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Ferromagnetic insulator induced by Peierls instability at orbital order transition

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Abstract. The origin of the ferromagnetic insulating state of La\textsubscript{7/8}Sr\textsubscript{1/8}MnO\textsubscript{3} is investigated. Based on the tight-binding model, it is shown that this state can be attributed to the Peierls instability arising from the interplay of spin and orbital ordering. The importance of the hole–orbiton–phonon intercoupling in doped manganites is revealed. This picture explains well the recent experimental finding of re-entrance of the ferromagnetic metal state at low temperatures (\textit{Phys. Rev. Lett.} \textbf{96} 097201).

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Table 1. Phase transitions of La$_{7/8}$Sr$_{1/8}$MnO$_3$. P, paramagnetic; FM, ferromagnetic; I, Insulator; and M, Metallic.

| Phase | Temperature | Structure | Magnetism | Transport |
|-------|-------------|-----------|-----------|-----------|
| I     | $T > T_{JT}$ | Orthorhombic | P         | I         |
| II    | $T_C < T < T_{JT}$ | Monoclinic | P         | I         |
| III   | $T_{OO} < T < T_C$ | Monoclinic | FM        | M         |
| IV    | $T_R < T < T_{OO}$ | Triclinic | FM        | I         |
| V     | $T < T_R$    | Unknown   | FM        | M         |

1. Introduction

R$_{1-x}$A$_x$MnO$_3$ (R being rare-earth ions and A being divalent ions, e.g. A=Ca, Sr, Ba or Pb) have been intensively studied for more than a decade because of their rich physics, such as unusual colossal magnetoresistance (CMR) [1], interesting ferromagnetic (FM) and antiferromagnetic phases and charge and/or orbital ordering. Despite intensive research and progress made so far in understanding the system, the origin of the ferromagnetic insulating (FMI) phase observed in lightly doped La$_{7/8}$Sr$_{1/8}$MnO$_3$ [2] is still controversial and unknown. CMR can be qualitatively understood in terms of the celebrated double exchange (DE) model [3], which means the simultaneous appearance of ferromagnetism and metallic behavior. Thus, FMI is not compatible with the DE model, at least not in a direct way. Although it is generally recognized that the FMI state may relate to the interplay of charge, spin and orbital degrees of freedom, no concrete picture is available. Finding such a picture is the focus of this paper.

It will be useful to first summarize the experimentally observed phases of La$_{7/8}$Sr$_{1/8}$MnO$_3$ (solid). Lowering the temperature, the first structural phase transition from orthorhombic to monoclinic order occurs at $T_{JT}$ $\sim$ 283 K. The system is in the orthorhombic paramagnetic insulating phase (phase I) above $T_{JT}$ and the monoclinic paramagnetic insulating phase (phase II) below $T_{JT}$ but above the FM transition temperature $T_C$ $\sim$ 183 K. The second structural phase transition from monoclinic to triclinic order occurs at $T_{OO}$ $\sim$ 150 K, separating the monoclinic FM metallic phase [4, 5] (phase III) from the triclinic FMI state (phase IV) having a superstructure with unit cell $2a_c \times 4b_c \times 4c_c$ ($a_c \times b_c \times c_c$ is the unit cell of the high-temperature orthorhombic phase) [6]. The FMI state of phase IV is supported by thermal activated exponential $T$ dependence [2, 7] of the resistivity that increases rapidly with a decrease of temperature for $T < T_{OO}$, and the metallic nature of phase III is confirmed by the fact that the resistivity decreases with temperature below $T_C$ [2]. The system undergoes another metal–insulator transition from the FM insulator to FM metal (phase V) at temperature $T_R$ $\sim$ 30 K. Phase V is a re-entrance of the FM metallic (FMM) state through the FMI phase at $T_R < T < T_{OO}$, newly discovered by the nuclear magnetic resonance technique [8]. The crystal structure below $T_R$ is still unknown. Table 1 lists all five phases, characterized by four critical temperatures. So far, phases I–III have been widely studied and well understood in terms of the crystal structure and magnetic and transport properties.

