Quantum decoherence in strongly correlated electron system

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Abstract

Physical phenomena in the vicinity of metal-to-insulator transition are analyzed by considering decoherence process between the localized state, $|L>$ and the itinerant state, $|I>$ in strongly correlated electron system. Collective modes such as spin density wave suppress the disappearance of the off-diagonal components of the density matrix, and thus for compensating this effect superconducting pairing can take place. Both competing behaviors are generated within the uncertainty principle, which invokes the metastable states as like pseudogap phase and electronic inhomogenity.

Electrodynamics of strongly correlated electron system has been known to be very complicate,[1,2] and especially, in cuprates exotic behaviors such as pseudogap state and sperconductivity appear with doping concentration. Understanding of these properties is still evolving, but satisfactory explanation did not exist yet because it has difficulty in finding the consistent method to describe the duality of charge dynamics simultaneously. The dual behaviors of localization and itinerancy of charge particles in the correlated system are general feature. Nevertheless, recent theoretical approaches[3–5] to study this phenomenon have mainly considered one side of the duality where the other is supplementary only, which is a fundamental limitation of its analysis.

Previously, we reported on the basic concept of consistent description of dual effects on charge dynamics simultaneously.[6] Based on the formalism of one-particle Green function,[7] each component of Hamiltonian for localization and itinerancy is extracted from simply using the renormalization constant, Z. The physical phenomena generated by two components are not independent each other and connected through this factor. In this study, we note its role of the quantum decoherence in abnormal behaviors in the proximity of metal-to-insulator transition. As the correlated metal approaches the insulator, decoherence process between localized and itinerant states undergoes, where the collective modes and superconducting pairing can play a complementary role in decoherence process.

Spectral representation of electrodynamics of charge carriers clearly shows two parts of spectral density consisting of quasiparticle and localized peaks.[8] The former peak represents the renormalized spectral weight of the quasiparticle in the Landau Fermi liquid and the latter indicates the Hubbard bands extracted from the Hubbard Hamiltonian including onsite Coulomb repulsion in lattices. The model calculation also exhibits that the spectral density of single-particle Green function is divided into two parts.[3] Generally, two peaks of the spectral density are apparently discriminated as the correlated metal goes close to the fully localized state, named as the Mott insulator.

Figure 1 shows the schematic diagram of spectral density divided into itinerant state, $|I>$ and localized state, $|L>$. As above mentioned, the splitting of the spectral density is typical phenomenon appearing at the strong correlation. Even though two states can be the integral quasi-states induced by the interaction among charge particles, it must become the preferred states well describing the itinerant and localized behaviors of electrodynamics. Therefore, the wave function of charge particle is simply written as the superposition of both states as like two-level system.

$$|\Psi\rangle = \alpha|I\rangle + \beta|L\rangle \tag{1}$$

where α and β can be expressed by using the renormalization constant, Z. Previously, based on the single-particle formalism we simply extracted that the coherent part of the Green function is weighted by the renormalization factor Z, and the incoherent part by the factor $1 - Z$, because both parts of the spectral density $A(k,\omega)$ are related to the expression as follows, the coherent part, $\int A_{ch}(k,\omega)d\omega = Z$ and the incoherent background, $\int A_{inch}(k,\omega)d\omega = 1 - Z$. From this, the complex numbers α and β are represented as $Z^{1/2}$ and $(1-Z)^{1/2}$ except for the phase factor, respectively and satisfied with normalization condition, $|\alpha|^2 + |\beta|^2 = 1$. The Hilbert space of this system is spanned by the orthonormal states $|I\rangle$ and $|L\rangle$.

We find that two-level system evolves into the possible states at ultimate region of the correlation strength, that is, the Mott insulator or the Landau Fermi liquid state. Prior to arrival at the ultimate states, the intermediate phase consisting of the superposition of two states can be effectively formed by its interaction with environment. This process resembles quantum decoherence and einselection that describe the mechanism by which quantum system interacts with the environment to exhibit the possible outcomes.[9] Decoherence indicates the destruction of the coherence of the possible states, which is generally represented by the disappearance of the off-diagonal element of the density matrix. The density operator is a useful tool for describing the probability distribution over the possible outcomes. The most general density operator, ρ is of the form representing a statistical mixture of pure states.

$$\rho = \sum_i p_i |\Psi_i\rangle\langle\Psi_i| \tag{2}$$

where the coefficient p_i is the proportion of the ensemble being in the state $|\psi_i\rangle$. Considering the pure state $|\Psi\rangle$ in eq. (1), the reduced density matrix can be simply expressed as below,

$$\rho = \alpha\alpha^*|I\rangle\langle I| + \alpha\beta^*|I\rangle\langle L| + \beta\alpha^*|L\rangle\langle I| + \beta\beta^*|L\rangle\langle L| \tag{3}$$

