Charge ordering in half-doped Pr(Nd)$_{0.5}$Ca$_{0.5}$MnO$_3$ under magnetic field

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Recent experiments in Pr(Nd)$_{0.5}$Ca$_{0.5}$MnO$_3$ thin films exhibited (multiple) reentrant charge ordering (CO) transitions with change of temperature $T$ under fixed magnetic field $H$, which are in contrast to the results for the corresponding bulk materials. To explain the experimental findings, a model including the double-exchange mechanism, intersite Coulomb interaction and electron-phonon coupling is proposed, for which the reentrant CO is naturally obtained due to the temperature dependence of the band-type coherent polaron hopping. Various results for the CO in the ($H$, $T$) plane are extensively discussed. The theory is considered to be valid for both thin films and bulk materials.

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I. INTRODUCTION

The colossal magnetoresistance manganites $R_{1-x}A_xMnO_3$ (R: rare-earth element like La, Pr, Nd; A: divalent alkali like Ca, Sr) and $R_n$-$n_x$A$_{1+n_x}$Mn$_n$O$_{3n+1}$ ($n = 1, 2$) have attracted great interest for both bulk materials and thin films in recent years. Due to the complex interplay of charge, orbital, spin, and lattice degrees of freedom, intriguing phenomena have been discovered. Among them, charge ordering (CO) with alternating Mn$^{3+}$ and Mn$^{4+}$ ions in real space is one of the most remarkable findings. It has been observed for optimal doping $x = 0.5$ in various (R, A) compositions, where the concentrations of Mn$^{3+}$ and Mn$^{4+}$ ions are equal, and was also found in the doping region $0.3 < x < 0.75$, depending on R and A. The CO may be melted by external magnetic fields, which are favorable to a ferromagnetic (FM) metallic state.

The CO in manganite thin films has been studied very recently. Due to strain effect, different properties from those in bulk materials are expected. Pelleir et al. studied the CO instability under magnetic field $H$ in Pr$_{0.5}$Ca$_{0.5}$MnO$_3$ thin films and found a spectacular reduction of the melting field $H_c$ for CO under tensile strain. This is ascribed to an enhanced electron itinerancy. On the other hand, the critical $H_c$, as a function of temperature $T$, is found to be non-monotonous. From the phase diagram in the plane ($H$, $T$), which is replotted in Fig. 1 by the solid line, a more interesting phenomenon, i.e., reentrant CO transitions with change of $T$ under fixed $H$, can be clearly seen. For example, at $H = 6$ T, the CO appears at about $T = 210$ K but later melts at $T = 100$ K. The profile for $H = 3.5$ T is even more remarkable: the CO appears at about $T = 220$ K, and later melts at $T = 60$ K, but finally reappears at $T = 20$ K, i.e., multiple (twice) reentrant CO transitions are expected through the whole temperature region.

A similar phase diagram with possible single reentrant behavior was also reported for Nd$_{0.5}$Ca$_{0.5}$MnO$_3$ thin films and is reproduced in Fig. 1 by the dotted line. In contrast, no obvious reentrant CO was found for the two corresponding bulk materials. Naturally, a theoretical investigation of the experimental findings is required.

It should be pointed out that the reentrant CO under magnetic field was clearly observed in bulk $R_{1-x}A_xMnO_3$ (R=Pr, Nd) for doping away from 0.5, e.g., $0.3 < x < 0.45$ for R=Pr. Although this issue is not fully understood either, it was argued by Khomskii et al. that phase separation into an electron-rich region (due to extra Mn$^{3+}$ ions) and a CO region, as that for $x = 0.5$, is a relevant mechanism. On the other hand, even in the half-doped ($x = 1/2$) case, (multiple) reentrant CO was found before in bi-layered manganite LaSr$_2$Mn$_2$O$_7$ under zero magnetic field. A mechanism for this scenario was proposed by us. The idea is to ascribe the CO to the competition of electronic kinetic energy and intersite Coulomb interaction, and simultaneously take electron-phonon (e-p) coupling into account, i.e., consider polaron ordering. Due to the inherent temperature-dependent band-type polaron motion, the kinetic energy may be small compared to the...
Coulomb energy at some temperatures (favoring CO), but dominates at other temperatures (favoring the homogeneous state) so that a reentrant behavior may appear. Here, the same idea will be generalized to study the CO under magnetic field. The experimental phase diagrams are interpreted and, more generally, various results for CO under magnetic field for half-doped manganites are discussed.

