

Scaling behavior in the optical conductivity of two-dimensional systems of strongly correlated electrons based on the U(1) slave-boson approach to the t - J Hamiltonian

Jae-Hyeon Eom¹ and Sung-Ho Suck Salk²

¹*Department of Physics, Probang University of Science and Technology, Probang, Youngest 790-784, Korea*

²*Korea Institute of Advanced Studies, Seoul 130-012, Korea*

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The U(1) holon-pair boson theory of Lee and Salk [Phys. Rev. B **64**, 052501 (2001)] is applied to investigate the quantum scaling behavior of optical conductivity in the two-dimensional systems of strongly correlated electrons. We examine the role of both the gauge field fluctuations and spin pair excitations on the ω/T scaling behavior of the optical conductivity. It is shown that the gauge field fluctuations but not the spin pair excitations are responsible for the scaling behavior in the low-frequency region $\omega/T \ll 1$. The importance for the contribution of the nodal spinons to the Drude peak is discussed. It is shown that the ω/T scaling behavior is manifest in the low-frequency region at low hole concentrations close to a critical concentration at which superconductivity arises at $T=0$ K.

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I. INTRODUCTION

The quantum phase transition (QPT) is a zero-temperature ($T=0$) phase transition induced by quantum fluctuations which can be controlled by “external” parameters such as magnetic field, pressure, phase stiffness, doping, etc. These external parameters correspond to some coupling constant g in the Hamiltonian and the QPT occurs as a result of the change of the ground state at a critical value g_c . The QPT is a subject of great interest, particularly in the area of strongly correlated electron systems involving superconductor-insulator transitions, metal-insulator transitions, integer and fractional quantum Hall transitions, and magnetic transitions.¹ Various studies concerned with the QPT in the high- T_C cuprates have been made concerning with electron fractionalization,^{2–6} magnetic properties,^{7–11} transport properties,^{12–14} time-reversal symmetry breaking,^{15–18} and phenomenological quantum critical point (QCP) near the optimal doping concentration.^{19–22} One of the most interesting studies in the QPT is to see if there exists a universal ω/T scaling behavior of response functions in the quantum critical region of $|g-g_c|/T \ll 1$.^{1,23} In the quantum critical region the energy gap Δ satisfies $\Delta \sim T$ and the response function shows the ω/T scaling behavior—for example, $\sigma(\omega, T, g) \sim T^{d-2} \Sigma(\omega/T, \Delta/T) \sim T^{d-2} \Sigma(\omega/T)$ in optical conductivity, σ at frequency ω .^{1,12} In the high- T_C cuprates, the external parameter can be the hole doping concentration x . The high- T_C cuprates show diversified phases of antiferromagnetism, pseudogap, and superconductivity. Hole doping to the parent compound of the antiferromagnetic (AF) Mott insulator induces frustration of the AF order and as a result the pseudogap (PG) phase occurs. Further hole doping results in the superconductivity (SC), and the superconducting transition temperature T_C increases to a maximum at an optimal concentration, beyond which T_C decreases until SC disappears, thus showing an arch shape of the superconducting transition temperature over a limited range of doping. In the present work we investigate the ω/T scaling behavior of the in-plane optical conductivity at very low frequency by apply-

ing the U(1) slave-boson theory of Lee and Salk^{24–26} which has been successful in reproducing various observations, including the arch-shaped superconducting transition temperature in the phase diagram of high- T_C cuprates. This theory is different from other previous slave-boson theories^{27–30} in that coupling between the charge and spin degrees of freedom is manifested in the expression of the Heisenberg interaction term in the slave-boson representation.^{24–26} Both the U(1) and SU(2) theories of Lee and Salk²⁴ showed that the hump structure in the optical conductivity originates from antiferromagnetic spin fluctuations of short range, including the spin-singlet pair excitations.^{25,26} In the present work we show that the optical conductivity at low frequency reveals a ω/T scaling behavior with a bell shape by satisfying the back flow condition under the enforcement of gauge field fluctuations. In addition, we discuss that the nodal quasiparticle excitations in the cold spot of the Brillouin zone at low hole doping concentrations and low temperatures sufficiently below the pseudogap (spin gap) temperature are responsible for the quantum phase transition.

