I. INTRODUCTION

Perovskite materials are quite ubiquitous and exhibit a variety of interesting and intriguing phenomena such as superconductivity or charge ordering (or their coexistence), colossal magnetoresistance, ferroelectricity, spin-dependent transport, and the interplay among magnetic, structural, and transport properties.\(^1\) Many oxides that have the formula \(ABO_3\) assume a perovskite structure where two adjacent \(BO_6\) octahedra share an oxygen which leads to cooperative octahedral distortions. Simple systems that manifest such cooperative electron-phonon phenomena are the barium bismuthates (\(BaBiO_3\)). Here, only the 6\(s\) electrons are involved in transport and these electrons produce only a single normal mode distortion, namely, the breathing mode. In pure \(BaBiO_3\), the \(BO_6\) octahedra alternately dilate and contract with Bi-O bonds of adjacent octahedra differing by about 10\% which is indicative of strong electron-phonon interaction (EPI).\(^1\)

Thus the relevant physics is dominated by a one-band three-dimensional cooperative breathing-mode (CBM) system. There is also compelling evidence of strong EPI in manganites (from extended x-ray absorption fine structure\(^6\) and pulsed neutron diffraction\(^5\) measurements) and in cuprates (through angle-resolved photoemission spectroscopy).\(^6\)

In copper oxides, as pointed out in Refs. \(7\) and \(8\), the dynamics of the Zhang-Rice singlet can be described by a one-band system with orbitals centered on copper sites. Furthermore, the on-site energy is modulated by the movement of oxygen closer or further from the neighboring copper ion. Thus the breathing mode is relevant to describe the linear modulation of the on-site energy. Consequently the copper-oxygen planes represent a one-band two-dimensional CBM system.

In the context of the two-band Jahn-Teller manganite systems as well, when C-type antiferromagnetism manifests as in \(La_{1-x},Sr_xMnO_3\) for 0.65 \(\leq x \leq 0.9\) (Ref. \(10\)), the \(d_{z^2}\) orbitals participate in the C-chain ordering. A ferromagnetic C chain can be looked upon as a one-band (i.e., \(d_{z^2}\) orbital band) and one-dimensional (1D) CBM system that is however Jahn-Teller coupled to neighboring C chains whose spin alignment is antiparallel.

Using a controlled analytic nonperturbative treatment that accounts for the quantum nature of the phonons, we derive a model that generically describes the cooperative breathing-mode at strong electron-phonon interaction in one-band one-dimensional systems. The effective model involves a next-nearest-neighbor hopping (that dominates over the nearest-neighbor hopping at strong coupling) and a nearest-neighbor repulsion that is significantly enhanced due to incompatibility of neighboring dilations/compressions. At non-half-filling, upon tuning the electron-phonon coupling, the system undergoes a period-doubling second-order quantum phase transition from a Luttinger liquid to a conducting commensurate charge-density-wave state: a phenomenon absent in both the Holstein model and the \(t-V\) model. Using fidelity to study the nature of the quantum phase transition, we find that the fidelity susceptibility shows a superextensive power law divergence as well as a remarkable scaling behavior; both together establish a second-order transition.

Understanding the CBM phenomena in systems such as the bismuthates, the cuprates, and the manganites is still an open question. The main purpose of this paper is to study the CBM physics in the simpler case of a one-band 1D system by taking account of the quantum phonons [see Fig. \(1(b)\)]. In fact, a controlled analytic treatment of the many-polaron effects produced by quantum phonons in a one-band 1D Holstein model [see Fig. \(1(a)\)]\(^{11}\) (which is a simpler noncooperative EPI system) has been reported not long ago.\(^{12,13}\) However, definite progress has been made in numerically treating the Holstein model at half filling (by employing a variety of techniques)\(^{14-19}\) and, to a limited extent, away from half filling.\(^{20}\)

Owing to its cooperative nature, the EPI leads to nonlocal distortion effects which can change the very nature of long-range order. While a weak interaction is amenable to a Migdal-type of perturbative treatment, the strong interaction (even for a one-band system) necessitates a nonperturbative approach.\(^12\) As a step towards modeling CBM distortions in real systems (such as the bismuthates, the cuprates, and the manganites), the present work builds on our previous work on the Holstein model\(^{11}\) to obtain the effective Hamiltonian for a one-band 1D CBM system.\(^{21-23}\) Upon inclusion of cooperative effects in the strong EPI, we show that the system changes its dominant transport mechanism from one of nearest-neighbor (NN) hopping to that of next-nearest-neighbor (NNN) hopping while the effective NN electron-electron interaction becomes significantly more repulsive due to incompatibility of NN breathing-mode distortions. Away from half filling in rings with an even number of sites (while the Holstein system without cooperative effects remains a Luttinger liquid at all interaction strengths), our model (at strong interaction) produces a commensurate charge-density-wave (CDW) state which is surprisingly conducting and whose period is independent of density. Furthermore, using scaling of the fidelity susceptibility (FS), we demonstrate that the CDW transition is a second-order quantum phase transition (QPT).

The paper is organized as follows. We derive an effective polaronic Hamiltonian starting from a CBM model in Sec. II. Next, we present the relevant formulas for the density-density
correlation function and the structure factor in Sec. III. We then analyze the strong-coupling limiting case of our CBM model in Sec. IV. The nature of the QPT and the long-range order in our CBM model are discussed in Sec. V. Finally, we close in Sec. VI with our conclusions.

