Edge-induced strongly correlated electronic states in two-dimensional Hubbard model: Enhancement of magnetic correlations and self-energy effects

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To understand nontrivial edge electronic states in strongly-correlated metals such as cuprate superconductors, we study the two-dimensional Hubbard models with open edge boundary. The position-dependences of the spin susceptibility and the self-energy are carefully analyzed self-consistently, by using the fluctuation-exchange (FLEX) approximation. It is found that spin susceptibilities are strongly enlarged near the (1,1) open edge when the system is near the half-filling. The enhancement is large even if the negative feedback from the self-energy is considered in the FLEX approximation.

The present study predicts the emergence of nontrivial spin-fluctuation-driven phenomena near the edge, like the quantum criticality, edge superconductivity, and the bond-density-wave order.

Keywords: high-$T_c$ superconductors, cluster Hubbard model, edge electronic states, fluctuation-exchange approximation

In strongly correlated electron systems, many-body electronic states are drastically modified by introducing real-space structures, such as the defects and domain boundaries. To predict exotic electronic properties created by introducing the defects in real space, it is important to develop theoretical methods of analyzing the strongly correlated metals without translational symmetry. In cuprate high-$T_c$ superconductors, for example, single nonmagnetic impurity on Cu-site induces the local moment with $\sim \mu_B$ in both YBa$_2$Cu$_3$O$_{7-x}$ (YBCO) [1] and La$_{2−x}$Sr$_x$CuO$_4$ (LSCO) [2]. It was revealed by the NMR study [3–5] that both the local and the staggered spin susceptibilities are strongly enhanced around the impurity site. In addition, dilute nonmagnetic impurities cause huge residual resistivity beyond the s-wave unitary scattering limit in cuprate superconductors [6] and heavy-fermion systems [7, 8]. Thus, the system approaches to the magnetic quantum-critical point (QCP) by introducing dilute point defects. [9].

In systems near the magnetic QCP without randomness, various interesting non-Fermi liquid phenomena are driven by spin fluctuations, such as the $T$-linear resistance above the pseudo-gap temperature $T^*$ in cuprates [10–12]. It was recently revealed that spin fluctuations drive nontrivial “nematic transitions”, such as the rotational symmetry breaking at $T = T^*$ [13] and the axial charge-density-wave (CDW) formation at $T_{\text{CDW}}(< T^*)$ [14–19], which attract increasing attention recently. The idea of the “spin-fluctuation-driven CDW” due to higher-order many-body effects (such as the vertex corrections) has been studied in various theoretical models. [20–29]. For cuprates, various bond CDW order states, which are the nematic transitions given by the symmetry-breaking in the self-energy, have been proposed in Refs. [22, 30, 31]. The “effective hopping integrals due to self-energy” have in-plane anisotropy in the bond CDW state. Since spin fluctuations drive various fundamental phenomena, it is significant to understand how the spin fluctuations are modified by the real-space structures. However, theoretical studies performed so far has been limited.

Effects of point defects in cuprates have been studied by many theorists [32–38]. In the random-phase-approximation (RPA), the antiferromagnetic (AFM) spin fluctuations are enlarged around the impurity site in the square-lattice Hubbard model, when the impurity potential is nonlocal [36–38]. The impurity-induced enhancement of AFM fluctuations is obtained in the strongly correlated region even if the impurity potential is local, by calculating the site-dependent self-energy based on the GV$^I$ method [9]. These results indicate that the AFM fluctuations strongly develop near the open edge of the cluster Hubbard model, since the edge potential is given by the impurity sites in a straight line. However, detailed theoretical analysis of the “open edge Hubbard model” based on the spin fluctuation theories has not been performed yet. (Note that the effect of the nonmagnetic impurities and open edges in graphene have been discussed in Refs. [39, 40].)

In the present paper, we study the site-dependent spin susceptibility and self-energy in the open edge Hubbard model, by using the RPA and the fluctuation-exchange (FLEX) approximation [41]. In both approximations, the AFM fluctuations are found to be strongly enlarged near the open edge, especially in the (1,1) open edge model. For this reason, both the mass-enhancement $(Z = m^*/m = 1 − \partial \Sigma(ε)/\partial ε|_{ε=0})$ and the quasiparticle damping $(\gamma^* = \text{Im} \Sigma(-iδ)/Z)$ given by the spin-fluctuation-induced self-energy takes large value near the open edge. These results indicate the emergence of exotic edge electronic states in strongly-correlated metals, like the quantum-critical phenomena, enhancement of superconductivity, and spin-fluctuation-driven CDW order.