II. THEORY

A. Derivation of the optical conductivity in the U(1) slave-boson theory

To point out differences with other proposed slave-boson theories we briefly present only the rudimentary part of the U(1) slave-boson theory proposed by Lee and Salk²⁴ and the derivation of the optical conductivity in the U(1) slave-boson theory.^{25,26} The t - J Hamiltonian in the presence of the external electromagnetic field \mathbf{A} is written

$$H = -t \sum_{\langle i,j \rangle, \sigma} (e^{iA_{ij}} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \text{H.c.}) + J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) - \mu \sum_{i, \sigma} c_{i\sigma}^\dagger c_{i\sigma}, \quad (1)$$

with $\mathbf{S}_i = \frac{1}{2} \sum_{\alpha\beta} c_{i\alpha}^\dagger \sigma_{\alpha\beta} c_{i\beta}$. Here A_{ij} is the external electromag-

netic field, $\tilde{c}_{i\sigma}$ ($\tilde{c}_{i\sigma}^\dagger$) the electron annihilation (creation) operator at each site, $\sigma_{\alpha\beta}$ the Pauli spin matrix, and μ the chemical potential. It is noted that the t - J Hamiltonian is the effective Hamiltonian in the large- U (on-site Coulomb repulsion energy) limit of the Hubbard model. Thus the electron cannot hop to another singly occupied site. Rewriting the electron operator as a composite of spinon (f) and holon (b) operators,

$$c_{i\sigma} = f_{i\sigma} b_i^\dagger, \quad (2)$$

the partition function is written as

$$Z = \int \mathcal{D}f \mathcal{D}b \mathcal{D}\lambda \exp\left(-\int_0^\beta d\tau \mathcal{L}\right), \quad (3)$$

where $\mathcal{L} = \sum_i (\sum_{\sigma} f_{i\sigma}^* \partial_\tau f_{i\sigma} + b_i^* \partial_\tau b_i) + H_{t-J}$ is the Lagrangian with H_{t-J} , the U(1) slave-boson representation of the above t - J Hamiltonian [Eq. (1)],

$$\begin{aligned} H_{t-J} = & -t \sum_{\langle i,j \rangle, \sigma} (e^{iA_{ij}} f_{i\sigma}^\dagger f_{j\sigma} b_j^\dagger b_i + \text{c.c.}) \\ & - \frac{J}{2} \sum_{\langle i,j \rangle} b_i b_j b_j^\dagger b_i^\dagger (f_{i\uparrow}^\dagger f_{j\uparrow}^\dagger - f_{i\downarrow}^\dagger f_{j\downarrow}^\dagger) (f_{j\uparrow} f_{i\downarrow} - f_{j\downarrow} f_{i\uparrow}) \\ & - \mu \sum_{i,\sigma} f_{i\sigma}^\dagger f_{i\sigma} + i \sum_i \lambda_i \left(\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i - 1 \right). \end{aligned} \quad (4)$$

Here λ_i is the Lagrange multiplier field which enforces the single-occupancy constraint.

Applying the Hubbard-Stratonovich transformations involving hopping, spinon pairing, and holon pairing orders we obtain the partition function

$$Z = \int \mathcal{D}f \mathcal{D}b \mathcal{D}\chi \mathcal{D}\Delta^f \mathcal{D}\Delta^b \mathcal{D}\lambda \exp\left(-\int_0^\beta d\tau \mathcal{L}_{eff}\right), \quad (5)$$

where $\mathcal{L}_{eff} = \mathcal{L}_0 + \mathcal{L}_f + \mathcal{L}_b$ is the effective Lagrangian with

$$\begin{aligned} \mathcal{L}_0 = & \frac{J(1-x)^2}{2} \sum_{\langle i,j \rangle} \left\{ |\Delta_{ij}^f|^2 + \frac{1}{2} |\chi_{ij}|^2 + \frac{1}{4} \right\} \\ & + \frac{J}{2} \sum_{\langle i,j \rangle} |\Delta_{ij}^f|^2 (|\Delta_{ij}^b|^2 + x^2) \end{aligned} \quad (6)$$

for the Lagrangian involved only with order parameters,

$$\begin{aligned} \mathcal{L}_f = & \sum_{i,\sigma} f_{i\sigma}^\dagger (\partial_\tau - \mu^f) f_{i\sigma} - \frac{J(1-x)^2}{4} \sum_{\langle i,j \rangle, \sigma} \{ \chi_{ij}^* f_{i\sigma}^\dagger f_{j\sigma} + \text{c.c.} \} \\ & - \frac{J(1-x)^2}{2} \sum_{\langle i,j \rangle} \{ \Delta_{ij}^{f*} (f_{i\uparrow} f_{j\uparrow} - f_{i\downarrow} f_{j\downarrow}) + \text{c.c.} \} \end{aligned} \quad (7)$$

