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Thermodynamic properties of the *d*-density-wave order in cuprates

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We solve a popular effective Hamiltonian of competing *d*-density-wave and *d*-wave superconductivity orders, self-consistently at the mean-field level for a wide range of doping and temperatures. The theory predicts a temperature dependence of the *d*-density wave order parameter seemingly inconsistent with the neutron-scattering and muon scattering resonance experiments of the cuprates. We further calculate thermodynamic quantities, such as chemical potential, entropy, and specific heat. Their distinct features can be used to test the existence of the *d*-density-wave order in cuprates.

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Unconventional charge and spin-density-wave orders were extensively investigated in correlated electron systems.[1] Recently, Chakravarty *et al.*,[2] proposed that the pseudogap phenomena in the high-T_c superconductors may originate from a hidden long-range order, *d*-density wave (DDW).[3] This state is also related to the staggered-flux state of Lee and Wen,[4] but the latter is dynamically fluctuating in their SU(2) gauge theory of the cuprates. According to Ref. 2, the pseudogap is a consequence of the competition between two independent orders DDW and *d*-wave superconductivity (DSC), which are transformable to each other in a three-dimensional order-parameter space and may coexist in the underdoped cuprates. A theory of DDW seems natural to account for a possible quantum critical point near the optimal doping level that marks the onset of the pseudogap, put forward by Tallon and Loram[5] by examining the data of photoemission, thermodynamic, and transport properties, etc.

This DDW scenario has recently attracted much attention about its nature and experimental consequences.[6–10] Some investigations[8] seem to indicate that various experiments in yttrium boruim copper oxide (YBCO) systems[11–13] support this idea. The neutron-scattering experiment[11] shows that the elastic signal around the in-plane wave vector $Q=(\pi,\pi)$ in the underdoped YBCO appears well above T_c. The muon scattering resonance (μSR) experiment[12] also confirms that a small internal magnetic field appears above T_c in the underdoped YBCO but below T_c in the optimally doped samples. Since internal magnetic fields are very weak and spin fluctuations are too fast to couple with muon's spins, it is reasonable to attribute them to DDW. However, both experiments also show that the magnetic signal is enhanced when the temperature drops across T_c. Such a behavior is not expected intuitively from the DDW picture, since the DSC and DDW orders compete each other. It thus becomes quite interesting to understand how this temperature-dependent puzzling behavior happens and, in particular, to see whether it can be understood in terms of the existing self-consistent DDW mean-field theory.[6–10]

In this communication, we shall study the temperature dependence of the DDW order at the mean-field level. We find that it cannot give the expected temperature dependence in the above experiments. Instead, our results show that the DDW order parameter is always suppressed when the temperature drops below T_c, and that this is a robust behavior, independent of the choice of parameters. Thermodynamic quantities (e.g., chemical potential, entropy, specific heat) are also investigated. Their distinct temperature dependences are discussed.

Consider following the mean-field Hamiltonian[6–10]

$$H_{MF}=\sum_{\langle ij\rangle\sigma}(-t_{\rm eff}-V_1\chi_{ij}^*)c_{i\sigma}^\dagger c_{j\sigma}+\text{H.c.}$$
$$-V_2\sum_{\langle ij\rangle\sigma}\Delta_{ij}(c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger-c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger)+\text{H.c.}$$
$$-\mu\sum_{i\sigma}c_{i\sigma}^\dagger c_{i\sigma}+V_1\sum_{\langle ij\rangle}\chi_{ij}^*\chi_{ij}+V_2\sum_{\langle ij\rangle}\Delta_{ij}^*\Delta_{ij},$$

where $\langle ij\rangle$ indicates summation over the nearest neighbors only. Δ_{ij} and the imaginary part of χ_{ij} play the role of the DSC and DDW order parameters, respectively. They are related to the electron operators via $\Delta_{ij}=\langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger-c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger\rangle$ and $\chi_{ij}=\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle$. V_1 and V_2 are positive in order to have a nonzero DDW and DSC order. We have used an effective hopping amplitude $t_{\rm eff}=t\delta$ with δ the doping concentration and t the bare hopping amplitude to take account of the reduction of t near half-filling due to the strong Coulomb repulsion. Loosely speaking, the effective theory described above is equivalent to the fermion part of the slave-boson mean-field theory of the *t*-*J* model[14,15] in which the *J* term is decoupled into particle-hole and particle-particle channels with different weights.