The off-diagonal elements are related to their interference effects of possible states. It indicates that the coherence of two states subsists. The simple matrix form of the density operator is given by,

$$\begin{pmatrix} \alpha\alpha^* & \alpha\beta^* \\ \beta\alpha^* & \beta\beta^* \end{pmatrix} \tag{4}$$

The matrix elements $\alpha\beta^*$ and $\beta\alpha^*$ have the relative phase factor, $e^{i\theta}$. In the many-particle system, the density operator can be obtained from the ensemble average, $\overline{\rho_{ij}}$ where the subscript are α and β. The interaction of particles makes the off-diagonal elements to have a random phase. The average cancels out these terms and thus, the density matrix becomes diagonalized to vanish the interference effects. The system will be in the state $|I\rangle\langle I|$ with probability $|\alpha|^2$ and in the state $|L\rangle\langle L|$ with probability $|\beta|^2$.

$$\rho = |\alpha|^2|I\rangle\langle I| + |\beta|^2|L\rangle\langle L| \tag{5}$$

Decoherence is a natural process of the loss of information from a system into the environment. The system tends to progress in the direction of increasing entropy. The quantum state of the system is apparently forced into one of the diagonal eigenstates with a probability, the collapse of the wave function. Doping concentration or the variation of the lattice constant controlling the correlation strength may play a role of its environment in strongly correlated system. This can lead to the emergence of observables finally, named as einselection.

On the whole, decoherence process evolves at fast timescale. But, the symmetry breaking or other degrees of freedom can impede the decoherence process. In cuprates, collective modes such as spin wave are known to form in the intermediate phase prior to arrival at the fully localized state, Mott insulator. These collective modes will have a finite-range ordering, which is experimentally observed in the same way. The two-dimensional behaviors of charge carrier arising from the layered structure should be most possible origin in this property.

We note that the collective modes limit the decoherence process because they have the coherent feature of the charge carriers, which makes it difficult to randomize the phase. It is very interesting that for compensating the disturbance of vanishing the off-diagonal element of the density matrix, the superconducting pairing can form with equal and opposite momentum of k and $-k$. In this case, the charge pairing is resulted from only the statistical possibility, not needed for some mediator as like phonon. Namely, the origin of charge pairing is related to the fact that the system tends toward achieving a state with a maximum of entropy. The parameter of forming the charge pairing becomes a kind of the entropy force.

$$S = -\mathrm{Tr}\rho \log \rho \tag{6}$$

In microscopic analysis, the collective modes and superconductivity are described by means of the electron-hole and electron-electron pairs in the conventional Hamiltonian with kinetic energy ε_k and interacting energy V_q.

$$H = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_{k,k',q} V_q c_{k+q}^\dagger c_{k'-q}^\dagger c_{k'} c_k \tag{7}$$

where $c_k^\dagger$ and c_k are creation and annihilation operators, respectively. Within the framework of the broken-symmetry Hartree-Fock approach, the mean-field Hamiltonian including the spin-density wave ordering and the singlet superconductivity is given by

$$H_M = \sum_k \varepsilon_{a,k} a_k^\dagger a_k + \sum_k \varepsilon_{b,k} b_k^\dagger b_k + \Delta_{DW} \sum_{k,\gamma} b_{k+Q,\gamma}^\dagger \sigma b_{k,\gamma} + \Delta_{SC} \sum_k a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger \tag{8}$$

The gap parameter for the singlet pairing Δ_{SC} is represented as $\sum_q V_{kq} \langle a_{k\uparrow} a_{-k\downarrow} \rangle$. The superconductivity comes from the itinerant state, while the density wave with gap parameter Δ_{DW} comes from the localized state. This is different from previous studies by various researchers where the Hamiltonian corresponding to the density wave and superconductivity are coupled by the common operators. The result shows that two physical phenomena compete in general. But, above description shows that both parts does not rely on together because they have independent eigenstates in time. Therefore, both physical phenomena can be analyzed separately. From the analysis of the expectation value, the quasiparticle pairing and collective mode are linked by the renormalization factor Z. The superconducting gap equation is expressed as below,[10]

$$\Delta_{SC} = 2\hbar\omega_C \exp(-\frac{1}{NV}) \tag{9}$$

where N is the density of states at the Fermi surface and $\hbar\omega_C$ is the cutoff energy of the interacting parameter. The cutoff energy and the interaction energy relate to the entropy change expressed at the density matrix formalism in some way. From this, we simply extract that the critical temperature T_c of the superconductivity has the proportional factors, Z and $(1-Z)$. Assuming that the factor Z increases with the doping carrier, the T_c variation is similar to the experimental results.[2] We find that the variation of the kinetic energy rather than potential energy strongly effects on the superconducting state because of the superconducting pairing dependent on the renormalization constant. This is in agreement with the analysis of the spectral weight transfer by using the optical spectroscopy.[11]

