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Enhanced superconductivity by near-neighbor attraction in the doped extended Hubbard model

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Recent experiment has unveiled an anomalously strong electron-electron attraction in one-dimensional copper-oxide chain $Ba_{2-x}Sr_xCuO_{3+\delta}$. While the effect of the near-neighbor electron attraction V in the one-dimensional extended Hubbard chain has been examined recently, its effect in the Hubbard model beyond the one-dimensional chain remains unclear. Here, we report a density-matrix renormalization group study of the extended Hubbard model on long four-leg cylinders on the square lattice. We find that the near-neighbor electron attraction V can notably enhance the long-distance superconducting correlations while simultaneously suppressing the charge-density-wave correlations. Specifically, for a modestly strong electron attraction, the superconducting correlations become dominant over the CDW correlations with a Luttinger exponent $K_{sc} \sim 1$ and strong divergent superconducting susceptibility. Our results provide a promising way to realize long-range superconductivity in the doped Hubbard model. The relevance of our numerical results to cuprate materials is also discussed.

The origin of unconventional superconductivity is one of the greatest mysteries since the discovery of high-T_c cuprates [1]. Contrary to the conventional BCS superconductors, it is widely believed that the strong electronic Coulomb repulsions in the $3d$ orbitals play the dominant role in the d-wave pairing mechanism in cuprates. Along this line, spin fluctuations generated by the doped antiferromagnetic state may provide the pairing glue [2–5]. Based on the minimal model describing the correlations effect – the single-band Hubbard model [6–10], this pairing mechanism has been proposed based on perturbation theory and instabilities on small clusters [11, 12]. However, the ultimate verification requires the exact proof of long-range orders d-wave superconductivity in the thermodynamic limit.

To address these questions, advanced numerical simulations have been applied to the Hubbard model and its low-energy analog – the t-J model, in the past few years[9, 10]. Many unusual phases in cuprates, such as a striped phase [13–17] and a strange metal phase [18–20], have been identified recently by unbiased and exact methods on clusters such as density matrix renormalization group (DMRG) and determinantal quantum Monte Carlo (DQMC). However, the search for d-wave superconducting (SC) phase is not been quite as successful.[21] Quasi-long-range SC order has been found in the Hubbard and t-J models on four-leg square lattice cylinders,[22–30] that may be tuned by the band structure and in the striped Hubbard model[31]. However, when a similar study was extended to the wider six and eight-leg t-J cylinders on the square lattice, which is closer to two dimensions, superconductivity is found to disappear in the hole-doped side [27–29]. Therefore, the original Hubbard and t-J models themselves might be insufficient to resolve the high-T_c puzzle.

Meanwhile, experimental efforts have been devoted to the search of new insights. In a very recent photoemission experiment, a strong near-neighbor electron attractive interaction was identified in 1D cuprate chains, which may be mediated by phonons [32, 33]. Such an interaction is likely to be a missing ingredient also in high-T_c cuprates. Intuitively, the extended Hubbard model (EHM) with on-site repulsion and near-neighbor electron attraction may favor nonlocal Cooper pairs [34, 35]. Moreover, a recent DMRG study has identified dominant p-wave SC correlations in the pairing channel in the one-dimensional (1D) EHM [36]. These recent experimental and theoretical discoveries motivate the investigation of d-wave superconductivity with the presence of a near-neighbor attractive electron interaction.

Principal results – Previous DMRG studies [22–24] have shown that the ground state of the lightly doped Hubbard model on four-leg square cylinders with next-nearest-neighbor (NNN) electron hopping t' is consistent with that of a Luther-Emergy liquid (LE)[37] which is characterized by quasi-long-range SC and charge-density-wave (CDW) correlations but exponentially decaying spin-spin and single-particle correlations. However, while both the CDW and SC correlations are quasi-long-ranged, the former dominates over the latter in all cases, which suggests that CDW order may be realized in two dimensions. In this paper, we show that the presence of a finite nearest-neighbor (NN) electron attraction V can notably enhance the SC correlations, while suppressing the CDW correlations simultaneously. This demonstrates the mutual competition relation between the SC and CDW orders in the Hubbard model. More importantly, we find that the SC correlations become dominant over the CDW correlations when the electron attraction is modestly strong. Our results provide a promising pathway to potentially realize long-range superconductivity in the Hubbard model.