In order to explain the FMI state of La$_{7/8}$Sr$_{1/8}$MnO$_3$, many different models were proposed in the literature, including charge polarons order [9], checkerboard-like charge order [10], orbital order without charge order [11], etc. Most of them are not consistent with the recent resonant x-ray scattering (RXS) experiments, which observed an orbital polaron lattice (OPL)
in phase IV [12]. This observation is the basis of the FMI–orbital polaron model proposed by Kilian and Khalilullin [13]. Orbital polarons can be viewed as charge carriers (holes) dressed by the interconnected orbital states. In light doping manganites, one Mn\(^{4+}\) site is surrounded by six neighboring Mn\(^{3+}\) sites, equivalent to one hole (with e\(_g\) orbits unoccupied) surrounded by six (occupied) e\(_g\) orbits. The strong hole–orbital coupling will polarize those e\(_g\) orbits and make them point toward the hole to minimize the interaction energy as well as the kinetic energy [13]. The formation of OPL in La\(_{7/8}\)Sr\(_{1/8}\)MnO\(_3\) emphasizes the importance of hole–orbital interaction for the FMI state [12]–[14].

Obviously, the genuine mechanism of the FMI state should explain the following experimental features: (i) the measured \(\rho–T\) curves [2, 7], (ii) the giant phonon softening [15], and (iii) the re-entrance of the FMM state (IV \(\rightarrow\) V) [8]. It is difficult for the orbital polaron model to explain features (i) and (iii). The reasons are as follows. Firstly, the orbital polaron cannot reproduce the measured \(\rho–T\) curves of La\(_{1–x}\)Sr\(_x\)MnO\(_3\) at \(T < T_{00}\) (cf figure 3). The polaron hopping model yields \(\rho = \rho_0 \exp(E_a/k_B T)\), where \(E_a\) is the activation energy of polarons, from which the binding energy \((E_b = 2E_a)\) of a polaron can be deduced. The fitting to experimental data [7, 12] with the hole–polaron hopping model gives \(E_b \sim 0.06–0.12\) eV, about an order of magnitude smaller than the theoretical value \((E_b \sim 0.6\) eV in [13]). Secondly, the observed re-entrance of the FMM state at lower temperatures is inconsistent with the polaron model, since polaron hopping becomes more and more difficult when the temperature is lowered. Therefore, the orbital polaron itself is not sufficient to explain the FMI state, and the origin of the metal–insulator transitions at \(T_{00}\) remains intriguing and controversial.

The above difficulties can be removed by including electron–phonon (e–ph) interaction in the simple electron–orbit coupling model. We argue that the mechanism of the FMI state is the e–ph coupling-induced Peierls instability [16] that opens an energy gap at \(T < T_{00}\). In this paper, we shall show that the Peierls instability can explain the observed re-entrance of FMM state quantitatively, and the other experimental features at the qualitative level.

2. Theory

Our theoretical model is based on the quasi-one-dimensional (1D) confinement of the motion of holes in La\(_{7/8}\)Sr\(_{1/8}\)MnO\(_3\), which has been demonstrated by the following experiments: (i) the convergent-beam electron diffraction and selected-area electron diffraction seeing the superstructure \((2a_c \times 4b_c \times 4c_c)\) of the FMI phase [6] (anisotropic 3D motion); (ii) the RXS showing an alternation of hole-rich and hole-poor planes in the c-direction [12], which confines holes to move in the 2D hole-rich \(a–b\) planes (2D motion); and (iii) the RXS also revealing the formation of OPL [12], which further confines holes to move along the 1D charge stripes in the \(a\)-direction (1D motion, see figure 1 and the following explanations). It is known that the quasi-1D confinement originates from the orbital order and its induced effective coupling between adjacent Mn\(^{3+}\) and Mn\(^{4+}\) sites. The inset of figure 1 depicts two possible configurations of one Mn\(^{4+}\)–O\(^2–\)–Mn\(^{3+}\) unit with different e\(_g\) orbital occupations on the Mn\(^{3+}\) site. Configuration II corresponds to e\(_g\) orbit pointing toward the hole along the axis of oxygen 2p orbit, while configuration I corresponds to e\(_g\) orbit pointing toward other directions. Due to orbital anisotropy, configuration II results in a maximized overlapping of wavefunctions of occupied e\(_g\) and 2p orbits. That induces two direct effects: (i) lower energy of configuration II than that of I with an energy difference \(\Delta_{\text{orb}}\) [13]; and (ii) effective Mn\(^{4+}\)–Mn\(^{3+}\) coupling with considerable transfer integration \((t \neq 0)\). As a result, configuration II is stable and favors the motion of
holes along the \(a\)-axis. In the hole-rich planes shown in figure 1, configuration II periodically repeats itself along the \(a\)-direction, thus forming the quasi-1D \(\text{Mn}^{3+}\text{O}^2-\text{Mn}^{4+}\text{O}^2-\) chain-like pathways of hole transport. Please note that weak interchain couplings (\(t_\perp\)) in the \(b\)- and \(c\)-directions also exist, resulting from the hole transfer between unoccupied and occupied \(e_g\) orbits \[12\]. Why can the orbital order-induced quasi-1D confinement only be observed around \(x = 1/8\)? Qualitatively speaking, the orbital disorder–order transition takes place at light hole doping provided that the Jahn–Teller phonons and superexchange processes mediate an effective coupling between orbits on neighboring sites \[13\].

