Exciton Mott transition and pair condensation in the electron-hole system

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Abstract. We investigate the exciton Mott transition and pair condensation in the spinless electron-hole Hubbard model by means of the dynamical mean field theory combined with the noncrossing approximation. By investigating the single-particle density of states, we find the crossover between the metallic electron-hole plasma and the exciton-like insulator. We also investigate the electron-hole pair condensation transition and the optical response, by calculation of the two-particle Green's function for the pair correlation with vertex corrections. It is shown that the excitonic peak in the optical response function gets strongly enhanced around the electron-hole pair condensation transition.

1. Introduction

The electron(e)-hole(h) system in photoexcited semiconductors has attracted much interest for many years. In this system, emergence of various interesting properties has been suggested, depending on e-h density, temperature, etc., and they have been studied both experimentally and theoretically [1]. Among them, one of important physics is the exciton Mott transition from an exciton or biexciton insulating gas phase to a metallic e-h plasma phase with increasing e-h density. Another is the transition from the normal phase to an e-h pair condensed one. In spite of the extensive studies for many years, these phase transitions have not yet been sufficiently understood, because of theoretical difficulties of describing these different phases in the unified theoretical framework.

Recently, the dynamical mean field theory (DMFT) [2] has been successfully applied to the issues of the exciton Mott transition and pair condensation transition in the e-h system [3]. However, in these studies, the exciton Mott transition and the pair condensation have been described by different theoretical methods. Also, the two particle Green’s function for the optical response is approximately calculated using ladder type Feynman diagrams. Therefore, it is desirable to describe these phase transitions by unified theoretical treatment and obtain the correct optical response function around these phase transitions.

In this paper, we study the exciton Mott transition and pair condensation transition by means of DMFT combined with the noncrossing approximation (NCA) [4]. By calculation of the single-particle density of states (DOS), we investigate the Mott transition. In addition, we formulate a general two-particle Green’s function using NCA, and discuss the e-h pair condensation and optical response.
2. Model and method

In the recent studies of e-h system by DMFT [3], the spinful e-h Hubbard model has been used. For simplicity, we here consider the spinless model equivalent to the well-known attractive Hubbard model,

\[ H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} - U' \sum_i \epsilon_{ie} c_{ie}^\dagger c_{ih}^\dagger c_{ih} c_{ie}, \]

where \( c_{ie(h)}^\dagger \) creates a conduction-band electron (a valence-band hole) at the \( i \)th site, and \( t \) and \( U' \) are the transfer integral of electrons and holes and the on-site e-h attractive interaction, respectively. The angle bracket \( \langle \rangle \) denotes taking the sum of adjacent sites. For simplicity, we assume that the transfer integral of electrons is the same as that of holes (mass of holes is the same as that of electrons) and the number of electrons is also the same as that of holes.

Within DMFT, the original lattice model is mapped onto an effective impurity model with the effective medium determined self-consistently. Following the DMFT procedure, we obtain the self-consistent equation, \( G^{-1}(\omega) = G^{-1}(\omega) + \Sigma(\omega) \), where \( G, \Sigma \) and \( G \) are the effective medium, self-energy and local Green’s function, respectively. The local Green’s function is obtained in terms of the self-energy by \( G(\omega) = \int d\varepsilon \rho_0(\varepsilon)[\omega + \varepsilon - \Sigma(\omega)]^{-1} \). Here, \( \mu \) is the chemical potential and \( \rho_0(\varepsilon) = \sum_k \delta(\varepsilon - \varepsilon_k) \) is DOS for free electrons and holes with dispersion \( \varepsilon_k \). For given effective medium \( G \), we calculate the self-energy \( \Sigma \) by means of NCA, and recompute \( G \) using the above equations. This procedure is iterated until numerical convergence is reached.