Model and Method – We use the DMRG method[38] to study the ground state properties of the single-band extended Hubbard model on the square lattice, defined by the Hamilto-

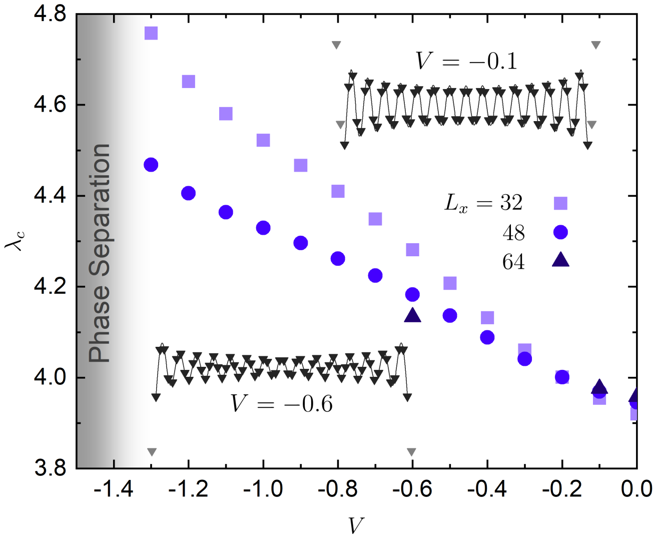

FIG. 1. (Color online) The CDW wavelength λ_c as a function of V. The length of the cylinder is $L_x = 32$, 48, and 64, and the hole doping concentration is 1/8. Inset: charge density profiles for $V = -0.1$ and -0.6, respectively. The fitting curves are obtained using Eq.2. Note that a few data points close to the boundaries (in grey) are removed in the fittings to minimize boundary effects. The gray shaded area denotes phase separation.

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$$H = - \sum_{ij,\sigma} t_{ij}(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + h.c.) + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + V\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j. \quad (1)$$

Here, $\hat{c}^\dagger_{i\sigma}$ ($\hat{c}_{i\sigma}$) is the electron creation (annihilation) operator with spin-σ ($\sigma =\uparrow,\downarrow$) on site $i = (x_i, y_i)$, $\hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$ and $\hat{n}_i = \sum_\sigma \hat{n}_{i,\sigma}$ are the electron number operators. The electron hopping amplitude t_{ij} equals t when i and j are the nearest neighbors, and equals t' for next-nearest neighbors. U is the on-site repulsive Coulomb interaction. V is NN electron interaction where $V < 0$ and $V > 0$ represent electron attraction and repulsion, respectively. We take the lattice geometry to be cylindrical with a lattice spacing of unity. The boundary condition of the cylinders is periodic along the $\hat{y} = (0, 1)$ direction and open in the $\hat{x} = (1, 0)$ direction. Here, we focus on four-leg cylinders where the width is $L_y = 4$ and length up to $L_x = 64$, with L_x and L_y are the number of lattice sites along the $\hat{x}$ and $\hat{y}$ directions, respectively. The doped hole concentration is defined as $\delta = N_h/N$, where $N = L_y \times L_x$ is the total number of lattice sites and N_h is the number of doped holes. For the present study, we consider the lightly doped case with hole doping concentration $\delta = 12.5\%$. We set $t = 1$ as an energy unit, and focus on $U = 12$ and $t' = -0.25$ as a representative parameters set. In our calculations, we keep up to $m = 16000$ number of states in each DMRG block with a typical truncation error $\epsilon \sim 10^{-6}$. We provide more numerical details in the Supplemental Material[39].