II. EFFECTIVE POLARONIC HAMILTONIAN

To bring out the essential physics, we begin with a 1D model of spinless electrons hopping in a one-band system of $d_{z^2}$ orbitals which are coupled to the oxygens in between, via CBM as shown in Fig. 1(b). The Hamiltonian is expressed as $H = H_i + H_{ep} + H_1$ where the hopping term $H_i$, using standard notation, is given by

$$H_i = -t \sum_j (c_j^\dagger c_{j+1} + \text{H.c.}),$$

(1)

with $c_j$ ($c_j^\dagger$) being the destruction (creation) operator of an electron in a $d_{z^2}$ orbital at site $j$. The EPI term $H_{ep}$ is expressed as

$$H_{ep} = -g \omega_0 \sqrt{2M} \omega_0 \sum_j n_j q_j,$$

(2)

where $g$ is the electron-phonon coupling (EPC), $n_j = c_j^\dagger c_j$, $q_j = u_j - u_{j-1}$ represents the expansion of the oxygens around the $d_{z^2}$ orbital, and the right-hand side oxygen displacement $u_j = (a_j^\dagger + a_j) / \sqrt{2M} \omega_0$. Furthermore, the lattice term $H_1$ representing simple harmonic oscillators is of the form

$$H_1 = \frac{K}{2} \sum_j u_j^2 + \frac{1}{M} \sum_j p_j^2 = \omega_0 \sum_j a_j^\dagger a_j.$$

(3)

The main difference between the Holstein model and the above cooperative Hamiltonian is that in the Holstein model electrons at different sites are coupled to different on-site molecular distortions whereas in the present system the electrons on adjacent sites are coupled to the displacement of the same in-between oxygen. Thus in our system, to produce an effective polaronic Hamiltonian, we need to devise a modification of the usual Lang-Firsov transformation so as to take into account the cooperative nature of the distortions. To meet this end, we used the following canonical transformation $\hat{H} = \exp(S)H \exp(-S)$ where $S$ now contains the difference in densities on adjacent sites

$$S = g \sum_j (a_j - a_j^\dagger)(n_j - n_{j+1}).$$

(4)

Then, one obtains $\hat{H} = H_0 + H_1$ where

$$H_0 = \omega_0 \sum_j a_j^\dagger a_j - 2g^2 \omega_0 \sum_j n_j + 2g^2 \omega_0 \sum_j n_j n_{j+1}$$

$$-t e^{-3\rho} \sum_j (c_j^\dagger c_{j+1} + \text{H.c.})$$

(5)

and

$$H_1 = \sum_j H_{1j} = -t e^{-3\rho} \sum_j (c_j^\dagger \{T_{j+1}^\dagger T_j - 1\} + \text{H.c.}),$$

with $T_{j+1}^\dagger = \exp[\pm g(2a_j - a_{j-1} - a_{j+1})]$. On account of the cooperative nature of the EPI we obtain an additional term $2g^2 \omega_0 \sum n_j n_{j+1}$ involving NN repulsion in $H_0$ and the perturbation $H_1$ now involves phonons at three sites as opposed to phonons at only two sites as in the noncooperative case. We consider the case $t \exp[-3\rho] \ll \omega_0$ and perform second-order perturbation theory similar to that in Refs. 12 and 25. The eigenstates of $H_0$ relevant for perturbation theory are $|n,m\rangle = |n\rangle_{el} \otimes |m\rangle_{ph}$ where NN occupied electronic states are projected out and $|0,0\rangle$ is the ground state (GS) with no phonons. The corresponding eigenenergies are $E_{n,m} = E_{n,el} + E_{m,ph}$. The treatment to perform second-order perturbation theory is an extension of the method followed in Refs. 12 and 25 and yields the following effective Hamiltonian for polaronic:

$$H^{(2)} = \sum_{i,j} \sum_m \langle 0|_{el} H_{ii} |m\rangle_{el} \langle m|_{ph} H_{ij} |0\rangle_{ph} E_{m,ph} - E_{n,el}.$$

(6)

Here (as shown by using Schrieffer-Wolff transformation in Appendix A of Refs. 25 and 26), it must be mentioned that when $t \exp[-3\rho] \ll \omega_0$, $H_0 + H^{(2)}$ represents the exact Hamiltonian up to second order in perturbation (even for finite antiadiabatic values $t/\omega_0 \lesssim 1$), the small parameter $|t/(g\omega_0)|$ of the perturbation will be derived below. In the above equation (6), unlike in Ref. 12, the term $H_1$ produces phonons at sites $j, j - 1$, and $j + 1$. Hence, we get nonzero contributions only when the index $i = j - 2, j - 1, j + 1$, or $j + 2$. Then after some tedious algebra one obtains

$$-H^{(2)} = \frac{\omega_0}{12 e^{-6\rho}}$$

$$= \sum_j \sum_{n_j = 1} \{n_j(1 - n_{j+1}) + (1 - n_j)n_{j+1}\} F_2(4,1,1)$$

$$+ 2 F_2(4,1) + F_1(4) + 2 F_1(1) + F_2(1,1)$$

$$+ \{c_{j+1}^\dagger (1 - 2n_j)c_{j+1} + \text{H.c.}\} [2 F_2(1) + F_2(2,2)]$$

$$+ \{c_{j-1}^\dagger (1 - 2n_{j-1})c_{j-1} + \text{H.c.}\} F_1(1)$$

$$+ \{2c_{j-1}^\dagger c_{j-1}^\dagger c_{j+1} + \text{H.c.}\} F_1(-1)$$

(7)