In this paper, we study the square-lattice cluster Hubbard model

\[
H = \sum_{i,j,σ} t_{ij} c_{iσ}^\dagger c_{jσ} + U \sum_i n_{i↑} n_{i↓},
\]

(1)
The spin (charge) susceptibility is given as
\[ \chi^s(q_y, \omega_l) = \sum_{q_y, l} G_{x,x'}(q_y, k_y, \omega_l + \epsilon_n) \times G_{x',x}(k_y, \epsilon_n), \]
where \( k_y = 2lT \) and \( \epsilon_n = (2n - 1)\pi T \) are the boson and fermion Matsubara frequencies. In RPA, the self-energy \( \Sigma(k_y, \epsilon_n) = \left( (\epsilon_n + \mu - H_0 - \hat{\Sigma}(k_y, \epsilon_n))^{-1} \right) \) is the local Green function. The spin (charge) susceptibility is given as
\[ \chi^s(q_y, \omega_l) = \chi^0(q_y, \omega_l) \left( -i \omega_l \right), \]
where \( \chi^0(q_y, \omega_l) = \sum_{q_y, l} G_{x,x'}(q_y, k_y, \omega_l + \epsilon_n) \times G_{x',x}(k_y, \epsilon_n), \) and \( U \) is the onsite Coulomb interaction. In the RPA and FLEX approximations, the self-energies \( \Sigma(q, \omega_l) \) and \( \Sigma(q, \omega_l) \) are given by
\[ \Sigma(q, \omega_l) = \sum_{q_y, l} G_{x,x'}(q_y, k_y, \omega_l + \epsilon_n) \times G_{x',x}(k_y, \epsilon_n). \]

In the FLEX approximation, the self-energy is
\[ \Sigma(q, \omega_l) = \sum_{q_y, l} G_{x,x'}(q_y, k_y, \omega_l + \epsilon_n) \times G_{x',x}(k_y, \epsilon_n), \]
where \( V(q_y, \omega_l) = U^2 \chi^s(q_y, \omega_l) + \frac{1}{2} \chi^c(q_y, \omega_l) - \chi^0(q_y, \omega_l) \). In the FLEX approximation, we solve Eqs. (2)-(4) self-consistently.

Hereafter, we perform the RPA and FLEX analyses for the cluster Hubbard models. The (1,0) edge cluster model is shown in Fig. 1 (b). For the (1,1) edge model, we analyze the one-site unit cell structure shown in the right-hand-side of Fig. 1 (c). In both models, we set the size of the \( x \)-direction as \( N_x = 64 \), and assume the translational symmetry along \( y \)-direction. The number of \( k_y \)-meshes is \( N_y = 64 \), and the number of Matsubara frequencies is 1024 (Figs. 2-4) or 2048 (Fig. 5). We set the electron filling \( n = 0.95 \), and the temperature \( T = 0.02 \). Here, the unit of the energy is \( |t| \), which corresponds to ~0.4eV in cuprate superconductors without renormalization.

First, we study \( \chi^s(q_y) \) at \( \omega_l = 0 \) using the RPA. Figures 2 (a) and (b) show the static RPA susceptibilities \( \chi^s_{x,x}(q_y) \) for the LSCO TB model at \( U = 1.39 \). The Stoner factor is \( \alpha_S = 0.804 \) and \( \alpha_S = 0.900 \) for (a) (1,0) edge model and (b) (1,1) edge model, respectively. Since \( \alpha_S = 0.781 \) in the absence of edges, the system approaches to the magnetic QCP by introducing the edge. In Fig. 2 (a), \( \chi^s_{x,x}(q_y) \) in the (1,0) edge model has the largest peak in the second layer \( x = 2 \), at the wavevector \( q_y = \pi \). Thus, the AFM correlation increases in the second layer. In Fig. 2 (b), \( \chi^s_{x,x}(q_y) \) in the (1,1) edge model has large peak in the first layer \( x = 1 \) at \( q_y = 0 \). This result means that strong ferromagnetic (FM) fluctuations develop at the (1,1) open edge. That is, the original FM correlation between the next-nearest-neighbor sites in the bulk is enlarged at the edge layer.

