ(ω) = σ_0 \int dω' \int dσ\rho^{(0)}(σ, ω')\rho(σ, ω + ω')f(ω') - f(ω' + ω)$$

$$σ(ω) = \frac{2πω}{\epsilon}G(ω) - \frac{1}{\epsilon(ω)}$$

(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 $[5,7] Σ(ω) = ω - \frac{G(ω)}{2} - \frac{1}{G(ω)}$ and the on-site Green’s function is $G(ω) = -i\Xi_{jj}(z)|_z = -\omega + ν$. We show the results of the optical conductivity compared with experiment [1] in Fig.1.

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REFERENCES