Now we are ready to present our model Hamiltonian to describe the quasi-1D motion of particles (electrons/holes). As shown in figure 1, the particles moving along \(\text{Mn}^{3+}\text{O}^2-\text{Mn}^{4+}\text{O}^2-\) chains will simultaneously couple to the orbits on the manganese sites and lattice displacements (phonons) on the oxygen ones. Considering that the quasi-particles of the orbital degree of freedom are bosonic orbitons \[17, 18\], we can establish an electron–orbiton–phonon intercoupling model. For simplicity, only Mn sites are included in the model and the oxygen degree of freedom are integrated out, giving rise to the effective Mn–Mn coupling and the phonon modulation to it (cf equation \((1)\)). Then, the tight-binding model can be written as (\(\hbar = 1\) and \(k_B = 1\) are assumed, and they are restored in the final results),

\[
H = t \sum_j (c_j^+ c_{j+1} + \text{h.c.}) + \sum_q \epsilon_q a_q^+ a_q + \sum_j c_j^+ c_j Q_j + \sum_p \omega_p b_p^+ b_p + \sum_j (c_j^+ c_{j+1} P_j + \text{h.c.}),
\]

\[
Q_j = (Q_{j-1} + Q_{j+1}),
\]

\[
P_j = (P_{j+1} - P_j),
\]

\[1\]

Figure 1. The orbital order-induced quasi-1D confinement of the motion of holes in the \(a\)-direction. The dashed lines denote the weak interchain couplings in the \(b\)- and \(c\)-directions. The arrows near the \(\text{O}^2-\) ions indicate the displacement of the oxygen sublattice. The inset shows the orbital order-induced effective coupling between adjacent \(\text{Mn}^{3+}\) and \(\text{Mn}^{4+}\) sites mediated by the oxygen 2p orbit. Configurations I and II correspond to different occupations of \(e_g\) orbitals on the \(\text{Mn}^{3+}\) site. \(\Delta_{\text{orb}}\) is the splitting of energy between I and II \[13\].
with

\[ Q_j = \sum_q R_q e^{iq \cdot R_j} (a_q + a_{-q}^+), \]
\[ P_j = \sum_p G_p e^{ip \cdot R_j} (b_{-p} + b_p^+), \]

(2)

where \( c_j^+ \) is the creation operator of a particle on site \( j \) (\( R_j \) is the atom position), \( a_q^+ (b_p^+) \) the creation operators of an orbiton (phonon) with momentum \( q (p) \), \( \epsilon_q \) and \( \omega_p \) are the dispersion spectra of the orbiton and phonon, respectively. The third term is the e–orb coupling between a particle on site \( j \) and the orbitons on the nearest neighbor sites \( j \pm 1 \) and the last term describes the e–ph coupling due to the phonon modulation of the particle hopping between sites \( j \) and \( j + 1 \) [19] (see figure 1). \( R_q \) and \( G_p \) are the e–orb and e–ph coupling constants, respectively, which satisfy \( G_{-p}^* = G_p \) and \( R_{-q}^* = R_q \) to ensure the Hermitian character of equation (1).