where

$$F_n(\alpha_1, \ldots, \alpha_n) = \sum_{m_1 = 0}^{\infty} \ldots \sum_{m_n = 0}^{\infty} \frac{(\alpha_1 g^2)^{m_1} \ldots (\alpha_n g^2)^{m_n}}{m_1! \ldots m_n!(m_1 + \ldots + m_n)}.$$


which for large values of $g^2$ becomes $F_{n} \approx \exp(g^2 \sum_{i=1}^{n} \alpha_i)/(g^2 \sum_{i=1}^{n} \alpha_i)$ for $\sum_{i=1}^{n} \alpha_i \geq 1$. In the above Eq. (7), the last two terms are a direct consequence of the cooperative nature of the EPI and are negligible for large $g^2$. More importantly, the relative importance of the various coefficients is noticeably different from the case where no cooperative effect exists (as explained below). For large $g^2$, the effective polaronic Hamiltonian simplifies to be

$$H_{\text{eff}} = -\left[2g^2\omega_0 + \frac{t^2}{4g^2\omega_0}\right] \sum_{j} n_{j+1}(1-n_j) - t e^{-3g^2} \sum_{j}(c_j^\dagger c_{j+1} + \text{H.c.}) - t^2 e^{-2g^2} \sum_{j}(c_{j-1}^\dagger(1-2n_j)c_{j+1} + \text{H.c.}).$$  

Notice that the coefficient of the NN hopping is significantly smaller than the coefficient of the NNN hopping for large $g^2$ and not-too-small $t/\omega_0$. This is a key feature resulting from cooperative effects. The above effective Hamiltonian may be contrasted with the following Hamiltonian $H_{\text{eff}}$ for the case where there is no cooperative EPI [i.e., $H_{\text{eff}} = -\sqrt{2}g\omega_0 \sum_{j} n_{j}(a_j^\dagger + a_j)$] [see Ref. 12 and Fig. 1(a)]:

$$H_{\text{eff}} = -2g^2\omega_0 \sum_{j} n_{j} - \frac{t^2}{2g^2\omega_0} \sum_{j} n_{j+1}(1-n_j) - t e^{-3g^2} \sum_{j}(c_j^\dagger c_{j+1} + \text{H.c.}) - t^2 e^{-2g^2} \sum_{j}(c_{j-1}^\dagger(1-2n_j)c_{j+1} + \text{H.c.}).$$  

We now provide an explanation of the above results. In Eq. (9), the coefficient of the $\sum_{j} n_{j+1}(1-n_j)$ term can be understood as resulting from a hopping process where an electron at site $j+1$ hops to a neighboring site $j$ back, but the lattice has no time to distort/relax locally at site $j$ ($j+1$) and thus yields the second-order perturbation energy $-t^2/\text{(energy change)}$ (see Fig. 2 of Ref. 25). On the other hand, the coefficient of $\sum_{j} n_{j+1}(1-n_j) c_{j+1}$ results when, in the intermediate state, site $j$ does not distort/relax during hopping and thus yields $t \exp(-2g^2)/(t/2g^2\omega_0)$ where $t \exp(-2g^2)$ is due to time ($\hbar/t e^{-2g^2}$) taken to distort the site $j+1$ (see Fig. 2 of Ref. 25). In the above noncooperative case, the NN hopping dominates over the NNN hopping in the small polaron limit.

Using the above logic we see that the higher order terms in perturbation theory, for both cooperative and noncooperative cases, are dominated by the process where an electron hops back and forth between the same two sites. The dominant term to $k$th order is approximately given for even $k$ by

$$\omega_0 \left[\frac{t}{g\omega_0}\right]^k \sum_{j} n_{j+1}(1-n_j),$$  

while for odd $k$ by

$$t e^{-g^2} \left[\frac{t}{g\omega_0}\right]^k \sum_{j} (c_j^\dagger c_{j+1} + \text{H.c.}).$$  

where $\gamma$ is 2 for the noncooperative case and 3 for the cooperative one. Since each term in the perturbation theory should be smaller than $\omega_0$, we see that the small parameter in our perturbation theory is $t/(g\omega_0)$.13

Here, a few observations are in order. First, the cooperative effects, unlike in the Holstein model’s case, raise the potential of the site next to an occupied site and thus make it unfavorable for hopping. Consequently, in Eq. (8) as compared to Eq. (9), the exponent is larger for the NN hopping and also the denominators of the coefficients are similarly larger for the hopping-generated NN interaction and for the NNN hopping. Next, Lau et al.7 obtain the same energy expression for a single polaron as that given by Eq. (8) (when $n_j = 0$). Additionally, in Ref. 27, the authors explain the ferromagnetic insulating behavior in low-doped manganites by using the noncooperative hopping-generated NN interaction [i.e., second term on the right-hand side of Eq. (9)] after modifying the hopping term for double-exchange effects. From Eq. (8), we see that cooperative phenomenon must be taken into account as it reduces the ferromagnetism generating interaction strength by a factor of 1.5. Lastly, the authors of Refs. 28 and 29 study the formation of bipolarons using Fröhlich polarons with spin degrees of freedom; although they use a Lang-Firsov transformation followed by a Schrieffer-Wolff transformation (which is similar to our type of perturbation theory), they nevertheless do not consider the dominant NNN hopping effects which are central to our treatment.