for the spinon sector, and

$$\begin{aligned} \mathcal{L}_b = & \sum_i b_i^\dagger (\partial_\tau - \mu^b) b_i - t \sum_{\langle i,j \rangle} \{ \chi_{ij}^* b_i^\dagger b_j + \text{c.c.} \} \\ & - \frac{J}{2} \sum_{\langle i,j \rangle} |\Delta_{ij}^f|^2 \{ \Delta_{ij}^{b*} b_i b_j + \text{c.c.} \} \end{aligned} \quad (8)$$

for the holon sector. Here χ , Δ^f and Δ^b are the hopping, spinon pairing, and holon pairing order parameters, respec-

tively. μ^f (μ^b) is the spinon (holon) chemical potential and x the hole concentration.

We compute the optical conductivity $\sigma(\omega)$ directly from the current response function $\Pi(\omega)$,

$$\sigma(\omega) = \left. \frac{\partial J_x(\omega)}{\partial E_x(\omega)} \right|_{E_x=0} = -\frac{1}{i\omega} \left. \frac{\partial^2 F}{\partial A_x^2} \right|_{A_x=0} = \frac{\Pi_{xx}(\omega)}{i\omega}, \quad (9)$$

where J_x is the induced current in the x direction, $E_x(\omega)$ the external electric field with frequency ω , $F = -k_B T \ln Z$ the free energy, and $A_x(\omega)$ the external electromagnetic field. Here the isotropic current is taken into account. In the slave-boson theory the current response function $\Pi(\omega)$ is given solely by the holon current response function because the spinon has no electric charge. The hopping order parameter $\chi_{ij} = |\chi_{ij}| e^{iA_{ij}}$ defines the pure gauge field $a_{ij} = \partial_{ij} \theta = \theta_i - \theta_j$. The inclusion of the gauge field fluctuations guarantees the important backflow condition for the spinon and holon currents $J^f + J^b = 0$. Allowing only the kinetic energy term of the t - J Hamiltonian, the Ioffe-Larkin composition rule for the electron current response function³¹ was obtained to be

$$\Pi = \frac{\Pi^f \Pi^b}{\Pi^f + \Pi^b}, \quad (10)$$

where Π^f and Π^b are the spinon and holon current response functions, respectively.

The Heisenberg exchange interaction in the t - J Hamiltonian introduces the antiferromagnetic spin fluctuations. Thus to incorporate the influence of the spin fluctuations into the current response function we allow the amplitude fluctuations of the spinon-singlet pairing order parameter $|\Delta^f|$. Further the spin (spinon) degree of freedom is coupled with the charge (holon) degree of freedom as shown in Eqs. (6) and (8) above. Such coupling is manifested via the coupling of spin pairing field Δ^f to the holon pairing field Δ^b in the expression below. In passing we would like to stress that such coupling allows the composite of the holon pair field and the spinon pair field to be the Cooper pair field. With the inclusion of the two order parameter fields^{25,26} we find that the total current response function is given by

$$\Pi = \frac{\Pi^f \Pi^b}{\Pi^f + \Pi^b} + \frac{\left(\Pi_{a\Delta}^b - \frac{\Pi_{a\Delta}^b + \Pi_{a\Delta}^f \Pi^b}{\Pi^b + \Pi^f} \right)^2}{2 \frac{(\Pi_{a\Delta}^b + \Pi_{a\Delta}^f)^2}{\Pi^b + \Pi^f} - (\Pi_{\Delta\Delta}^0 + \Pi_{\Delta\Delta}^b + \Pi_{\Delta\Delta}^f)}, \quad (11)$$

where $\Pi_{a\Delta}^f = -\partial^2 F^f / \partial a \partial |\Delta^f|$ and $\Pi_{a\Delta}^b = -\partial^2 F^b / \partial a \partial |\Delta^f|$ are the spinon (holon) response functions associated with both the gauge fields and the spinon pairing field and $\Pi_{\Delta\Delta}^f$, $\Pi_{\Delta\Delta}^b$, and $\Pi_{\Delta\Delta}^0$ the response functions associated with the spinon pairing field. It is recalled that the first term of Eq. (11) represents the Ioffe-Larkin rule contributed only from the kinetic energy term, satisfying the backflow condition by allowing the gauge field fluctuations and the second term represents from the spin fluctuations. Further the second term contains the effects of coupling between the charge (holon) pair and spin (spinon) pair fields. We note that the first term solely

contributes to the Drude peak and the second term to the hump structure of the optical conductivity.^{25,26}