Before we start to work out the details it deserves to further clarify the validity of the above proposed theory. Actually, we notice that there are several alternative models to study CO (and concomitant orbital and magnetic orderings) in half-doped manganites currently. A natural model is to take the intersite Coulomb interaction as the driving force for CO. This modelling was adopted by many authors and also used for a discussion of other materials, e.g., the Verwey transition in magnetite Fe$_3$O$_4$. Another kind of model emphasizes the role of CE-type antiferromagnetic (AFM) spin order concomitant with CO, which was found in e.g., Nd$_{0.5}$Sr$_{0.5}$MnO$_3$. As derived by van den Brink et al., the on-site Coulomb interaction alone between electrons in different orbitals will lead to CO. And the experimental ($\pi,\pi,0$)-type CO, i.e., the checkerboard CO forms in the $xy$-plane and stacks in $z$-direction, can be explained within the same picture. However, this model is not well suited for Pr(Nd)$_{0.5}$Ca$_{0.5}$MnO$_3$, where the spins are not yet ordered when CO appears. Recently, a purely Jahn-Teller (JT) phononic model, even without direct electron correlations, was proposed by Yunoki et al. By treating the e-p coupling adiabatically, they have constructed the phase diagram of charge, orbital and magnetic orderings with change of JT coupling strength and AFM superexchange of the core spins. This model seems not to be generally accepted at the moment. Without relying on peculiar features of concrete materials (e.g., magnetic structure), the intersite Coulomb interaction, which is always present in reality, is regarded as the origin of CO as done by most authors. And on the other hand, another aspect of e-p coupling, i.e., polaron formation with dynamic phonons is addressed. Experimentally it has been verified that the CO should be viewed as the formation of a polaron lattice. A strong evidence is the isotope effect, where the CO transition temperature $T_{co}$ was changed by replacing $^{16}$O with $^{18}$O. Therefore, as the simplest model to study CO in manganites, the e-p coupling is indispensable, besides the intersite Coulomb interaction. This improves the one proposed by Khomskii where only the latter is included. Indeed, the model with both e-p and intersite Coulomb interactions has been successfully used to explain the experimental isotope effect renormalization of sound velocity around $T_{co}$ and reentrant CO in LaSr$_2$Mn$_2$O$_7$ mentioned above. Also, it is believed to have grasped much of the physics of the CO transitions in Pr(Nd)$_{0.5}$Ca$_{0.5}$MnO$_3$, addressed in this paper.

**II. MODEL HAMILTONIAN AND TECHNICAL TREATMENTS**

On the basis of the considerations in the introductory section, we write the Hamiltonian as

$$H = -t(\cos(\theta/2)) \sum_{\langle ij \rangle} (c_i^\dagger c_j + \text{h.c.}) + V \sum_{\langle ij \rangle} n_i n_j + g \sum_i n_i (b_i + b_i^\dagger) + \omega \sum_i b_i^\dagger b_i .$$

The first term is the double-exchange (DE) model, where $t$ is the nearest-neighbor (n.n.) hopping and $\theta$ is the angle between two n.n. core spins which is assumed uniform or an average on $b_{ij}$. $V$ is the intersite Coulomb interaction and $n_i = c_i^\dagger c_i$ is the electron number operator. Irrespective of the details for various types of e-p coupling (e.g., JT, breathing, etc.), we have used a simple on-site Holstein-type model with dispersionless phonons as shown by the third term to describe an essential effect of e-p coupling. Then $b_i$, $b_i^\dagger$ are local phonon operators at site $i$, $q$ is the e-p coupling constant and $\omega$ is the Einstein phonon frequency. The band is half-filled, i.e., one electron per two sites. Note that the effect of external magnetic field $H$ has been implied in the factor $\langle \cos(\theta/2) \rangle$, which becomes larger with increasing $H$ due to enhanced FM order (i.e., $\theta \to 0$).

In the following, we consider the Hamiltonian in the two-dimensional (2D) case since the checkerboard CO was found only in the basal plane as mentioned above. Moreover, we mainly focus on the qualitative results in this work, thus no sophisticated techniques will be elaborated. The quantitative aspects of the results obtained should not be trusted literally, but they are qualitatively correct. Throughout the paper we set $\hbar = k_B = 1$ and $t$ is taken as the energy unit.