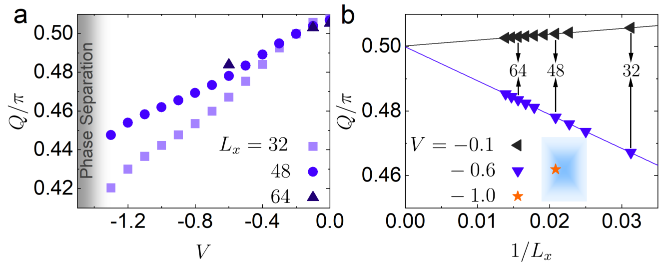

FIG. 2. (Color online) The CDW ordering wavevector Q as a function of electron attraction V in (**a**) and the inverse of the cylinder length L_x for different V in (**b**), respectively. The blue shaded area labels the CDW wavevector $Q = (0.462 \pm 0.01)\pi$ and charge stripe correlation length $\xi_{co} = (10.5 \pm 1.5)\lambda_c$ for $La_{2-x}Ba_xCuO_4$ with $x = 0.125$ [40].

Charge density wave order – To describe the charge density properties of the ground state of the system, we have calculated the charge density profile $n(x, y) = \langle \hat{n}(x, y)\rangle$ and its local rung average $n(x) = \sum_{y=1}^{L_y} n(x, y)/L_y$. For relatively weak electron attraction V, e.g., $V = -0.1$ as shown in the inset of Fig.1, the charge-density distribution $n(x)$ is consistent with the "half-filled" charge stripe [22, 26, 41, 42] of wavelength $\lambda_c = \frac{1}{2\delta}$, i.e., spacings between two adjacent stripes, with half a doped hole per unit cell. This is consistent with previous DMRG studies of the single-band Hubbard model in the absence of electron attraction, i.e., $V = 0$ [22–24]. Accordingly, the ordering wavevector $Q = 2\pi/\lambda_c$ can be obtained by fitting the charge density oscillation induced by the boundaries of the cylinder[43, 44]

$$n(x) \approx \frac{A\cos(Qx + \phi_1)}{[L_{\text{eff}}\sin(\pi x/L_{\text{eff}} + \phi_2)]^{K_c/2}} + n_0. \quad (2)$$

Here A is a non-universal amplitude, ϕ_1 and ϕ_2 are the phase shifts, K_c is the Luttinger exponent, and n_0 is the mean density. We find that an effective length of $L_{\text{eff}} \sim L_x - 2$ best describes our results. As expected, we find that $\lambda_c \sim 4$ ($Q = 4\pi\delta \sim \pi/2$) for the "half-filled" charge stripe.

When the electron attraction becomes relatively strong, the CDW wavelength λ_c starts deviating notably from the"half-filled" charge stripes on finite cylinder (see Fig.1 insets). We note that such a deviation for both λ_c and Q from their half-filled stripe values becomes smaller with the increase of the length of cylinders, suggesting that this deviation could be a finite-size effect. This is indeed supported by the finite-size scaling of Q as shown in Fig.2(b). It is clear that in the long cylinder limit, i.e, $L_x \to 0$ or $1/L_x \to 0$, Q for all different V will converge to the same value $Q = 4\pi\delta = \pi/2$ where $\lambda_c = 1/2\delta = 4$ at $\delta = 12.5\%$. As a result, the"half-filled" charge stripes may restore in the thermodynamic limit. It is also interesting to note that for cuprates such as $La_{2-x}Ba_xCuO_4$ and $La_{2-x}Sr_xCuO_4$ near 12.5% hole doping, the CDW wavevector Q determined from scattering measurements is always smaller than that expected for the "half-filled" charge stripe