B. Scaling behavior of the conductivity in two dimensions

The dimensional analysis shows that the conductivity $\sigma(\omega)$ has scaling dimension of $d-2$ and the conductivity has the scaling form,^{1,12}

$$\sigma(\omega, T, g) = \frac{Q^2}{\hbar} \left(\frac{k_B T}{\hbar c} \right)^{d-2} \Sigma \left(\frac{\hbar \omega}{k_B T}, \frac{\Delta}{k_B T} \right), \quad (12)$$

where $\Sigma(\hbar\omega/k_B T, \Delta/k_B T)$ is the scaling function, with $\Delta \sim \xi^{-z}$ the energy gap and Q the charge of the charge carrier. Here ξ is the correlation length and z the dynamics critical exponent. In the critical region of $\Delta \sim k_B T$, the conductivity shows universal scaling behavior

$$\sigma(\omega) = \frac{Q^2}{\hbar} \left(\frac{k_B T}{\hbar c} \right)^{d-2} \Sigma \left(\frac{\hbar \omega}{k_B T} \right). \quad (13)$$

In this work we are concerned with the two-dimensional system of the high- T_C cuprates and the conductivity has no scaling dimension in temperature. Thus we obtain

$$\sigma(\omega) \sim \Sigma \left(\frac{\omega}{T} \right). \quad (14)$$

Numerical calculations of the scaling function by Damle and Sachdev showed a bell-shaped feature in the plot of Σ'_l vs ω/T , where Σ'_l is the real part of the scaling function for low frequency $\omega/T \ll 1$ in two spatial dimensions.¹²

III. COMPUTED RESULTS OF IN-PLANE OPTICAL CONDUCTIVITY

Here we present the predicted ω/T scaling behavior of the conductivity $\sigma(\omega, T)$ with the inclusion of both the gauge field fluctuations and the spin pair excitations based on the U(1) slave-boson theory. In order to see whether the quantum phase transition occurs, we choose a low hole concentration of $x=0.02$ near a critical doping at which the superconducting transition was shown to occur at $T=0$ K.²⁴ The temperature range is chosen between $0.015t$ and $0.045t$, which is sufficiently below $T^*(0.07t)$, based on the predicted phase diagram obtained by Lee and Salk.²⁴ Figure 1 shows the ω/T scaling behavior of the optical conductivity for temperatures between $0.015t$ and $0.045t$. We see that the ω/T scaling behavior becomes markedly clear for $\omega/T \ll 1$ in the region of low temperature as shown in Fig. 1. Encouragingly we obtained a bell shape in the plot of $\sigma(\omega)$ vs ω/T in agreement with the bell shape feature demonstrated by Damle and Sachdev (see Fig. 6 in Ref. 12).

Although not shown here we find that the neglect of the spin-singlet pair excitations (the fluctuations of the spinon-singlet pair order) does not appreciably affect the scaling behavior of the conductivity. Such excitations affect largely the hump structure in the optical conductivity. This indicates that the spin fluctuations contribute only to higher-energy (-frequency) charge dynamics involved with a midinfrared band in the high- T_C cuprates. For further analysis of the scal-

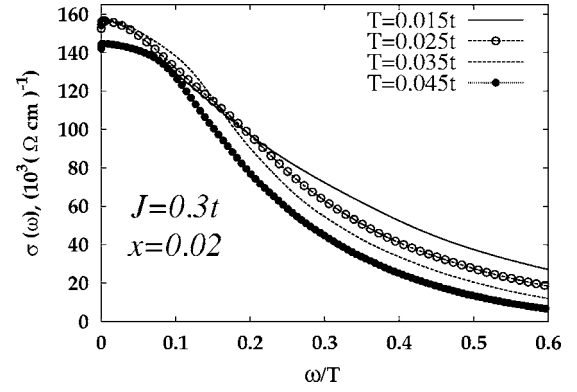


FIG. 1. ω/T scaling behavior of the optical conductivity with the inclusion of both the gauge field fluctuations and the spin pair excitations based on the U(1) slave-boson theory at $x=0.02$.