First, the usual Lang-Firsov (LF) transformation is acted upon Hamiltonian, i.e., $\tilde{H} = UHU^\dagger$ with

$$U = \exp[-(g/\omega) \sum_i n_i (b_i - b_i^\dagger)] .$$

Then, thermally averaging on the phonon states, one obtains the following effective electronic Hamiltonian:

$$H_{\text{eff}} = -\tilde{t} \sum_{\langle ij \rangle} (c_i^\dagger c_j + \text{h.c.}) + V \sum_{\langle ij \rangle} n_i n_j$$

with the renormalized hopping $\tilde{t} = t(\cos(\theta/2))P(T)$.

Here

$$P(T) = \exp[-(g^2/\omega) \coth(\omega/2T)]$$

is the polaron narrowing factor and a constant $-(g^2/\omega) \sum_i n_i^2$ is ignored in Hamiltonian. Thus the effect of e-p coupling is contained exclusively in $P(T)$. 


Note that \( P(T) \) has a strong temperature dependence, which is plotted in Fig. 2. Although the narrowing effect is overestimated by the LF method for \( \omega/t \ll 1 \), i.e., the absolute value of \( P(T) \) is too small, the \( T \)-dependent property is qualitatively correct, i.e., \( P(T) \) increases monotonically with decreasing \( T \) because of smaller and smaller phonon occupation number. Due to the same reason, \( P(T) \) is seen to be nearly flat at very low temperatures, about \( T/\omega < 0.2 \), where the phonons are hardly excited. If acoustic phonons are considered, as in some references, a rapid variation of \( P(T) \) with \( T \) should be still possible up to \( T = 0 \), as schematically shown by the dashed line in Fig. 2. We emphasize here that the \( T \)-dependent \( P(T) \) is the essence of our theory, which may render the CO to melt with decreasing \( T \) by quickly enhancing the hopping \( \tilde{t} \). In principle, the thermal average \( \langle \cos(\theta/2) \rangle \) is also \( T \)-dependent, but it is assumed to be quite weak compared to \( P(T) \). Actually in the CO states in Fig. 2, there is no indication for noticeable changes of the spin order under fixed fields, especially in the reentrant temperature region. Thus the possible tiny change of \( \langle \cos(\theta/2) \rangle \) with \( T \), even in the correct direction (i.e., increasing with decreasing \( T \)), is argued impossible for a melting of the CO, and thus not important. In what follows, \( \langle \cos(\theta/2) \rangle \) will be simply considered as a function of \( H \), i.e., \( \langle \cos(\theta/2) \rangle = F(H) \). Finally, a minor point is that, for the current model \( 2 \text{ and } 3 \), no phonon-mediated intersite interaction has been derived. For other types of e-p coupling, such an extra interaction may be obtained, leading to a shift of the parameter \( V \) \text{ and } \gamma \).

For the effective Hamiltonian \( 2 \) and \( 3 \), we make use of the Hartree mean-field (MF) theory to study the CO. For a bipartite lattice with sublattices A and B, it is assumed

\[
\langle n_i \rangle = \begin{cases} 
1/2 + x, & i \in A \\
1/2 - x, & i \in B
\end{cases},
\]

where \( x \) characterizes the deviation from the uniform electron distribution. The final self-consistent equation for the order parameter \( x \) is obtained as follows (trivial solution \( x = 0 \) is ignored)

\[
1 = \frac{2V}{\pi^2} \int_0^{1} \frac{\tanh[2\sqrt{(tx)^2 + (Vx)^2}/T]}{\sqrt{(tx)^2 + (Vx)^2}} K(\sqrt{1 - z^2}) \, dz,
\]

where \( K \) is the complete elliptic integral of the first kind.

### III. Results and Discussions

The above equation can be easily evaluated numerically. For manganites, the bare hopping \( t \approx 0.2-0.5 \) eV, and the intersite interaction \( V/t \approx 0.1-0.2 \) due to a large dielectric constant. The optical phonon frequency \( \omega \) ranges \( \sim 10-70 \) meV. For example, a soft mode at \( \omega \approx 7 \) meV was reported by Zhao \textit{et al.} for \( \text{La}_{1-x}\text{Ca}_x\text{MnO}_3 \) \((x = 0.25, 0.4) \) thin films. We point out that the high frequency modes play no role for the melting of CO here because, as discussed above, they only contribute to a nearly flat \( P(T) \) in the temperature scale for the reentrance to occur.