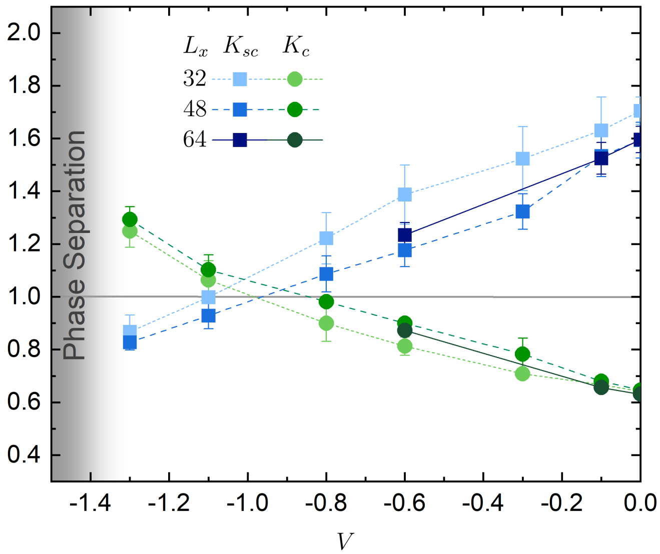

FIG. 3. (Color online) The extracted Luttinger exponents K_{sc} and K_c as a function of the strength of electron attraction V on different cylinders of length L_x. The gray shaded area denotes phase separation.

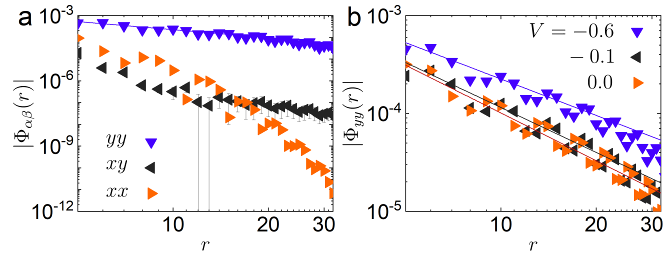

FIG. 4. (Color online) The superconducting pair-field correlation function for $V = -0.6$ in (**a**) and charge density profile for $V = -0.6, -0.1$ and 0.0 in (**b**). The cylinder length is $L_x = 64$ and the solid lines are power-law fitting using $\Phi_{yy}(r) \sim r^{-K_{sc}}$.

of $4\pi\delta$ [40, 45–47]. Considering the fact that experimentally the charge order in cuprates is short-ranged with a correlation length of $\xi_{\rm co} \approx 11\lambda_{\rm c}$ in LBCO[40] and $\xi_{\rm co} \approx 3\lambda_{\rm c}$ in LSCO[45–47]. Our results shown in Fig.2(b) on finite-length cylinders (with L_x comparable to $\xi_{\rm co}$ in cuprates) are suggestive of significant electron attraction V in these materials, where the estimated values of electron attraction (in the context of single-band Hubbard model) are $V \approx -1.0(2)$ in LBCO and $V \approx -0.40(5)$ in LSCO.

Importantly, another prominent observation in our study is that while "half-filled" charge stripes may be restored in the thermodynamic limit, their amplitude and strength is monotonically suppressed by the electron attraction. This is supported by the fact that the CDW exponent K_c defined in Eq. (2) increases notably with the increase of electron attraction $|V|$ as shown in Fig.3. For instance, we find that $K_c = 0.65(1)$ for $V = -0.1$ while $K_c = 0.87(1)$ for $V = -0.6$ on the four-leg cylinder of length $L_x = 64$, with an apparent insensitivity to the length of the ladders used in this study. It is worth mentioning that when $V \lesssim -1.0$ the CDW order is sufficiently suppressed to be secondary, where the SC correlation becomes dominant, as shown in Fig. 3.