What are the different roles of the e–orb and e–ph interactions in equation (1)? One can see that the orbiton couples to the on-site charge density \( n_j \), which promotes the formation of Holstein-like small polarons in the strong-coupling limit [20]. That is the physical origin of the formation of orbital polarons [12, 13]. The essential effect of Holstein-like small polarons is reducing the electron bandwidth (or enlarging the electron effective mass). This interaction predicts a transition from band transport to thermal-activated hopping of polarons at high temperatures. However, the e–ph interaction in equation (1) can take the role of opening the energy gap, since the phonon modulation of the electron transfer predicts the Peierls instability in quasi-1D systems at low temperatures [16, 21]. A kind of generalized Peierls instability has been found to play an important role in the ground-state orbital ordering of LaMnO\(_3\) [22]. For \( \text{La}_{7/8}\text{Sr}_{1/8}\text{MnO}_3 \), when the orbital order effectively confines the particles to move along quasi-1D pathways (see figure 1), the strong e–ph interaction distorts the oxygen sublattice to make \( \text{O}^{2-} \) ions displace toward Mn\(^{4+}\), which enhances the polarization of orbits and helps us to stabilize the orbital order (see figure 1). There thus forms the quasi-1D charge-density-wave (CDW) state in the manganese sublattice accompanied by the bond-order-wave (BOW) state in the oxygen sublattice with twice the period of the original lattices (dimerization). An analogous material with a similar CDW/BOW ground state is the halogen-bridged mixed-valence metal complex, which has been well studied with this kind of e–ph interaction in the literature [23].

At \( T < T_C \), the FM \( t_{2g} \) spins of Mn ions exclude the opposite spin to occupied \( e_g \) orbitals due to Hund’s rules, i.e. only carriers with the majority spin contribute to the charge transport. Before coupling to orbitals and phonons, the Mn\(^{4+}\)–Mn\(^{3+}\) transfer (the first term in equation (1)) in the majority-spin subspace conduces to a half-filled metallic energy band and the bare particle spectrum \( \xi_{k}^0 \) can be written as

\[ \xi_{k}^0 = \gamma_{k}^0 + \delta_{k}^0 \]

(3)

with

\[ \gamma_{k}^0 = -2t \cos k_x a, \]
\[ \delta_{k}^0 = -2t \eta (\cos k_y b + \cos k_z c), \]

(4)

where the effect of weak interchain coupling (\( t_\perp = \eta t, \eta \ll 1 \)) has been included in \( \delta_{k}^0 \). Here \( \eta \) is a dimensionless parameter denoting the relative strength of the interchain coupling to the intrachain one.
The orbitons and phonons then couple to the tight-binding particles, as described in equation (1), and change the above metallic band to an insulator one. The simultaneous couplings between two bosons to one fermion are technically difficult to solve, even though the direct orbiton–phonon coupling has been ignored in equation (1). Thus, we make two approximations for e–orb coupling in the following calculations. The first one is the \( q \)-independence \( \epsilon_q(=\epsilon) \) and \( R_q(=r) \), based on the theoretical result that the orbiton is almost dispersionless at strong e–orb couplings [24]. The second one is the perturbation theory of small polarons [19] at strong e–orb couplings, which conduces to

\[
\xi_k = \xi_k^0 \exp\left(-\frac{r^2}{\epsilon^2}\right) - \frac{r^2}{\epsilon} \equiv A\xi_k^0 - B,
\]

where \( A \) denotes the electron bandwidth reduction (or effective-mass enhancement) and \( B \) the energy shift due to strong e–orb couplings. The above approximations have captured the essential physics of e–orb coupling: electron effective-mass enhancement \( (A) \) and energy shift \( (B) \), so that it should produce reasonable results in the limit of strong e–orb interactions. Please note that the above approximations are only valid at finite \( \epsilon \) to avoid \( B \) being unphysically large.