The solution for \( V = 0.1 \), \( \omega = 0.05 \) is displayed in the phase diagram Fig. 3 in the plane of \( T \) and \( F(H) \). The results for different \( g \) values are presented. The reentrant CO is clearly seen within a finite region of \( F(H) \) for \( g = 0.04, 0.042, \) and \( 0.043 \), while not for \( g = 0.035 \) for any \( 0 \leq F(H) \leq 1 \). For a careful analysis of the reentrant behavior, the value \( g = 0.042 \) is taken as an example and enlarged in Fig. 3. We fix \( F(H) = 0.8 \) as indicated by the arrow and check how the CO state evolves with decreasing \( T \). At the highest energy scale, the entropic term dominates the free energy and the homogeneous state is stable. For temperatures of the order of \( V \), where the coherent polaron motion is nearly frozen (i.e., \( \tilde{t} \to 0 \)), a charge order transition takes place. On decreasing \( T \) the band-type hopping \( \tilde{t} \) becomes larger, and moreover, it increases fast enough to dominate \( V \) so that the CO state is destabilized. Thus the second transition, where the CO melts into the homogeneous state (hs) takes place. With continuing decrease of \( T \), the third transition occurs to recover the CO since the ground state must be charge ordered, which will be discussed in detail later. To summarize, in the whole temperature region, the system goes through a series of transitions: hs → CO → hs → CO with decreasing \( T \). The corresponding \( x \) vs. \( T \) is shown in the inset of Fig. 3 by the solid line, where the order parameter takes on alternating zero and non-zero values. Interestingly, the double reentrance of the CO at fixed \( F(H) \) or external field obtained here is a remarkable experimental observation shown in Fig. 3. In addition, in the inset of Fig. 4, the curves \( x \) vs. \( T \) for two examples without reentrance, i.e., \( F(H) = 0.7, 0.9 \), are also shown. An analysis of them is helpful. For \( F(H) = 0.7 \), as shown by the dashed line, \( x \) decreases with decreasing \( T \) (due to increasing \( \tilde{t} \)) in the intermediate region but does not approach zero. This means that the increase of \( \tilde{t} \) is not sufficient to melt the CO. The case for \( F(H) = 0.9 \) is different. Now the absolute value of \( \tilde{t} \) becomes relatively large, even at high temperatures. Although it is reduced at higher \( T \), the simultaneously enhanced thermal fluctuation will prohibit CO. Thus the CO can not be stabilized at a relatively high temperature as the cases for
$F(H) = 0.7$ and 0.8. It remains unstable with decreasing $T$, and appears only at very low temperatures to realize the charge ordered ground state, as seen by the dotted line.

**FIG. 3.** The phase diagram in the plane of $T$ and $F(H)$ for $V = 0.1$, $\omega = 0.05$. The solid curves from left to right correspond to $g = 0.035$, 0.04, 0.042, and 0.043, respectively. The dashed line shows a correction to the phase boundary of $g = 0.035$ (see text).

**FIG. 4.** The enlarged phase diagram for $g = 0.042$ in Fig. 3. The two dashed lines 1 and 2 show two possibilities for a correction to the phase boundary (see text). In the inset the order parameters $x$ vs. $T$ are plotted for $F(H) = 0.7$, 0.8, and 0.9.

As for the ground state, it is always charge ordered for any $V/\tilde{t} > 0$ because of the perfect nesting property at half-filling for the model Hamiltonian (2,3). This conclusion can be drawn from Eq. (3), which is proven to always give a solution of nonzero $x$ at $T = 0$. On the other hand, it must be noted that the perfect nesting property may be easily broken in real materials, for example, by inclusion of the next n.n. hopping which is usually present. In situations away from perfect nesting, a natural conclusion for the ground state is that the CO only appears when $V$ exceeds a critical value, or equivalently it vanishes if $\tilde{t}$ becomes large. Correspondingly, in the phase diagram of Fig. 3, a critical value of $F(H)$ (or a critical field $H_c$) is expected at $T = 0$ to separate the CO and homogeneous states. With this in mind, the phase boundary may be reasonably corrected in two ways, 1 and 2, as shown by the dashed lines. For line 1, only the possibility of one reentrance is obtained. And for line 2, a double reentrance is still possible. These two possible phase diagrams are qualitatively consistent with the experimental findings in Fig. 1. At the same time, a similar correction is valid for the phase boundary of $g = 0.035$ in Fig. 3, as shown by the dashed line. This corrected phase boundary is the same as usually observed in half-doped manganites in the $(H,T)$ plane, e.g., the bulk Pr$_{0.5}$Ca$_{0.5}$MnO$_3$. For concrete calculations including all above corrections, a model beyond perfect nesting is needed, which is left for future studies.