After we obtain convergence of \( G \), we calculate the pair correlation function defined as,

\[ \chi_p(q, \tau) = \langle 1/N \rangle \sum_{k,l} \langle T_\tau c_{ke}(\tau) c_{q-kh}(\tau) c_{q-h}^\dagger(0) c_{k\epsilon}^\dagger(0) \rangle. \]

In order to incorporate the vertex correction into the correlation function, we consider the two-particle Green’s function in the effective impurity model [2]. We define the two-particle Green’s function as,

\[
g(\nu_n; \nu_l, \nu_m) = \frac{1}{\beta} \int_0^\beta \int_0^\beta \int_0^\beta d\tau_1 d\tau_2 d\tau_3 e^{i\nu_n(\tau_1 - \tau_3)} e^{i\nu_l(\tau_1 - \tau_2)} e^{i\nu_m(\tau_3 - \tau_4)} \langle T_\tau A(\tau_1) B(\tau_2) C(\tau_3) D(\tau_4) \rangle,
\]

where \( \beta = 1/T \) is the inverse temperature. For the pair correlation function, the fermionic operators \( A, B, C \) and \( D \) are \( c_{0e}, c_{0h}, c_{ih}^\dagger \) and \( c_{0e}^\dagger \), respectively. Applying the standard diagrammatic rules of NCA [4, 5] to the two-particle Green’s function (2), we obtain

\[
g(\nu_n; \nu_l, \nu_m) = \frac{1}{Z_0} \sum_{n_1,n_2,n_3,n_4} \langle n_1 | A | n_2 \rangle \langle n_2 | B | n_3 \rangle \langle n_3 | C | n_4 \rangle \langle n_4 | D | n_1 \rangle \]

\[
- R_{n_1}(z) R_{n_2}(z + i\nu_n + i\nu_l) R_{n_3}(z + i\nu_n) R_{n_4}(z + i\nu_m) \\
+ R_{n_1}(z) R_{n_2}(z + i\nu_n + i\nu_l) R_{n_3}(z + i\nu_n + i\nu_l) R_{n_4}(z + i\nu_n - i\nu_m) \\
+ R_{n_1}(z) R_{n_2}(z + i\nu_n + i\nu_l) R_{n_3}(z + i\nu_n + i\nu_l + i\nu_m) R_{n_4}(z + i\nu_m) \\
- R_{n_1}(z) R_{n_2}(z + i\nu_n + i\nu_l) R_{n_3}(z + i\nu_n + i\nu_l + i\nu_m) R_{n_4}(z + i\nu_m) \\
- R_{n_1}(z) R_{n_2}(z + i\nu_n + i\nu_l) R_{n_3}(z + i\nu_n + i\nu_l - i\nu_m) R_{n_4}(z + i\nu_n - i\nu_m) \\
+ R_{n_1}(z) R_{n_2}(z + i\nu_n + i\nu_l) R_{n_3}(z + i\nu_n + i\nu_l - i\nu_m) R_{n_4}(z + i\nu_m),
\]

where \( R_n(z) \) is the ionic resolvent and \( Z_0 \) denotes the ‘impurity’ contribution of the partition function in the effective impurity model [4]. The contour C surrounds all singularities of the integrands anticlockwise, and the sums of \( |n_1\rangle, |n_2\rangle, |n_3\rangle, |n_4\rangle \) are performed over \( |0\rangle, c_{0e}^\dagger |0\rangle, c_{0h}^\dagger |0\rangle, c_{0e}^\dagger c_{0h}^\dagger |0\rangle \).
We first calculate the two-particle Green’s function (2) using equations (3), and extract the vertex function $\Gamma(i\nu_n; i\omega_l, i\omega_m)$ via the Bethe-Salpeter equation, $\hat{\Gamma} = \hat{g}_0 - \hat{g}^{-1}$, where $g_0$ is the bare two-particle Green’s function, $g_0(i\nu_n; i\omega_l, i\omega_m) = \beta G(i\omega_l)G(i\nu_n - i\omega_l)\delta_{l,m}$. Here, $\hat{O}$ denotes a $N_f \times N_f$ matrix, and $N_f$ is the number of the Matsubara frequency. On the other hand, the bare two-particle Green’s function in the lattice model is calculated as, $g_0(q, i\nu_n; i\omega_l, i\omega_m) = (\beta/N) \sum_k [i\omega_l - \varepsilon_k + \mu - \Sigma(i\omega_l)]^{-1} [i\nu_n - i\omega_l - \varepsilon_{q-k} + \mu - \Sigma(i\nu_n - i\omega_l)]^{-1} \delta_{l,m}$. Using this equation and the Bethe-Salpeter equation, we compute the two particle Green’s function in the lattice model as, $\hat{g}(q, i\nu_n) = \hat{g}_0(q, i\nu_n)^{-1} - \hat{\Gamma}(i\nu_n)$. We finally obtain the pair correlation function, $\chi_p(q, i\nu_n) = \beta^2 \sum_{l,m} g(q, i\nu_n; i\omega_l, i\omega_m)$.