Figures 2 (c) and (d) show the static \( \chi^s_{x,x}(q_y) \) for the LSCO TB model at \( U = 2.13 \). Here, \( \alpha_S = 0.707 \) in the (c) (1,0) edge model, and \( \alpha_S = 0.900 \) in the (d) (1,1) edge model, respectively. Since \( \alpha_S = 0.639 \) in the absence of edges, the spin fluctuations are strongly enlarged near the edge. The obtained \( (x,q_y) \)-dependence of the spin susceptibility in the YBCO TB model is essentially similar to those in the LSCO TB model. (In Fig. 2 (c), \( \chi^s_{x,x}(q_y) \) has the largest peak in the first edge layer \( x = 1 ) \) To summarize, in the RPA, strong magnetic fluctuations are induced near the open edge, insensitive to the detail of the TB model parameters.

In Figs. 2 (a)-(d), we see that the \( x \)-dependence of \( \chi^s_{x,x}(q_y) \) well corresponds to that of Friedel oscillation of the local density-of-states (LDOS), \( D_x(\epsilon) = \frac{1}{2\pi^2} \int_{-\pi}^{\pi} dk_y \text{Im} G_x^0(k_y, \epsilon - i\delta), \) at \( \epsilon = 0 \). Thus, the edge-induced spin-fluctuation enhancement originates from the large LDOS spot due to the Friedel oscillation [9]. In the Supplemental Material (SM) [42], we verify that \( \chi^s_{x,x}(q_y) \) tends to become large at which \( D_x(\epsilon) \) is large.

Now, we study \( \chi^s(q_y) \) using the FLEX approximation, in order to understand the negative feedback effect due to...
local quasiparticle damping rate at Fermi en-

troducing the (1,1) edge model and (b) (1,0) edge model, respectively. (c)(d) In YBCO TB model: \( \chi_{x,x}^{s}(q_{y}) \) for the (c) (1,0) edge model and (d) (1,1) edge model, respectively.

the site-dependent self-energy. Figures 3 (a) and (b) show the obtained static \( \chi_{x,x}^{s}(q_{y}) \) in the LSCO TB model at \( U = 1.78 \), in the (a) (1,0) edge model and (b) (1,1) edge model. The Stoner factor \( \alpha_{S} \) is 0.900 for both (a) and (b). Note that \( \alpha_{S} = 0.896 \) in the absence of edges. Figures 3 (c) and (d) show the static \( \chi_{x,x}^{s}(q_{y}) \) in the YBCO TB model at \( U = 3.54 \), in the (c) (1,0) edge model \( \alpha_{S} = 0.880 \) and (d) (1,1) edge model \( \alpha_{S} = 0.900 \), respectively. Note that \( \alpha_{S} = 0.836 \) in the absence of edges.

Therefore, the enhancement of the spin susceptibility near the edge given by the RPA is also verified by the FLEX approximation. In the YBCO TB model, by introducing the (1,1) edge, \( \alpha_{S} \) increases from 0.836 (0.641) to 0.900 in the FLEX approximation (RPA). The increment of \( \alpha_{S} \) becomes smaller compared to the RPA, because of the negative feedback between \( \chi^{s} \) and self-energy.

Hereafter, we discuss the site-dependence of the self-energy \( \Sigma(k_{y}, \epsilon - i\delta) \) given by the FLEX approximation. First, we show the numerical results in the LSCO TB model. Figure 4 (a) shows the local mass-enhancement factor \( Z_{x} = 1 - \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_{y} \frac{\partial}{\partial \epsilon} \text{Re} \Sigma_{x,x}(k_{y}, \epsilon - i\delta)|_{\epsilon=0} \) in LSCO at \( U = 1.78 \). In the (1,0) edge model, \( Z_{x} \approx 1.3 \) for any \( x \geq 1 \). In the (1,1) edge model, in contrast, \( Z_{x} \) increases to 1.75 at the edge. Figure 4 (b) shows the local quasiparticle damping rate at Fermi energy, which we defined as \( \gamma_{x}^{*} \equiv \gamma_{x}/Z_{x} \), where \( \gamma_{x} = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_{y} \text{Im} \Sigma_{x,x}(k_{y}, 0 - i\delta) \). In the (1,0) edge model, the site-dependence of \( \gamma_{x}^{*} \) is moderate. In contrast, \( \gamma_{x}^{*} \) at the edge \( (x=1) \) takes large value in the (1,1) edge model, due to the strong spin fluctuations near the edge.