The *t*-*J* model at half-filling has a (hidden) local SU(2) symmetry,[16] which rotates (Imχ, ReΔ, ImΔ) as a three-vector. Thus the DDW(π-flux) phase is degenerate with the DSC phase. Finite doping breaks this local SU(2) symmetry explicitly and favors DSC order,[14] because the Fermi-surface nesting is destroyed. Ubbens and Lee[15] showed that at finite temperatures the DDW (flux) state is stable only when very close to the half-filling. The boundary between the DDW-(flux) and DSC phases is of the first order in nature. Thus there is no coexistence phase. In the model we are considering, $V_1>V_2$ is needed to have DSC and DDW coexist as

pointed out in Ref. 7. Although the Heisenberg term equally favors DDW and DSC orders, the repulsion between the nearest sites favors DDW over DSC. Hence the mean-field Hamiltonian above is reasonably postulated.

Because the DDW order breaks the translational symmetry, the Brillouin zone is reduced into one half and the operators $(c_{k\uparrow}, c_{k+Q\uparrow}, c^{\dagger}_{-k\downarrow}, c^{\dagger}_{-k-Q\downarrow})$ are mixed to give two branches of Bogoliubov quasiparticle excitations: $E(k)_{\pm}=\{(-\mu \pm W_k)^2+(2V_2\Delta\phi_k)^2\}^{1/2}$, where $W_k=\sqrt{\epsilon_k^2+(2V_1\mathrm{Im}\chi\phi_k)^2}$, $\epsilon_k=-(t_{\mathrm{eff}}+V_1\mathrm{Re}\chi)\gamma_k$, and $\phi_k=\cos k_x-\cos k_y$, $\gamma_k=\cos k_x+\cos k_y$ (ϵ_k is the tight bond band energy.). The corresponding self-consistent equations of Reχ, Imχ, and Δ are

$$\mathrm{Re}\chi=\frac{1}{2N}\sum_k{}' \frac{-\epsilon_k\gamma_k}{W_k}\left\{\tanh\left(\frac{\beta E_{k+}}{2}\right)\frac{-\mu+W_k}{E_{k+}} - \tanh\left(\frac{\beta E_{k-}}{2}\right)\frac{-\mu-W_k}{E_{k-}}\right\},$$

$$\mathrm{Im}\chi=\frac{1}{2N}\sum_k{}' \frac{2V_1\mathrm{Im}\chi\phi_k^2}{W_k}\left\{\tanh\left(\frac{\beta E_{k+}}{2}\right)\frac{-\mu+W_k}{E_{k+}} - \tanh\left(\frac{\beta E_{k-}}{2}\right)\frac{-\mu-W_k}{E_{k-}}\right\},$$

$$\Delta=\frac{1}{2N}\sum_k{}' \left\{\tanh\left(\frac{\beta E_{k+}}{2}\right)/E_{k+}+\tanh\left(\frac{\beta E_{k-}}{2}\right)/E_{k-}\right\} \times 2V_2\Delta\phi_k^2,$$

$$\delta=\frac{1}{N}\sum_k{}' \left\{\tanh\left(\frac{\beta E_{k+}}{2}\right)\frac{-\mu+W_k}{E_{k+}}+\tanh\left(\frac{\beta E_{k-}}{2}\right) \times\frac{-\mu-W_k}{E_{k-}}\right\},$$

where the summation is restricted within the reduced Brillouin zone and $\beta=1/T$. Below we denote the energy gaps $\Delta_{\mathrm{DSC}}=2V_2\Delta$ and $W_{\mathrm{DDW}}=2V_1\mathrm{Im}\chi$ for the DSC and DDW orders, respectively.

After solving the self-consistent equations at $V_1=0.38$ and $V_2=0.25$ with energy scale set as $t\equiv 1$, we obtain the dependence of the Δ_{DSC} and W_{DDW} gap vs doping δ at zero temperature as shown in Fig. 1 of Ref. 2. Δ_{DSC} begins to develop after $\delta>0.06$ and reaches maximum at $\delta\approx 0.18$. W_{DDW} also drops to zero around there. The phase diagram of temperature vs δ is similar to Ref. 7, and we shall not reproduce it here.