After the electron is coupled to orbital degree of freedom,

\[
\xi_k = \gamma_k + \delta_k,
\]

where

\[
\gamma_k = A\gamma_k^0,
\delta_k = A\delta_k^0 - B.
\]

Let us make some further comments on the e–orb interactions of concern in the present work. Our model Hamiltonian describes electrons coupled to two bosonic fields (orbitons and phonons), which is formally similar to the model of electrons coupled to two kinds of phonons for cuprates [25]. The key feature of orbitons distinguishing them from usual phonons is the strong spatial anisotropy due to the symmetry of \( e_g \) electron wave functions, which has been qualitatively considered in building up our quasi-1D Hamiltonian (see figure 1 and equation (1)). The quantitative description of orbitons by means of pseudospin operators, which may be required for a more general study [13], has been beyond the scope of this paper. The parameter characterizing the orbital ordering coming into play due to orbitons is \( \lambda_o \equiv r/t \). In our calculations, \( \lambda_o \approx 0.2–0.65 \), which is realistic for manganites and consistent with the literature [13].

Particles with a new energy spectrum in equation (6) then couple to phonon degree of freedom. Now, we can analytically solve the Hamiltonian by transforming it into momentum space

\[
H = \sum_k \xi_k c_k^+ c_k + \sum_p \omega_p b_p^+ b_p + \sum_{k,p} g_{pk} c_{k+p}^+ c_k (b_p + b_{-p}^+),
\]

where \( g_{pk} \) is the e–ph coupling constant in momentum space and its dependence on \( k \) is to be neglected in what follows \( (g_p = g_{-p}^* \propto M_p) \), as in the literature [27]. That Hamiltonian for 1D systems indicates a Peierls superstructure that, described by introducing the following anomalous average [26], breaks the translational symmetry of the initial lattice:

\[
\Delta = g_{2k_f} (b_{2k_f} + b_{-2k_f}^+) \neq 0,
\]
where angular brackets denote the thermodynamic average that can be obtained by performing Gibbs average to the Matsubara equations of motion for the operators $b_K$ and $b_{-K}^\dagger$ ($K = 2k_F$ for the Peierls phase transition) [27],

$$\left(-\frac{\partial}{\partial \tau} - \omega_K\right) \langle b_K(\tau) \rangle = \sum_k F(k, \tau = -0),$$

$$\left(-\frac{\partial}{\partial \tau} + \omega_K\right) \langle b_{-K}^\dagger(\tau) \rangle = -\sum_k F(k, \tau = -0),$$

where $F(kt) = -i\langle Ta_k(t)a_{-K}^\dagger(0)\rangle$ is the anomalous Green’s function describing the elementary Umklapp scattering process $k - K \to k$.

After Fourier transformation over Matsubara ‘time’ to equation (10), we have

$$\langle b_K + b_{-K}^\dagger \rangle_{\omega_n} = \frac{2g_k \omega_K T}{\omega_n^2 + \omega_K^2} \sum_{k,n} F(k, \varepsilon_n).$$

The condition for the Peierls phase transition is $\omega_n = 0$ at $K = 2k_F$, i.e.

$$\Delta = g_k \langle b_K + b_{-K}^\dagger \rangle_{\omega_n=0} = -\frac{2g_k^2 T}{\omega_K} \sum_{k,n} F(k, \varepsilon_n).$$

In coordinate representation, equation (9) describes the Peierls deformation potential characterized by the wave vector $K$: $V(x) = \Delta e^{iKx} + \Delta^* e^{-iKx}$. The anomalous Green’s function $F$ can be derived from the Gorkov equations for Matsubara Green’s functions (limit to first order in $V$) under the ‘nesting condition’: $\gamma_{k-K} = \gamma_{k-2k_F} = -\gamma_k$ [27],

$$G(k, \varepsilon_n) = G_0(k, \varepsilon_n) + G_0(k, \varepsilon_n) \Delta F(k, \varepsilon_n),$$

$$F(k, \varepsilon_n) = G_0(k - K, \varepsilon_n) \Delta^* G(k, \varepsilon_n),$$

which gives the following solutions:

$$G(k, \varepsilon_n) = \frac{i\varepsilon_n - \delta_k + \gamma_k}{(i\varepsilon_n - \delta_k)^2 - \gamma_k^2 - \Delta^2},$$

$$F(k, \varepsilon_n) = \frac{\Delta^*}{(i\varepsilon_n - \delta_k)^2 - \gamma_k^2 - \Delta^2}.$$