Superconducting correlation – To describe the superconducting properties of the ground state of the system, we have calculated the equal-time spin-singlet SC correlation function

$$\Phi_{\alpha\beta}(r, y) = \langle \Delta^\dagger_\alpha(x_0, y_0)\Delta_\beta(x_0 + r, y_0 + y)\rangle. \qquad (3)$$

Here, $\Delta^\dagger_\alpha(x, y) = \frac{1}{\sqrt{2}}[\hat{c}^\dagger_{(x,y),\uparrow}\hat{c}^\dagger_{(x,y)+\alpha,\downarrow} - \hat{c}^\dagger_{(x,y),\downarrow}\hat{c}^\dagger_{(x,y)+\alpha,\uparrow}]$ is spin-singlet pair creation operator on the bond $\alpha = \hat{x}$ or $\hat{y}$. (x_0, y_0) is the reference bond with $x_0 \sim L_x/4$, r is the distance between two bonds in the $\hat{x}$ direction and y is the displacement between two bonds in the $\hat{y}$ direction. We have calculated different components of the SC correlation, including Φ_{xx}, Φ_{xy} and Φ_{yy} and find that the pairing symmetry is consistent with the plaquette d-wave symmetry [24, 25]. This is characterized by $|\Phi_{yy}(r, 0)| \gg |\Phi_{xy}(r, 0)| \gg |\Phi_{xx}(r, 0)|$ and $\Phi_{yy}(r, 0) = -\Phi_{yy}(r, 1)$.

Similar to the CDW correlation, at long distances, $\Phi_{yy}(r)$ is characterized by a power law as shown in Fig.4(a) with the appropriate Luttinger exponent K_{sc} defined by

$$\Phi_{yy}(r) \sim r^{-K_{sc}}. \qquad (4)$$

As mentioned, previous studies[22–24] on 4-leg square cylinders have shown that without electron attraction, that is, $V = 0$, the CDW correlations dominate over the SC correlations as $K_c < K_{sc}$. It is hence highly nontrivial to find a way to enhance the SC correlations while suppressing the CDW order.

In the previous section, we have shown that CDW correlations can be notably suppressed by NN electron attraction V. Accordingly, we would expect that the SC correlations can be enhanced by the NN electron attraction V since the CDW and SC orders are mutually competing [48]. Our numerical results are indeed consistent with this expectation. As shown in Fig.3, SC correlations become dominant over CDW correlations when $V \lesssim -1.0$, where $K_{sc} < K_c$. While a slow decay of SC correlations with $K_{sc} < 2$ implies a SC susceptibility that diverges as $\chi \sim T^{-(2-K_{sc})}$ as the temperature $T \to 0$, a much smaller K_{sc}, i.e., $K_{sc} \sim 1$, would lead to a much more divergent SC susceptibility. It is worth mentioning that while adding a near-neighbor attraction flips the dominant order, the ground state of the system is still consistent with that of a LE liquid phase where $K_{sc}K_c \sim 1$.

Spin-spin and single-particle correlations – To describe the magnetic properties of the ground state, we calculate the spin-spin correlation function defined as

$$F(r) = \langle \vec{S}_{x_0,y_0} \cdot \vec{S}_{x_0+r,y_0}\rangle. \qquad (5)$$

Here $\vec{S}_{x,y}$ is the spin operator on site $i = (x, y)$ and $i_0 = (x_0, y_0)$ is the reference site with $x_0 \sim L_x/4$. Fig.5(**a**) shows $F(r)$ for four-leg cylinder of length $L_x = 64$. It is clear that $F(r)$ decays exponentially as $F(r) \sim e^{-r/\xi_s}$ at long-

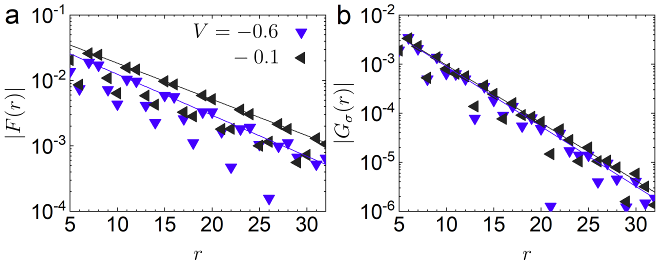

FIG. 5. (Color online) (**a**) The spin-spin and (**b**) single-particle correlation functions with electron attraction $V = -0.6$ and $V = -0.1$. The length of cylinder is $L_x = 64$. Solid lines denote exponential fit $F(r) \sim e^{-r/\xi_s}$ and $G_\sigma(r) \sim e^{-r/\xi_G}$, where ξ_s and ξ_G are corresponding correlation lengths.