In the next few sections, we will analyze the effective polaronic Hamiltonian given by Eq. (8) and show that there is a period-doubling QPT from a Luttinger liquid to a conducting CDW when the coupling $g$ increases at fixed adiabaticity $t/\omega_0$. The transition is a consequence of enhanced NNN hopping and pronounced NN repulsion. We employ a modified Lanczos algorithm30 [and use antiperiodic (periodic) boundary conditions for even (odd) number of fermions] to study the QPT in the system. In all our numerical calculations involving the effective polaronic Hamiltonian, we used the series $F_n(\alpha_1, \ldots, \alpha_n)$ given in Eq. (7) and not the approximate coefficients in Eq. (8).

III. DENSITY-DENSITY CORRELATION FUNCTION AND STRUCTURE FACTOR

In this section, to characterize correlations and analyze QPT, we present the relevant formulae for the density-density correlation function and the structure factor. The two-point correlation function for density fluctuations of electrons at a distance $l$ apart is given by

$$W(l) = \frac{4}{N} \sum_j [\langle n_j n_{j+l} \rangle - \langle n_j \rangle \langle n_{j+l} \rangle],$$  

with filling fraction (FF) $\langle n_j \rangle = \frac{N}{N_p}$ where $N$ is the total number of sites and $N_p$ is the total number of electrons in the system. Then the structure factor, which is the Fourier
transform of $W(l)$, is given by

$$S(k) = \sum_{l} e^{ikl} W(l),$$  

(13)

where wave vector $k = \frac{2n\pi}{N}$ with $n = 1, 2, \ldots, N$. Now, we observe that

$$S(\pi) = \left( \sum_{l_{\text{even}}} - \sum_{l_{\text{odd}}} \right) W(l),$$

with

$$\sum_{l_{\text{even}}} W(l) = \frac{2((\hat{N}_e - \hat{N}_o)^2)}{N},$$

and

$$\sum_{l_{\text{odd}}} W(l) = -\frac{2((\hat{N}_e - \hat{N}_o)^2)}{N},$$

where $\hat{N}_e = \sum_{l_{\text{even}}} n_j$ and $\hat{N}_o = \sum_{l_{\text{odd}}} n_j$ is the number operator which gives the total number of electrons at even (odd) sites. Hence, we obtain the simple expression

$$S(\pi) = \frac{4((\hat{N}_e - \hat{N}_o)^2)}{N}.$$  

(14)

We will now analyze the situation where only one sublattice is occupied and obtain some exact results. When we consider odd values of $l$, we note that

$$\langle n_j n_{j+1} \rangle = 0.$$  

Hence, from Eq. (12) we get

$$W(l_{\text{odd}}) = -\frac{4N_p^2}{N^2}.$$  

(15)

Next, we observe that the GS becomes an eigenstate of the operators $\hat{N}_e$ and $\hat{N}_o$ with the eigenvalues $N_p$ (0) and 0 ($N_p$) respectively if the even-site (odd-site) sublattice is occupied. Consequently, we get

$$[S(\pi)]_\text{max} = \frac{4N_p^2}{N},$$  

(16)

where $[S(\pi)]_\text{max}$ is the maximum value that $S(\pi)$ can attain.

To analyze the QPTs, we can treat the rescaled value of $S(\pi)$ as the order parameter $S^*(\pi)$ defined as follows:

$$S^*(\pi) = \frac{S(\pi) - [S(\pi)]_\text{min}}{[S(\pi)]_\text{max} - [S(\pi)]_\text{min}},$$  

(17)

where $[S(\pi)]_\text{min}$ is the minimum value of $S(\pi)$; consequently, $S^*(\pi)$ varies from 0 to 1 during the phase transition.

In the next section, we will study the limiting case of large EPC values where the NNN hopping is the only relevant transport mechanism in the CBM model leading to the $t_2$-$V$ model [see Eq. (19)].

IV. ANALYSIS OF THE $t_2$-$V$ MODEL—A LIMITING CASE OF THE CBM MODEL

The effective Hamiltonian for the CBM model contains three terms, namely, NN hopping, NNN hopping, and NN repulsion [as can be seen from Eq. (8)]. There are two possible extreme cases of the CBM model corresponding to small and large values of the EPC $g$. For small values of $g$ ($\sim 1$), NN hopping dominates over NNN hopping; consequently, Eq. (8) reduces to

$$H_{t_2} \equiv -t \sum_{j} (c_{j}^\dagger c_{j+1} + \text{H.c.}) + V \sum_{j} n_j n_{j+1},$$  

(18)

which is the well-studied $t$-$V$ model with $t/V \ll 1$ at the small values of $g$ ($\sim 1$) considered.