There exists a coexisting region of both orders. However, in this region the behavior W_{DDW} vs temperature (T) is subtle [see Fig. 1(a)]. In comparison, Fig. 1(b) shows how Δ_{DSC} varies with T. For very low doping ($\delta=0.05$) where $\Delta_{\mathrm{DSC}}=0$, W_{DDW} is monotonically enhanced when T is reduced. When the coexisting region is entered, W_{DDW} becomes maximum around T_c where Δ_{DSC} starts developing. This feature is general for competing orders, which also happens in the competition of *s*- and *d*-wave pairing orders.[17] When either

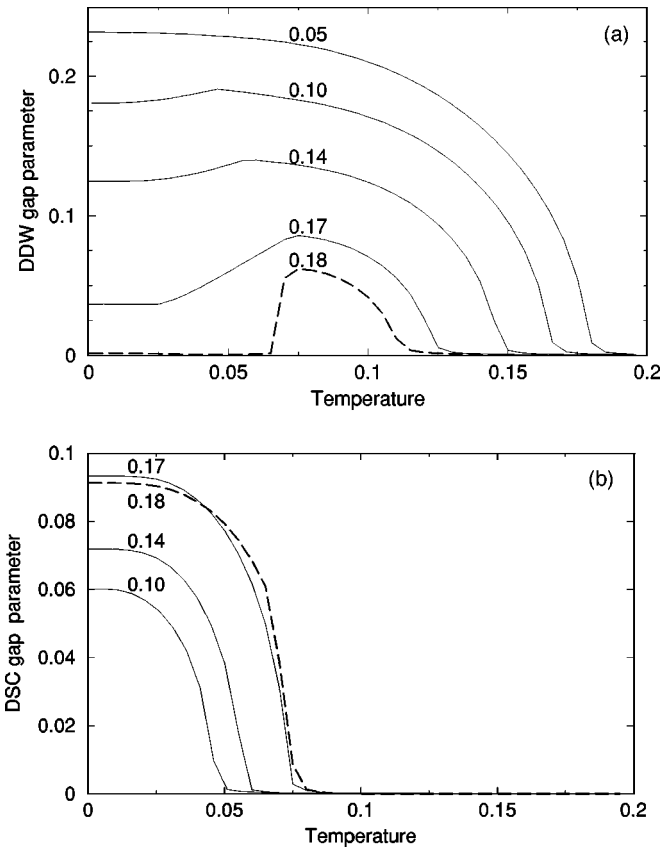

FIG. 1. (a) W_{DDW} vs temperature for various doping levels. From top to bottom, $\delta=0.05,0.10,0.14,0.17,0.18$. (b) Δ_{DSC} vs temperature for various doping levels. From bottom to top, $\delta=0.10,0.14,0.18,0.17$. Curves of $\delta=0.18$ are plotted with dashed lines for the aid of eyes.

order develops, it generates a gap near the Fermi surface. Consequently, it becomes difficult for the other to form. When T slightly drops from T_c, Δ_{DSC} increases fast as $(1-T/T_c)^{1/2}$. W_{DDW} loses more weight to DSC than it gains from lowering temperature. When T drops well below T_c, Δ_{DSC} increases very slowly and W_{DDW} changes little as well. In the underdoped region, W_{DDW} still has a substantial residual value at $T=0$ K, which gets significantly reduced and may even become zero near the optimal doping. When $\delta=0.18$ in Fig. 1(a), W_{DDW} only exists in a small range around T_c. In other words, something as the reentry phenomenon occurs here with varying temperatures: W_{DDW} vanishes at $T=0$ K, begins to increase from a finite temperature to T_c, and then decreases to zero again when $T>T_c$. We never see W_{DDW} developing with decreasing T within the superconducting region. These are just opposite to what the neutron scattering and μSRR experiments indicated.

We have to take it seriously as to why the experimental signals are enhanced when $T<T_c$. There seem to be only two possibilities. The first one is that these signals are really related to the DDW order. Then a modified mean-field theory is needed for a mechanism wherein the two orders can somehow enhance each other around T_c. Or if these signals have other origins such as from spin, then they cannot be used as evidence for the existence of the DDW order.