distances, with a finite correlation length ξ_s. This is consistent with a finite excitation gap in the spin sector. Moreover, we find that ξ_s decreases with increasing $|V|$, e.g., $\xi_s = 7.8(1)$ for $V = -0.1$ and $\xi_s = 7.0(2)$ for $V = -0.6$. This suppression of short-range antiferromagnetic correlations may thus help to destabilize CDW order and promote SC order. Consistent with previous studies[22–24], $F(r)$ displays spatial modulations with wavelengths twice that of the charge.

We have also calculated the single-particle Green function, defined as

$$G_\sigma(r) = \langle c^\dagger_{x_0,y_0,\sigma} c_{x_0+r,y_0,\sigma}\rangle. \quad (6)$$

Examples of $G_\sigma(r)$ are shown in Fig.5(**b**). The long distance behavior of $G_\sigma(r)$ is consistent with exponential decay $G_\sigma(r) \sim e^{-r/\xi_G}$. Similar to ξ_s, we find that ξ_G also decreases with the increase of $|V|$. For instance, the extracted correlation lengths are $\xi_G = 3.7(1)$ for $V = -0.1$ and $\xi_G = 3.5(1)$ for $V = -0.6$, respectively. These are consistent with that of the LE phase.

Summary and discussion – In this paper, we have studied the ground state properties of the lightly doped extended Hubbard model on the four-leg square cylinders in the presence of near-neighbor electron attraction. Taken together, our results show that the ground state of the system is consistent with a LE liquid [37] where both CDW and SC correlations decay as a power-law and $K_{sc}K_c \sim 1$. However, previous studies[22–24] show that SC correlations are secondary when $V = 0$ compared with CDW correlations since $K_c < 1 < K_{sc}$. Interestingly, we find that the near-neighbor electron attraction V can notably enhance SC correlations while simultaneously suppress CDW correlations. As a result, when $V \lesssim -1.0$, SC correlations become dominant while CDW correlations become secondary as $K_{sc} < 1 < K_c$. To the best of our knowledge, to date, this is the first numerical realization of dominant superconductivity in doping the *uniform* Hubbard model on the square lattice of width wider than a 2-leg ladder. While in this paper we have focused on the effect of electron attraction V on the LE liquid phase on four-leg cylinders, it will also be interesting to study its effect on doping a qualitatively distinct phase such as the insulating "filled" stripe phases[49–51] with t'=0 as well as on wider six and eight-leg square cylinders to see whether a superconducting phase can be likewise obtained when V is sufficiently strong. Answering these questions may lead to a better understanding of the mechanism of high-temperature superconductivity.

We note that the critical V_c, where superconductivity starts to dominate in our simulation, is consistent with the recently identified attractive interaction in 1D cuprates $Ba_{2-x}Sr_xCuO_{3+\delta}$.[32] Considering the chemical similarity, it is reasonable to believe that the effective near-neighbor attraction in the CuO_2 plane is comparable to $V \sim -t$. Therefore, our finding suggests the importance of additional interactions beyond the Hubbard model to stabilize superconductivity over CDW. Future high-resolution experiments, such as photoemission and x-ray scattering, and their comparisons with numerical simulations may quantify this effective interaction V in high-T_c cuprates, in a similar way as for the 1D cuprate chains.

Another approach to estimating this effective V in realistic materials is a microscopic analysis of cuprates' crystal and electronic structure. Site phonons coupled with electronic density are possible candidates to mediate such an attractive interaction, which has been quantitatively discussed,[33, 52]. However, the combined impact of other phonons and other bosonic excitations may contribute to this effective interaction and ultimately result in the strong d-wave superconductivity in cuprates.

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