On the other hand, for large values of $g$, NNN hopping dominates over NN hopping and Eq. (8) can be simplified to

$$H_{t_2} \equiv -t_2 \sum_{j} [c_{j-1}^\dagger (1 - 2n_j) c_{j+1} + \text{H.c.}] + V \sum_{j} n_j n_{j+1},$$  

(19)

which we shall call the $t_2$-$V$ model; here, since EPC is large (i.e., $g \gtrsim 3$), $t_2/V \ll 1$. However, owing to the novelty of the model, we shall study it [i.e., Eq. (19)] for arbitrary values of $t_2/V$ in rings with even number of sites. Next, for $t_2/V \ll 1$, we note that the system always has alternate sites (i.e., one sublattice) occupied for less than half filling and above half filling the other sublattice gets filled. This can be explained, for less than half filling, as follows. At large repulsion, we shall compare the energy for the following two situations:

1. When there are $m_A > 0$ ($m_B > 0$) electrons in sublattice A (B).
2. When all the $m_A + m_B = N_p$ electrons are in one sublattice only.

In case 1, each electron in sublattice B has $m_B - 1$ sites blocked in B by other electrons in B and at least [at most] $m_A + 1$ ($2m_A$) sites blocked in B by electrons in sublattice A; one can similarly argue for the electrons in sublattice A. Thus in sublattice B(A), each electron can hop to at most $\frac{N}{2} - m_{A(B)} - m_{B(A)}$ unblocked sites and at least $\frac{N}{2} - 2m_{A(B)} - m_{B(A)} + 1$ unblocked sites.

In case 2, each electron has $m_A + m_B - 1$ sites blocked by the other electrons in the same sublattice. Hence, each electron has exactly $\frac{N}{2} - m_A - m_B + 1$ unblocked sites to hop to. At large repulsion, since case 2 gives electrons more number of unblocked sites to hop to, we see that the total energy is the lowest when all the electrons are present in the same sublattice. As for the other extreme situation $V = 0$, for an even number of electrons, the model has both sublattices equally occupied.

In the $t_2$-$V$ model, the ground-state energy has a slope discontinuity, with the energy increasing up to a critical value, after which it is constant for FFs $\frac{1}{3}$, $\frac{1}{3}$, and $\frac{1}{3}$ [as shown in Fig. 2(a)]. We will now show clearly that as the interaction strength increases, at a critical value of $V/t_2$, using $Z_3$ symmetry (i.e., both sublattices being equally populated) is broken and only a single sublattice is occupied. As depicted in Fig. 2(b), the structure factor $S(\pi)$ jumps from zero to its maximum value [given by Eq. (16) for FFs $\frac{1}{3}$, $\frac{1}{3}$, and $\frac{1}{3}$] indicating explosive first-order QPT from a Luttinger liquid to a CDW.

Next, we observe that the number of electrons in even and odd sublattices are conserved quantities for the $t_2$-$V$ model.
Therefore, the GS of the system is an eigenstate of both $\hat{N}_e$ and $\hat{N}_o$ with eigenvalues $N_e$ and $N_o$, respectively. Hence, Eq. (14) simplifies to

$$S(\pi) = \frac{4(N_e - N_o)^2}{N}.$$  \hspace{1cm} (20)

Then, when $Z_2$ symmetry is respected, for an even number of electrons $N_p = 2N_e = 2N_o$, we have $S(\pi) = 0$ and for an odd value of $N_p$ we have $S(\pi) = 4/N$. We find that at a critical interaction strength, as shown in Fig. 3, the following dramatic changes occur: (i) the structure factor $S(\pi)$ jumps from 0 to its maximum value $4N_p^2/N$; (ii) $W(l)$ odd also jumps to its large $V$ value of $-4N_p^2/N^2$; and (iii) $W(l)$ even (for $l \neq 0$) too jumps and its final value at half filling is 1. For a fixed $t_2$ and $N$, the critical value $V_C^2$ of $V$ increases monotonically as $N_p$ decreases. For $N = 16, N_p = 2$, and $t_1 = 1$, we get $V_C^2 \approx 4$. From finite-size scaling for half filling, using $V_C^N - V_C^\infty \propto 1/N^2$ and system size $N \leq 20$, we obtain $V_C^\infty \approx 2.83$.

We see from the above analysis that at a critical repulsion, the system undergoes a discontinuous transition to a conducting commensurate CDW state away from half filling while at half filling one obtains a Mott insulator. Usually commensurate CDWs are insulating (see Ref. 32) whereas our model surprisingly predicts a conducting commensurate CDW. Furthermore, quite unlike the Peierls transition, the period of the CDW is independent of density.

V. ANALYSIS OF THE CBM MODEL

To analyze the QPT at various FFs of a system governed by the effective polaronic Hamiltonian given in Eq. (8), we performed our calculations at values of the adiabaticity $t/\omega_0 < 1$ and $g \geq 1$ such that the small parameter $t/(g\omega_0) < 1$ and $\text{te}^{-3\gamma} \ll \omega_0$. Here we report only for the conservative case $t/\omega_0 = 0.1$ since the results at other values of $t/\omega_0 < 1$ are qualitatively similar (as shown in Appendix A).

As the value of $g$ increases (in the regime of study $1 \leq g \leq 3.5$), NN and NNN hoppings compete and the system gradually transits from a large-$V$ $t$-$V$ model to a large-$V$ $t_2$-$V$ model; thus, at values of $g \sim 1$ we expect the system to be a Luttinger liquid while at $g \sim 3$ we should get a CDW. In the next subsections we will demonstrate that the system indeed undergoes a Luttinger liquid to a conducting CDW transition with the QPT being second order in nature. The QPT discussed in this work is quite different from the metallic Luttinger liquid to insulating CDW transition studied by many authors\textsuperscript{33-35} in a system with only NN hopping and long-range Coulomb interaction.