As mentioned before, the reentrant CO on decreasing $T$ depends on the increasing strength of $\tilde{t}$ and its relative magnitude to $V$. Under which conditions it takes place is complicated, relying on the concrete parameters, i.e., $g$, $\omega$, $F(H)$ which control $\tilde{t}$, and the value of $V$. Some insight can be gained by comparing the phase diagrams with different values of $g$, $\omega$, and $V$. A few consequences seem clear: for relatively large $F(H)$, increasing $g$ helps the first CO transition to occur at a high temperature, and consequently favors the appearance of the reentrant behavior; a similar effect can be obtained by increasing $V$; large $\omega$ is unfavorable to the reentrant CO. Unfortunately, no quantitative criterion can be straightforwardly extracted.

So far, we have not addressed the observation that the reentrant CO is exhibited in Pr(Nd)$_{0.5}$Ca$_{0.5}$MnO$_3$ thin films, while it is not obvious for the corresponding bulk materials. The difference is understandable from the above results. For thin films, due to strain effects, the lattice parameters are modified (e.g., the in-plane parameter is elongated by the tensile strain). Correspondingly, the model parameters will change in thin films compared to bulk materials. We speculate that the reentrant behavior in thin films is due to the softened optical phonon modes.

Finally, we comment on the function $F(H)$, which was used throughout the results. Its explicit form is not known although its qualitative behavior is transparent. Above, spin order was fixed when the reduced Hamiltonian (4) was introduced. Strictly speaking, the effect of $H$ should be studied interactively with the CO under the same Hamiltonian by inclusion of the superexchange $J_{AF}$ of the core spins and the Zeeman energy. The explicit form of $F(H)$ can be roughly estimated in the following phenomenological way. We consider a Hamiltonian of the form $-\tilde{t}(\cos(\theta/2)) \sum_{i,j} (\hat{c}_i^\dagger \hat{c}_j + \text{h.c.}) + J_{AF} \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j - g\mu_B H \sum_i S_i^z$, with $\mathbf{S}_i$: core spin and $g$: Landé factor. Moreover, a uniform canted state from the competition between FM order due to the DE mechanism and AFM
superexchange is assumed in order to simulate the essential effect of the external field (i.e., favoring the FM order). In this way, a linear relation between $\langle \cos(\theta/2) \rangle$ and $H$ may be obtained.

IV. CONCLUSION

Based on a double-exchange model with intersite Coulomb interaction and e-p coupling, charge ordering has been studied under magnetic field $H$ in the context of polaron formation. A melting of the CO on decreasing $T$ under fixed $H$ can be naturally obtained due to the $T$-dependent band-type polaron hopping. More generally, various phase diagrams in the plane of $T$ and $F(H)$ with (single or double) or without reentrant behavior, depending on the concrete model parameters, have been extensively discussed. The experimental findings on the CO under magnetic field in the half-doped Pr(Nd)$_{0.5}$Ca$_{0.5}$MnO$_3$ can be explained for both thin films and bulk samples. Future work will have to address a number of important issues which are still not well comprehended: the orbital degree of freedom, a deviation from $(\pi, \pi)$ for the wavevector of the CO in thin films, and a possible magnetic phase separation in the CO state.

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52. For real quantification, it’d better to first elaborate the formulas like Eq. (3).
53. For example, the change of $t$ in thin films due to purely geometric factors is discussed in Q. Yuan, to be published.
54. See also L. J. Zou, Q. Q. Zheng, and H. Q. Lin, Phys. Rev. B 56, 13669 (1997).
55. G. Allodi, R. De Renzi, F. Licci, and M. W. Pieper, Phys. Rev. Lett. 81, 4736 (1998); F. Dupont, F. Millange, S. de Brion, A. Janossy, and G. Chouteau, Phys. Rev. B 64, 220403(R) (2001).