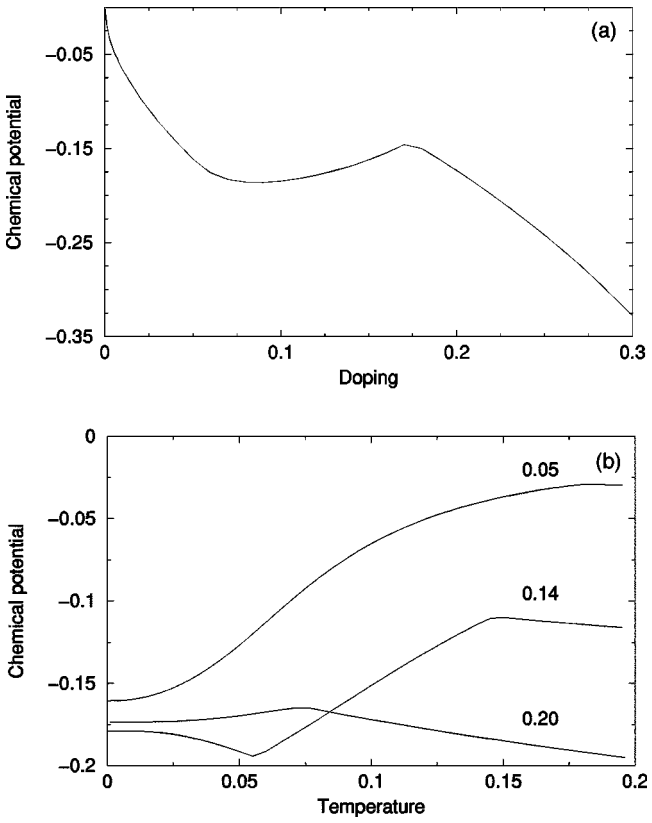

FIG. 2. (a) Chemical potential vs doping at zero temperature. (b) Chemical potential vs temperatures at characteristic doping levels. $\delta = 0.05,\ 0.14,\ 0.20$.

The behavior of chemical potential μ is also interesting. In Fig. 2(a), we show the dependence of μ with δ at zero temperature. μ decreases with increasing δ when $\delta \lesssim 0.06$, increases slowly in the underdoped region and drops quickly in the overdoped region. This can be understood as follows. The energy curve of quasiparticles is cone shaped in the momentum space with a Fermi pocket near $(\pi/2, \pi/2)$. After the onset of Δ_{DSC}, W_{DDW} drops faster with increasing δ, so that the density of states (DOS) increases. This keeps μ roughly unchanged while increasing doping. In the underdoped region, $\partial\mu/\partial n$ is small and becomes even negative, which means that the charge instability may develop here. Photoemission experiments[18] show that μ is almost fixed at the undoped value upon increasing δ in the underdoped region. Our result agrees with it qualitatively, but μ is not fixed at the value of the undoped case.

Figure 2(b) shows the temperature dependence of μ at three doping levels: low (nonsuperconducting) doping ($\delta = 0.05$), underdoped ($\delta = 0.14$), and overdoped ($\delta = 0.20$). In the low doping region, μ increases with temperature increasing. W_{DDW} is weakened by temperature while μ increases to fix the particle number. In the underdoped region, μ's behavior is subtle. It first drops when $T < T_c$, then increases when $T_c < T < T_{\mathrm{DDW}}$, and then drops again when $T > T_{\mathrm{DDW}}$, where T_{DDW} is the onset temperature for DDW. This can be explained by the temperature dependence of W_{DDW} (Fig. 1). W_{DDW} is enhanced (or weakened) by increasing temperature within the range $T < T_c$ (or $T_c < T < T_{\mathrm{DDW}}$).

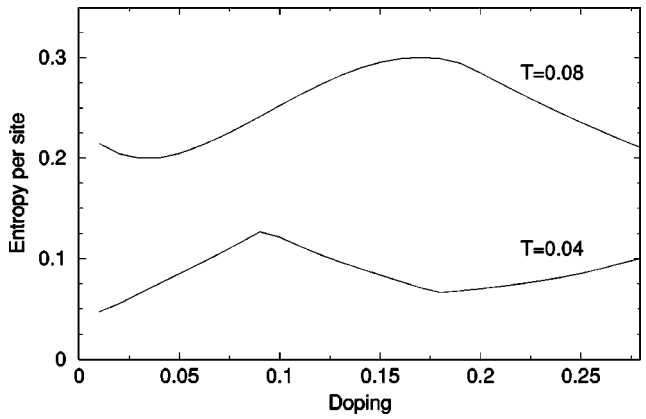

FIG. 3. Entropy per lattice site vs doping at fixed temperatures. From top to bottom, $T = 0.08,\ 0.04$.

Thus μ first drops and then increases. After T passes over T_{DDW}, μ drops, behaving as an ordinary Fermi gas. In the overdoped region, $W_{\mathrm{DDW}} = 0$. Thus μ is almost fixed when $T < T_c$ but drops when $T > T_c$.

The DDW order also has important effects on the entropy per site S vs δ, as shown in Fig. 3. The first curve is at the high temperature where $\Delta_{\mathrm{DSC}} = 0$ and only W_{DDW} exists. In the underdoped region, S decreases when δ is reduced, because W_{DDW} reduces the low-energy DOS. In the overdoped region, S drops when δ increases, which is the standard Fermi-liquid behavior. Thus S reaches maximum near the optimal doping. This agrees with experimental results of Loram *et al.*[19] Very close to half-filling, the hopping amplitude is reduced. As a result, the band width is reduced and DOS is enhanced. This effect tends to increase S. Simultaneously, the DDW order is enhanced by lowering doping, which has an effect to decrease S. At high temperatures where W_{DDW} is small, the first effect may overcome the second one and thus S increases when δ decreases. This phenomenon is absent at the low temperature where W_{DDW} is large, which is also shown in Ref. 19. Let us increase δ at the lower temperature as in the bottom curve. S increases at very low doping levels, since only W_{DDW} exists. In the coexistence or underdoped region, S drops because Δ_{DSC} develops. After passing the optimal point, Δ_{DSC} decreases and thus makes S increase again.