3. Results

we now investigate numerically the exciton Mott transition and pair condensation transition in the spinless electron-hole system (1) at typical low filling $n_e = n_h = 0.1$, where $n_e$ ($n_h$) is the number of electrons (holes) per site. We assume the free-particle DOS to be semicircular form, $\rho_0(\varepsilon) = \sqrt{4T^2 - \varepsilon^2}/(2\pi t^2)$, and take half the band width as the energy unit, $2t = 1$.

We first study the exciton Mott transition by investigating the single-particle DOS. In Figure 1, we show DOS of electrons $\rho(\omega) = -\text{Im}G(\omega + i0)/\pi$ at $T = 0.3$. We can clearly see the crossover from metal to insulator. As $U'$ increases, a dip gradually evolves near the Fermi level, and a gap opens between the Hubbard bands for $U' = 3$. The temperature dependence of DOS for $U' = 3$ is shown in Figure 2. As $T$ decreases, the chemical potential shifts, entering the inside of the gap, and the system becomes insulating at low temperatures $T < 0.4$. This behavior is qualitatively consistent with the previous studies of the infinite dimensional attractive Hubbard model at higher filling [6].

We next study the e-h pair condensation. By calculating the static and uniform pair susceptibility $\chi_{\text{static}} = \chi_p(q = 0, i\nu_n = 0)$, we determine the pair condensation transition temperatures. Divergence of $\chi_{\text{static}}$ indicates occurrence of the second order pair condensation transition. In Figure 3, we show the inverse susceptibility $1/\chi_{\text{static}}$ as a function of $T$. We find that $1/\chi_{\text{static}}$ goes to zero with lowering $T$. We thus determine the transition temperatures $T_c \sim 0.21, 0.30, 0.39$ for $U = 1, 2, 3$, respectively. The transition temperatures are higher than that obtained in the previous studies [6], which is due to our NCA approach.

Finally, we calculate the optical response function $\chi(\omega) = \text{Im}\chi_p(q = 0, \omega + i0)$, by applying
the pade approximation to $\chi_p(q = 0, i\nu_n)$. Figure 4 shows the optical response function $\chi(\omega)$ for $U' = 2.0$ at several temperatures. At high temperatures, the broad peak appears in $\chi(\omega)$. With lowering $T$, the peak becomes sharper and shifts toward lower energies. At much lower temperatures close to the transition temperature $T_c \sim 0.3$, the peak gets strongly enhanced and diverges at $T = T_c$. This behavior clearly demonstrates the evolution of the excitonic correlations with lowering $T$.

4. Summary
In this paper, we have described the exciton Mott transition and pair condensation transition and calculated the optical response function in the spinless e-h Hubbard model, using the unified theoretical framework, DMFT + NCA. By calculation of DOS, we have shown that the system crossovers from metal to insulator with increasing the e-h attraction. We have estimated the transition temperature for the e-h pair condensation by investigating divergence of the pair susceptibility. We also calculate the optical response function, and show that the excitonic peak gets strongly enhanced around the pair condensation transition.

The transition temperature obtained by our DMFT + NCA approach is too high. Therefore, we should employ a numerically exact impurity solver, such as the quantum Monte Carlo method, to obtain the quantitatively good results. This is our future work.

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