A. Study of density-density correlation function, structure factor, and order parameter

First, we calculated $W(l)$ and $S(k)$ at FFs $\frac{1}{4}$ and $\frac{1}{2}$ numerically and the results are displayed in Fig. 4. Upon tuning the EPC $g$, the density-density correlation function $W(l)$ gradually changes its nature from decaying to oscillatory thereby exhibiting long-range order; it then attains the value given by Eq. (15) at all odd values of $l$ corresponding to the state of only one sublattice being occupied [see Figs. 4(a) and 4(c)]. Furthermore, the structure factor value $S(\pi)$ increases upon increasing $g$ and attains the maximum value given by Eq. (16) [see Figs. 4(b) and 4(d)]. These observations assert...
that the system undergoes QPT from a Luttinger liquid to a conducting commensurate CDW state away from half filling with period doubling. Thus, at a critical value of $g$, the Ising $Z_2$ symmetry (i.e., both sublattices being equally populated) is broken. Quite surprisingly, our model predicts a conducting commensurate CDW state away from half filling and $N = 16$, and $N = 18$ in our CBM model and the Holstein model.

We will now compare $S(\pi)$ versus $g$ behavior manifested by our model and the Holstein model in Fig. 5. We see that while our CBM model appears to undergo a QPT, the Holstein model does not seem to do so. We observe that the coefficient of NNN hopping for the Holstein model [see Eq. (9)] becomes much smaller than that of the NN hopping as $EPC$ increases. Hence, the Holstein model, for sufficiently larger values of $g$, behaves like the $t$-$V$ model, whereas our model can be approximated by the $t_2$-$V$ model at large $g$. We know that the $t$-$V$ model does not undergo a QPT away from half filling.\(^{31}\) Therefore, the Holstein model too will not undergo a QPT at a non-half-FF (which is consistent with the results of Ref. 12). Thus, the $Z_2$ symmetry breaking QPT (at non-half-filling) in our model is a unique feature which has no analog in either the Holstein model or the $t$-$V$ model. Furthermore, at half filling, the $t$-$V$ model undergoes a QPT when $V = 2t^{30,31}$ while the Holstein model suffers a QPT at $g > 1^{12,19}$ on the other hand our CBM model, for the range of $EPC$ considered (i.e., $g \geq 1$), is always deep inside the CDW phase since the coefficient of NN repulsion is much larger than the hopping terms.

Plots of the order parameter $S^*(\pi)$ displayed in Fig. 6 also reveal signatures of QPT at FFs $\frac{1}{2}$ and $\frac{3}{4}$ and at different system sizes. Moreover, we observe that the increase in $S^*(\pi)$ becomes sharper as the system size increases. From the figures it appears that there is either a continuous or weakly first order QPT for both the FFs.

**B. Ground-state fidelity; fidelity susceptibility and its scaling behavior**

Although the order parameter $S^*(\pi)$ depicts a QPT, the nature of the transition (whether it is first order, second order, or KT-like) is not clear. Therefore, we take recourse to the study of the ground-state fidelity (GSF) and FS to characterize the nature of the QPT. The GSF is defined as the overlap between GSs at two different but near values of the control parameter (say $g$ and $g + \delta$) as follows:

$$F(g, \delta) = |\langle \Psi_0(g) | \Psi_0(g + \delta) \rangle|,$$  \hspace{1cm} (21)

where $|\Psi_0\rangle$ is the GS of the system and $\delta$ is a small quantity.\(^{36}\) It is clear from Eq. (21) that $F(g, \delta)$ depends on $\delta$. On the other hand, the FS,\(^{37}\) defined below as the second derivative of GSF,

$$\chi_F(g) = \left[ \frac{\partial^2}{\partial g^2} F(g, \delta) \right]_{\delta=0} = 2 \lim_{\delta \to 0} \frac{1 - F(g, \delta)}{\delta^2},$$  \hspace{1cm} (22)

is independent of $\delta$.

The GS of the system, after transition, becomes twofold degenerate as either of the two sublattices, namely even and odd, can have the larger occupancy. Now, any linear superposition of the two degenerate states is also a GS. Therefore, the calculated GSF [i.e., the absolute value of the overlap of GS $|\Psi_0\rangle$ at two close by values of the control parameter ($g$ and $g + \delta$)] becomes arbitrary. To eliminate arbitrariness in the estimate of GSF, we start with $\Psi_0(g)$ as our initial guess in the modified Lanczos algorithm to get the GS $\Psi_0(g + \delta)$.

Next, we point out a mapping that will enable us to perform fidelity calculations in systems with sizes larger than the usual sizes accessible to the modified Lanczos technique. At $N_p/N$ filling in our CBM model, when NN repulsion is much larger than both the NN and the NNN hoppings, our model can be reduced to the following model at $N_p/(N - N_p)$ filling but without NN repulsion (for similar analyses, see the treatment of the $t$-$V$ model in Ref. 38 and the mapping of the $t$-$V_1$-$V_2$ model in Ref. 26):

$$H_{\text{eff}}^{RC} = -t e^{-3g^2} \sum_j (c_j^\dagger c_{j+1} + \text{H.c.})$$

$$- \frac{t^2 e^{-2g^2}}{4g^2\omega_0} \sum_j [c_{j-1}^\dagger (1 - n_j) c_{j+1} + \text{H.c.}],$$  \hspace{1cm} (23)
Hamiltonian contains only kinetic terms. Hence, the GS in the FFs we consider the following scaling relation

\[ \chi_F(g) \propto N^{\gamma} \]  

The logarithmic scale plot of the peak FS value \( \chi_{F_{\text{max}}}(N) \) with \( N \) shows a linear behavior [see Fig. 8(e)] which confirms a power-law divergence of \( \chi_{F_{\text{max}}}(N) \) at the extremum point \( g_{\text{max}} \).