There is also specific heat anomaly at the onset of W_{DDW}, as shown in Fig. 4. The jump of the specific heat coefficient $\gamma(T) = C(T)/T$ is large and can be compared with those at the onset of Δ_{DSC}. The jump at the DDW transition is larger at the more underdoped side, while that at the DSC transition's behavior is just opposite. However, the former is not seen in experiments and is a difficulty for the DDW scenario. It was argued that disorder removes the sharp transition and turns it into a smooth crossover in Ref. 2. Reference 20 suggests that a negatively large μ can weaken the jump by destroying the nesting of Fermi surface. However, from the Fig. 2(b), μ increases rapidly when $T \to T_{\mathrm{DDW}}$, and $|\mu|$ is much smaller at T_{DDW} than at zero temperature, especially at the low doping region. It is still difficult to understand why μ can be negatively large.

At last, we briefly discuss the condensation energy U_0. In

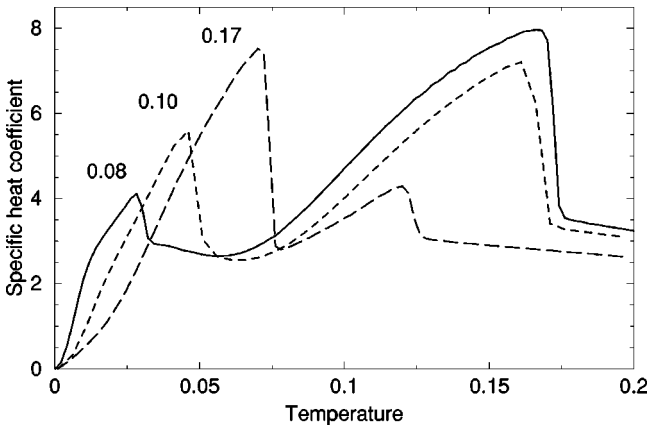

FIG. 4. Specific heat coefficient $\gamma(T)$ vs δ in the underdoped and optimal region, from left to right $\delta=0.08$, 0.10, 0.17.

the case of the pure DSC state, electrons near $(\pi,0)$ contribute much to U_0 and those near $(\pi/2,\pi/2)$ contribute little. However, in the DDW scenario, there is a preexisting W_{DDW} in the pseudogap region by assumption. Upon doping, the Fermi surface is a small pocket, which has not been seen in experiments yet. The same $d_{x^2-y^2}$ symmetry makes the vicinity of $(\pi,0)$ already far below the Fermi surface. Then the paring cannot affect them as significantly as is in the case of pure DSC, thus, U_0 is reduced. Let us study the contribution to U_0 along the curve of the minimum gap form the direction $(\pi/2,\pi/2)\rightarrow(\pi,0)$. At the beginning, it is proportional to $\Delta_{\mathrm{DSC}}\phi_k$, where $\phi_k=\cos k_x-\cos k_y$. After passing the point k_0 where the end of the Fermi pocket lies, the dependence changes into $\phi_k[\sqrt{W_{\mathrm{DDW}}^2(1-\phi_{k0}/\phi_k)^2+\Delta_{\mathrm{DSC}}^2}-W_{\mathrm{DDW}}(1-\phi_{k0}/\phi_k)]$. If W_{DDW} is large, the slope becomes softer and an apparent kink develops. This kink can be testified by studying the retreat of the leading edges of the high-resolution ARPEPS data deep in the superconducting region relative to those in the pseudogap region. If the pseudogap is caused by pair fluctuations, such kink will not exist.

In summary, we studied the DDW and DSC order parameters' dependence with temperature and thermodynamic quantities in detail by solving the mean-field Hamiltonian self-consistently. The DDW order is suppressed when temperature drops below T_c in the underdoped region because of their competing nature. The disagreement with experimental results was discussed. Behaviors of the chemical potential, entropy, and specific heat with temperature and doping are investigated. The increase of chemical potential is predicted when the temperature increases in the pseudogap region. We also showed the decrease of entropy when doping decreases in the underdoped region. The distribution of condensation energy in the momentum space has a kink along the direction from $(\pi/2,\pi/2)$ to $(\pi,0)$. These features may be used in experiments to testify the DDW scenario.

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