The respective phenomena generated from two states are affected by the uncertainty principle. It is reasonable that the uncertainty principle in the two-level system is extracted by using the Green function formalism. The single-particle Green function is represented as $G(xt, x't') = -i\langle\Psi_o|T[\hat{\psi}(xt)\hat{\psi}^\dagger(x't')]|\Psi_o\rangle$, where the $\hat{\psi}$ and $\hat{\psi}^\dagger$ are the annihilation (creation) field operators.[7] The expectation value of an operator $\widehat{Q}$ is formally represented as below,

$$\langle\widehat{Q}\rangle = -i \lim_{t\to t'^+} \lim_{x\to x'} \langle\widehat{Q}G(xt, x't')\rangle \tag{10}$$

By using the wave function in Eq. (1), the expectation value has the sum of two components of $\langle\widehat{Q}\rangle_I$ in the itinerant state $|I>$ and $\langle\widehat{Q}\rangle_L$ in the localized state $|L>$.

$$\langle\widehat{Q}\rangle = \langle\widehat{Q}\rangle_I + \langle\widehat{Q}\rangle_L \tag{11}$$

From this, the product, $\langle\Delta Q\rangle\langle\Delta P\rangle$ of the uncertainties of conjugate variables, ΔQ and ΔP has three parts. Two parts are related to the quantities for the itinerant and localized state, respectively. The rest is the product of the respective variable in each state and in this case, the uncertainty principle for position and momentum is given by,

$$\langle \Delta x \rangle_I \langle \Delta p \rangle_L \geq Z(1-Z)\frac{\hbar}{2} \tag{12}$$

where the factors Z or $1-Z$ are calculated from the expectation value by using the Green function formalism because as previously described, the Green functions of itinerant and localized states are expressed as having renormalization factors, Z or $1-Z$. At the ultimate region, that is, in case Z is zero or one, this type of the uncertainty relation disappears. Above uncertainty relation indicates that the physical phenomena generated by two possible states are not independent together. This invokes the system to have electronic inhomogenity, where the collective modes and superconducting pairing are generated within the extent of the uncertainty relation and coexist in space. Therefore, the electronic inhomogenity is an intrinsic property appeared by the basic quantum effects in the many-body system with strong correlation.

We find that ultimately, the tendency of the system to achieving the maximum entropy rather than other features such as the inhomogeneous charge distribution with the minimum energy causes the complexity of the system . Here, we can estimate the extent of the spatial distribution, δx of each physical phenomenon.

$$\delta x \simeq \frac{\hbar p_F}{m\Delta} \tag{13}$$

where the p_F and m are the Fermi wave vector and mass of the carrier. Considering the observed energy scale of about several decades meV of the density wave, the spatial scale of them extends over several decades Å.

In conclusion, the intermediate state of strongly correlated electron system can be understood by decoherence process. We find that decoherence process plays a key role in analyzing pseudogap phase and superconductivity.

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FIGURES

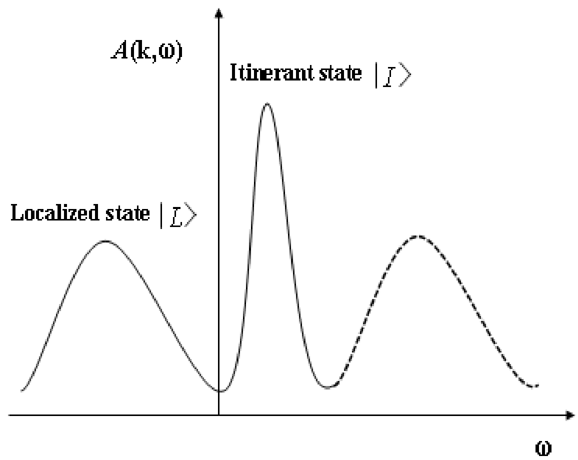

FIG. 1. The schematic diagram of spectral density separated into itinerant state, $|I>$ and localized state, $|L>$