Next, we show the numerical results in the YBCO TB model. Figure 4 (c) shows the obtained \( Z_{x} \) in YBCO at \( U = 3.54 \). In the (1,1) edge model, \( Z_{x} \) increases from 2 in the bulk to 3.2 at the edge. Figure 4 (d) shows the obtained \( \gamma_{x}^{*} \). In both (1,0) and (1,1) edge models \( \gamma_{x}^{*} \) increases near the edge layer. In the (1,1) edge model, \( \gamma_{x}^{*} \) drastically increases to 0.0072 at the edge layer.

Therefore, by introducing the open edge in metals with moderate AFM fluctuations \( (\alpha_{S} \sim 0.9) \), strong AFM or FM fluctuations are induced near the open edge. The in-
duced strong spin fluctuations give rise to huge quasiparticle damping rate and mass-enhancement near the open edge. The present study indicates that various extreme quantum critical phenomena are expected to emerge near the open edge.

Finally, we examine the $T$-dependences of the electronic states in detail based on the FLEX approximation. Figures 5 (a)-(d) show the Stoner factor $\alpha_S$ and the largest local mass-enhancement factor $Z_{\text{max}}$ in the YBCO TB model. In YBCO model, as shown in Figs. 5 (c) and (d), both $\alpha_S$ and $Z_{\text{max}}$ strongly increase as $T$ decreases in the presence of (1, 1) edge. These results mean the emergence of interesting edge-induced quantum critical phenomena.

In the SM [42] we present the numerical results for $n = 0.90 \sim 1.10$, and find that prominent edge-induced quantum criticality appears when the edge LDOS is large. This result is an useful guideline to realize the quantum criticality driven by real space structures. The large damping may be observed experimentally, as the pseudo-gap formation in the LDOS in (1, 1) open edge.

In summary, we studied the site-dependent spin susceptibility and self-energy in the open edge Hubbard model. The magnetic fluctuations are found to be strongly enlarged near the open edge, especially for the (1, 1) edge case. In the FLEX, both the local mass-enhancement factor $Z_x$ and the local quasiparticle damping $\gamma_x$ given by the spin-fluctuation-induced self-energy become huge near the open edge. Thus, interesting edge-induced quantum critical phenomena are predicted by the present study. We note that the impurity-driven enhancements of $\chi^\ast$ and $\gamma^\ast$ are underestimated in the FLEX, since the negative feedback between $\chi^\ast$ and $\Sigma$ is overestimated [9]. To overcome this problem, the GV method will be useful, since this method can successfully explain the impurity-induced magnetic quantum-critical phenomena in cuprate superconductors [9]. This is one of our important future problems. Another important future problem is to study the spin-fluctuation-driven nematicity discussed in Refs. [20, 22, 28, 31]. The present study indicates the emergence of the impurity- or edge-induced nematic orders, which are actually observed in several Fe-based superconductors [43, 44].

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In the main text, we present only the numerical results of the electron filling \( n = 0.95 \), which corresponds to under-doped region of hole-doping compounds. Interesting edge-induced quantum critical phenomena are realized in both LSCO TB and YBCO TB cluster Hubbard models. In this supplemental material (SM), we present the numerical results for \( n = 0.90 \sim 1.10 \) in order to understand the origin of the edge-induced quantum criticality. We find the realization condition of the prominent edge-induced quantum criticality.

**A: filling dependence in LSCO TB model**

First, we explain the numerical results for the LSCO TB model. We set \( T = 0.02 \) and \( U = 1.78 \) in unit eV, for \( n = 0.90, 0.95, 1.05 \) and 1.10. Figure S1 presents the (a) \( \chi_{x,x}^s(q_y) \) and (b) quasiparticle damping \( \gamma_{x,x}^s \), mass-enhancement factor \( Z_x \), and the bare local density of states (LDOS) at the Fermi level \( D_x(0) \). The obtained spin Stoner factors are shown in Fig. S1 (a). The oscillation in \( D_x(0) \) is understood as the Friedel oscillation caused by the open edge.