At large \( N \), we obtain \( \chi_{F_{\text{max}}}(N) \sim N^{2.601} \) at \( \frac{1}{3} \) filling, whereas at \( \frac{1}{4} \) filling we get \( \chi_{F_{\text{max}}}(N) \sim N^{1.868} \). The superextensive power law divergence of \( \chi_{F_{\text{max}}} \) along with the dynamical critical exponent value \( z \sim 1 \) rules out a KT-like transition (see Appendix B for details).

In order to examine the possibility of a second-order QPT, we consider the following scaling relation\(^{39,40} \) for \( \chi_F(g) \):

\[ \frac{\chi_{F_{\text{max}}}(N) - \chi_F(g,N)}{\chi_F(g,N)} = f[N^{1/\nu}(g - g_{\text{max}})], \]  

where \( \nu \) is the critical exponent of the correlation length. Interestingly, a plot of \( [\chi_{F_{\text{max}}}(N) - \chi_F(g,N)]/\chi_F(g,N) \) versus \( N^{1/\nu}(g - g_{\text{max}}) \), as depicted in Fig. 9, shows a nice scaling relation of \( \chi_F(g,N) \) with \( \nu \) taking the values 1.33 ± 0.01 and 1.41 ± 0.01 for the best fits to the universal curves at FFs \( \frac{1}{3} \) and \( \frac{1}{4} \) respectively. The superextensive power law divergence and the scaling behavior of \( \chi_F \) demonstrate that the QPT is second order in nature.

Furthermore, as pointed out in Refs. 39 and 40, average FS \( \chi_F(g,N) \) around the critical point \( g_c \) scale like

\[ \frac{\chi_F(g)}{N} \propto \frac{1}{|g_c - g|^\alpha}. \]  

in the thermodynamic limit, with \( \alpha \) being a critical exponent. The three exponents \( \alpha, \mu, \) and \( \nu \) are related as\(^{39,40} \)

\[ \alpha = \nu(\mu - 1). \]  

FIG. 7. (Color online) GSF \( F(g,\delta) \) in the CBM model at \( \frac{\omega}{\mu_0} = 0.1 \) for (a) \( \frac{1}{3} \) filling and \( N = 32 \), and (c) \( \frac{1}{4} \) filling and \( N = 30 \). FS \( \chi_F(g) \) for (b) \( \frac{1}{3} \) filling and (d) \( \frac{1}{4} \) filling correspond to the GSF plots in (a) and (c), respectively. For the sake of clarity, only selected points are shown for \( \delta = 0.02 \).

FIG. 8. (Color online) GSF \( F(g,\delta) \) in the CBM model at \( \frac{\omega}{\mu_0} = 0.1 \) and \( \delta = 0.05 \) for (a) \( \frac{1}{3} \) filling and (c) \( \frac{1}{4} \) filling. FS \( \chi_F(g) \) for (b) \( \frac{1}{3} \) filling and (d) \( \frac{1}{4} \) filling correspond to the GSF plots in (a) and (c). (e) Plot of the peak values of FS \( \chi_{F_{\text{max}}}(N) \) versus \( N \), on a logarithmic scale, at \( \frac{1}{3} \) filling and \( \frac{1}{4} \) filling and the corresponding power-law fits.

FIG. 9. (Color online) Scaling behavior of FS \( \chi_F(g,N) \) in the CBM model at \( \frac{\omega}{\mu_0} = 0.1 \) and for (a) \( \frac{1}{3} \) filling yielding \( \nu = 1.33 \pm 0.01 \) and for (b) \( \frac{1}{4} \) filling producing \( \nu = 1.41 \pm 0.01 \).
The values of the critical exponent $\alpha$, on using Eq. (27), turn out to be $\alpha \simeq 1.33$ and $\alpha \simeq 1.22$ for FFs $\frac{1}{4}$ and $\frac{3}{4}$, respectively. On using finite size scaling, we find the critical point $g_c$ values to be 2.785 and 2.594 for FFs $\frac{1}{4}$ and $\frac{3}{4}$, respectively [based on positions of dips (peaks) of GSF (FS) in Fig. 8].