By replacing $i\varepsilon_n$ with $\varepsilon$, the new energy spectrum is determined by the zero of denominators (pole) of equation (14):

$$\varepsilon = \delta_k \pm \sqrt{\gamma_k^2 + \Delta^2}.$$  \hfill (15)

Inserting equation (7) into equation (15) gives the energy gap $E_g$ of the system,

$$E_g = 2\Delta - 8A\eta t.$$  \hfill (16)

By inserting equation (14) into equation (12) and then performing standard calculations, we obtain the self-consistent equation of $\Delta$ (set to be real),

$$1 = \frac{g^2}{2} \sum_k \frac{\sinh \sqrt{\gamma_k^2 + \Delta^2}}{\cosh \frac{\sqrt{\gamma_k^2 + \Delta^2}}{T} + \cosh \frac{\delta_k}{T} \sqrt{\gamma_k^2 + \Delta^2}} \frac{1}{g_k \sqrt{2/\omega_K}}.$$  \hfill (17)
3. Discussion

So far we have derived the insulating state at $T < T_C$ resulting from the Peierls instability at the orbital order transition temperature $T_{OO}$. With this mechanism, we first quantitatively explain the observed re-entrance of FMM state. The key point is that a $T$-dependent interchain coupling $\eta(T)$ may induce two critical temperatures $T_{c1}$ and $T_{c2}$ of the metal–insulator transition. The former corresponds to the ordinary Peierls instability and the latter to the re-entrance of the metallic state. It is called stepped Peierls transition theory, with which Zhou and Gong explained the anomalous transport property in NbSe$_3$ [28]. With this theory, we can elucidate the re-entrance of FMM state in La$_{7/8}$Sr$_{1/8}$MnO$_3$. For strong $e$–orb coupling, the self-consistent equation of $T_{MI}$ (derived from $E_g(T_{MI}) = 0$) can be expressed as

$$\Delta(T_{MI}) = 4A\eta(T_{MI})t.$$  \hspace{1cm} (18)

In principle, $\eta(T)$ should increase with a decrease of temperature, in analogy with the role of pressure. Since the exact expression of $\eta(T)$ is hard to determine, we take the leading linear term of its series expansion at low temperature ($T < T_\Delta$),

$$\eta(T) = \eta_0(1 - \alpha T/T_\Delta),$$  \hspace{1cm} (19)

where $T_\Delta$ denotes the critical temperature of the charge order [$\Delta(T_\Delta) = 0$], which coincides with $T_{c1}$ at $\eta = 0$ (cf equation (16)) but is a little higher than $T_{c1}$ at $\eta > 0$. $\eta_0$ is the $T$-independent part of $\eta$ and $\alpha$ is a phenomenological parameter. In our calculations, we fix $T_\Delta = 180$ K by considering the experimental $T_{c1} = T_{OO} \sim 150$ K. Please note that at least two parameters in the self-consistent equation (equation (17)) are dependent on each other after $T_\Delta$ is fixed.

We then self-consistently solve equations (17)–(19) and illustrate the change of $T_{c1}$ and $T_{c2}$ with $\eta_0$ in figure 2. The parameters are chosen as $r = 0.2t$, $g = 1.1\sqrt{T}$, $\epsilon = 0.6t$, $\alpha = 0.5$ and $t = 0.4$ eV. As shown in figure 2, our calculations can yield $T_{c1} \sim 150$ K and $T_{c2} \sim 30$ K at $\eta_0 \sim 0.028$, comparing well with the experimental observation in [8] as indicated by the big arrows in the figure. No re-entrance of metallic state occurs at small interchain coupling ($\eta_0 < 0.024$), characterized by $T_{c2} = 0$. $T_{c1}$ decreases slightly with increasing $\eta_0$ in this limit. Nonzero $T_{c2}$ emerges at about $\eta_0 \sim 0.024$. Further increasing interchain coupling will induce a rapid increase of $T_{c2}$ and a rapid decrease of $T_{c1}$ meanwhile. When $T_{c1}$ and $T_{c2}$ coincide into one point at large interchain coupling, the Peierls phase transition disappears. This is just the interchain-coupling-induced delocalization of quasi-1D states, as occurs in conjugated polymers [29]. Since the value of $t$ for the e$_g$ electron system is believed to be $0.3$–$0.6$ eV [13, 30], our theory quantitatively explains the re-entrance of the FMM state with consistent parameters in the literature.