In the (1, 1) edge model, the edge-induced quantum criticality is prominent in both hole-doped case (\( n < 1 \)) and electron-doped case (\( n > 1 \)). \( \chi_{x,x}^s(q_y) \) is strongly enlarged at \( x = 1 \) and \( q_y = 0 \). By reflecting this fact, both \( \gamma_{x,x}^s \) and \( Z_x \) are strongly enlarged in both hole- and electron-doped cases. In the (1, 0) edge model, the edge-induced quantum criticality is moderate. In electron-doped case, \( \chi_{x,x}^s(q_y) \) takes the maximum at \( x = 1 \) and \( q_y = \pi \). In hole-doped case, in contrast, \( \chi_{x,x}^s(q_y = \pi) \) is moderately enlarged at \( x \geq 2 \). Both \( \gamma_{x,x}^s \) and \( Z_x \) show similar \( x \)-dependences to \( D_x(0) \).

The obtained nontrivial \( n \)-dependences for both (1, 1) and (1, 0) edge models are well understood in terms of the LDOS without interaction shown in Fig. S1 (b). In the (1, 0) edge model, the LDOS at \( x = 1 \) is strongly suppressed in hole-doped case. Due to this fact, the edge electronic states deviate from the quantum criticality. In electron-doped case, the LDOS at \( x = 1 \) is larger than the bulk DOS, so the edge effect becomes moderate. In the (1, 1) edge model, the \( x \)-dependence of the LDOS is essentially \( n \)-independent. For this reason, the edge electronic states approach to the quantum criticality in both hole-doped and electron-doped cases.

**B: filling dependence in YBCO TB model**

Next, we explain the numerical results for the YBCO TB model for \( n = 0.90, 0.95, 1.05 \) and 1.10. The obtained \( \chi_{x,x}^s(q_y), \gamma_{x,x}^s, Z_x, \) and \( D_x(0) \) are shown in Fig. S2. The YBCO TB model with \( n > 1 \) corresponds to the electron-doped cuprate superconductors, NCCO and PCCO. The obtained spin Stoner factors are shown in Fig. S2 (a).

In both (1, 0) and (1, 1) edge models, the obtained \( n \)-dependences are qualitatively similar to those obtained in the LSCO TB model. In the (1, 1) edge model, \( \chi_{x,x}^s(q_y = 0) \), are strongly enlarged at \( x \approx 1 \). Thus, the edge electronic states approach to the quantum criticality. This result originates from the large LDOS on the (1, 1) edge in YBCO model, shown in Fig. S2 (b). In the (1, 0) edge model, the edge-induced quantum criticality is moderate. For both \( n > 1 \) and \( n < 1 \) cases, \( \chi_{x,x}^s(q_y = \pi) \) takes the maximum at \( x = 1 \). In hole-doped case, in contrast \( \chi_{x,x}^s(q_y = \pi) \) is moderately enlarged at \( x \geq 2 \). Both \( \gamma_{x,x}^s \) and \( Z_x \) show similar \( x \)-dependences.

To summarize, prominent edge-induced quantum criticality is realized when the edge LDOS is large. This result is an useful principle to control the quantum criticality driven by real space structure, since it is easy to calculate the LDOS in non-interacting systems. The YBCO TB model with \( n > 1 \) corresponds to NCCO and PCCO. In YBCO TB model, very large quasiparticle damping rate \( \gamma_{x,x}^s \) is obtained in the (1,1) open edge. This result may lead to the pseudo-gap formation in the LDOS in the (1,1) open edge in YBCO, NCCO, and PCCO cuprate superconductors.
FIG. S1: (color online) (a) Obtained $\chi_{\alpha}^2(q_y)$ in LSCO TB model with (1,1) open edge and (1,0) open edge, respectively. The results for $n = 0.90, 0.95, 1.05,$ and 1.10 are shown. (b) Obtained filling-dependences of the mass-enhancement factor $Z_x$ and quasiparticle damping $\gamma_x^*$, and LDOS at the Fermi level $D_x(0)$ in the LSCO TB model ($n = 0.90 \sim 1.10$).
FIG. S2: (color online) (a) Obtained $\chi_{x,x}^*(q_y)$ in YBCO TB model with (1, 1) open edge and (1, 0) open edge, respectively. The results for $n = 0.90, 0.95, 1.05,$ and $1.10$ are shown. (b) Obtained filling-dependences of the mass-enhancement factor $Z_x$ and quasiparticle damping $\gamma_{x}^*$, and LDOS at the Fermi level $D_x(0)$ in the YBCO TB model ($n = 0.90 \sim 1.10$).