ing behavior of the optical conductivity in Fig. 2 we show the predicted result of $\sigma(\omega)$ vs ω/T with the exclusion of gauge field fluctuations—that is, the conductivity contributed only from the bare kinetic energy term of the holons. A universal scaling behavior with a bell shape is no longer predicted as shown in Fig. 2. Comparison of Figs. 1 and 2 shows that the scaling behavior originates from the kinetic energy term by satisfying the backflow condition guaranteed by the gauge fluctuations.^{31,32} As shown in Fig. 2 deviation from scaling behavior becomes increasingly larger as ω/T decreases to 0. We note that the nodal quasiparticle excitations for the Drude peak in the cold spot of the Brillouin zone are important for the ω/T scaling behavior of a bell shape, as shown in Fig. 1.

The gauge (pure gauge) invariance disappears in our mean-field treatment. In the present study the phase (gauge) fluctuations of the spin (spinon) pairing order parameters are taken into account. The coherence of the spinon pairing Higgs field leads to the acquirement of mass for the gauge field as a consequence of the Anderson-Higgs mechanism. Earlier Onoda and co-workers pointed out that a downward deviation from linearity in temperature³³ in the limit of $\omega \rightarrow 0$ is attributed to the acquirement of mass by the gauge

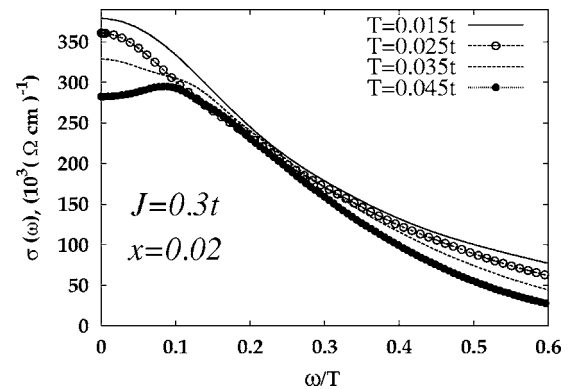


FIG. 2. Deviation from the ω/T scaling behavior of the optical conductivity in the low-frequency region with the exclusion of gauge field fluctuations.

field.³⁴ In the future it will be of great interest to make quantitative and qualitative comparisons with such a study on equal footing by direct calculations of resistivity in the limiting case of $\omega \rightarrow 0$.

Finally we would like to point out the essence of the present study. Unlike other theories, in our slave-boson theory the coupling of the spinon pair field with the holon pair field is taken care of in the treatment of the Heisenberg term of the t - J Hamiltonian. The backflow condition for the spin and charge currents is maintained—that is, $J^f + J^b = 0$ with J^f the spinon current and J^b the holon current. As mentioned above, our theory predicts the peak- (Drude-peak) dip-hump (midinfraband) structure in agreement with the observation of optical conductivity. The hump structure is attributed to the antiferromagnetic spin fluctuations of short range, which originate from the hot spot of the Brillouin zone. From the present study of the optical conductivity in the low-frequency region of ω we find that the Drude peak originates from the nodal point (the cold spot). Therefore we find that only the nodal quasiparticle excitations in the cold spot contribute to the scaling behavior of the conductivity and play a dominant role in the quantum phase transition. As shown in Fig. 1, the ω/T scaling behavior survives at a low hole doping concentration sufficiently below the pseudogap temperature T^* .

IV. SUMMARY

In the present study, we investigated the scaling behavior in the conductivity of the two-dimensional systems of strongly correlated electrons based on the holon-pair boson theory of Lee and Salk.²⁴ The scaling behavior with the bell-shaped structure of optical conductivity in the very-low-frequency region of $\omega \rightarrow 0$ is predicted near a critical doping concentration in the underdoped region at temperatures sufficiently below T^* . By observing the disappearance of the scaling behavior in the low-frequency region with the exclusion of the gauge field fluctuations, we find that the nodal quasiparticle excitations in the cold spot of the Brillouin zone contribute to the ω/T scaling behavior in the conductivity by satisfying the backflow condition and that the spin fluctuations from the hot spot quasiparticles are not responsible for both the bell-shaped optical conductivity and the scaling behavior in the low-frequency region.

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