In a recent experiment on the (011)-oriented La$_{7/8}$Sr$_{1/8}$MnO$_3$ films, Chen et al measured an energy gap opening at $T \sim 190$ K and increasing to $\sim 0.16$ eV at $T = 120$ K [31]. The absent physics mechanism in their experiment has already been elucidated in this paper, that is, the observed energy gap results from the Peierls instability at orbital order transition. To further clarify this point, we calculated the temperature dependence of the energy gap self-consistently and show the result in the inset of figure 2 together with the experimental data. Some of the above parameters are adjusted to fit Chen et al’s experiment: $T_\Delta = 200$ K, $r = 0.64t$ and $\eta_0 = 0.02$. As shown in the figure, our calculated $E_g$–$T$ curve is in good agreement with the experimental data.
Figure 2. Two critical temperatures of metal–insulator transitions ($T_{c1}$ and $T_{c2}$) as a function of interchain coupling strength $\eta_0$. The large dots are the coincident points of $T_{c1}$ and $T_{c2}$. The re-entrance of the ferromagnetic metal state is shown by the big arrow. The inset shows the temperature dependence of the energy gap. The line is the theoretical result, while the dots are experimental data from [31]. See the text for details of the parameters.

We then systematically studied the effect of the e–orb coupling on the Peierls phase transition and found that large $r$ increases $T_{c1}$ and decreases, meanwhile, $T_{c2}$. As a consequence, strong e–orb coupling will enlarge the phase area of the FMI state in figure 2. Sufficient strong e–orb coupling will annihilate the re-entrance of the FMM state by decreasing $T_{c2}$ to zero (the figure is not shown). That confirms the orbital order being in favor of the Peierls insulating phase. Please note that the Peierls instability cannot take place without the orbital order-induced quasi-1D confinement in La$_{7/8}$Sr$_{1/8}$MnO$_3$.

With our theory, we can also explain the other experimental features listed in the introduction at the qualitative level. The Peierls instability opens an energy gap (see equation (16)) and makes La$_{7/8}$Sr$_{1/8}$MnO$_3$ undergo a metal–insulator transition at $T_{OO}$. As a consequence, the charge carriers transport only through the localized gap states at $T < T_{OO}$, which will trigger the variable range hopping (VRH) [32]. That picture is confirmed by the good fit of the experimental $\rho$–$T$ curve [7, 12] with the VRH mechanism: $\rho = \rho_0 \exp(\sqrt{T_0/T})$ in figure 3. The exponent 1/2 results from a parabola density of states (DOS) with zero DOS at the Fermi level $E_F$ (called Coulomb gap). As regards the giant phonon softening of the Mn–O breathing mode [15], we comment that it results from the celebrated giant Kohn anomaly at Peierls instability, i.e. the suppression of phonon frequency at $p \sim 2k_F$ [33].

4. Summary

In summary, we have demonstrated that the FMI state of La$_{1-x}$Sr$_x$MnO$_3$ originates from the electron–phonon coupling-induced Peierls instability when the orbital order confines holes to move along quasi-1D pathways. With this picture, the re-entrance of the FMM state has
Figure 3. The fits of the experimental measurements of $\rho$ by $\rho = \rho_0 \exp(T_0/T)^{1/2}$. The experimental data are from [12] ($x = 0.125$) and [7] (for others).

been well explained quantitatively. The other experimental features of the FMI state, such as the temperature dependence of resistivity and the giant phonon softening, have also been understood at the qualitative level. Our theory supports the belief that the intercoupling of hole–orbital–phonon is critical in understanding the electronic properties of doped manganites.

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