VI. CONCLUSIONS

We derived an effective Hamiltonian for molecular chains involving CBM at strong EPI. The spinless fermion model considered here should be relevant to perovskite systems with large on-site Coulomb repulsion. Our analysis shows that our system has an effective Hamiltonian of the form

$$H_{t-V} = -t \sum_j (c_j^\dagger c_{j+1} + H.c.) - t_2 \sum_j [c_j^\dagger(1 - 2n_j)c_{j+1} + H.c.] + V \sum_j n_jn_{j+1},$$

with $t_2 \ll t$ for small $g$ ($\sim 1$), whereas $t_2 \gg t$ for large $g$ ($\gtrsim 3$); furthermore $V$ is significantly larger than both $t$ and $t_2$ for all values of EPC ($1 \leq g \leq 3.5$) considered. Thus, NN and NNN hoppings compete and the system transits from a large-$g$ $t-V$ model (with a Luttinger liquid GS) to a large-$V$ $t_2-V$ model (with a period-doubling CDW GS) as $g$ increases; our fidelity analysis shows that the QPT is second order in nature. In the past, a density-independent charge ordering has indeed been observed in manganite systems (see Fig. 2 in Ref. 41). However, since the dimensionality and number of bands are different, our findings are not directly related to these reported results. Although the reported calculations were performed for a conservative value of the adiabaticity $t/\omega_0 = 0.1$, we find that our results are qualitatively similar in the whole antiadiabatic regime of $t/\omega_0 < 1$ (as shown in Appendix A). Furthermore, we provide one more model system where the utility of GSF and FS in studying the nature of QPT is clearly demonstrated.

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APPENDIX A

In this Appendix, we study our CBM model at different values of the adiabaticity parameter $\frac{t}{\omega_0}$ and for system size $N = 16$ and FF $\frac{1}{4}$. First, we wish to point out that in the entire antiadiabatic regime, the $Z_2$ symmetry breaking captured by $S(\pi)$ is a novel feature of our CBM model which is not present in the Holstein model; this claim is endorsed by Figs. 5 and 10.

As depicted in Fig. 11, for various values of $\frac{t}{\omega_0}$, the order parameter $S^*(g)$ rises from 0 to 1 when the control parameter $g$ is increased; larger values of $\frac{t}{\omega_0}$ lead to QPT occurring at smaller values of $g$. The GSF $F(g, \delta)$ and the corresponding FS, at different values of $\frac{t}{\omega_0}$, are portrayed in Figs. 12(a) and 12(b), respectively. The dip (peak) in the GSF (FS) occurs at smaller values of $g$ when the adiabaticity $\frac{t}{\omega_0}$ assumes larger values.

From the above analysis, we find that our model exhibits qualitatively similar behavior for all values of the adiabaticity parameter $\frac{t}{\omega_0} \lesssim 1$. Furthermore, we expect similar behavior at other FFs and system sizes as well.

APPENDIX B

In this Appendix, we will describe a new general approach to identify a KT transition. The FS can also be written as

$$\chi_F(g) = \sum_{n \neq 0} \frac{|\langle \Psi_n(g) | H_I | \Psi_0(g) \rangle|^2}{[E_n(g) - E_0(g)]^2},$$

or

$$E_0^{(2)}(g) = \sum_{n \neq 0} \frac{|\langle \Psi_n(g) | H_I | \Psi_0(g) \rangle|^2}{[E_n(g) - E_0(g)]^2}.$$

At the KT-transition point, both the numerator and denominator of Eq. (B2) tend to zero with system size in exactly the same manner; hence no divergence results. At the extremum point, the mass gap typically vanishes with system size as

$$\Delta \equiv E_I(g_{\max}) - E_0(g_{\max}) \sim \frac{1}{N^z},$$

where $z$ is the dynamical critical exponent. Thus, for a KT transition the FS at the extremum point exhibits the following

FIG. 11. (Color online) Order parameter $S^*(\pi)$ in the CBM model at $\frac{1}{4}$ filling, $N = 16$, and for different values of $\frac{t}{\omega_0}$. 035453-8
behave

\[ \chi_{\text{Fmax}} \sim N^z. \]  

However (in contrast to the KT transition), for a first-order or a second-order transition, the numerator of Eq. (B2) (at the extremum point) does not tend to zero as fast as the denominator and hence divergence occurs in the thermodynamic limit. Therefore, the divergence in Eq. (B2) leads to an even stronger power-law divergence in the FS at the extremum point [as can be seen from Eq. (B1)]:

\[ \chi_{\text{Fmax}} \sim N^\mu, \]  

where \( \mu > z \). Now, in Fig. 13, we depict variation of the mass gap \( \Delta(N) \) with \( N \) on a logarithmic scale and observe linear behavior. At large \( N \), we obtain \( \Delta(N) \sim 1/N^{1.007} \) (i.e., \( z = 1.007 \)) at \( 1/4 \) filling while at \( 1/3 \) filling we get \( \Delta(N) \sim 1/N^{0.984} \) (i.e., \( z = 0.984 \)), whereas from Fig. 8(e), we find \( \chi_{\text{Fmax}}(N) \sim N^{2.001} \) (i.e., \( \mu = 2.001 \)) at \( 1/4 \) filling while at \( 1/3 \) filling we get \( \chi_{\text{Fmax}}(N) \sim N^{1.868} \) (i.e., \( \mu = 1.868 \)). Clearly, \( \mu > z \) for both the FFs which rules out the possibility of a KT transition. Hence, the QPT in our model is either first order or second order.

Lastly, we would like to mention that another approach, involving examining the global geometric entanglement, to detect the elusive KT quantum phase transition has been recently reported.22,43

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7. For a numerical investigation of single-polaron properties of the system in Fig. 1(b), see B. Lau, M. Berciu, and G. A. Sawatzky, Phys. Rev. B 76, 174305 (2007).
21. A different type of cooperative electron-phonon interaction effect corresponding to a distance-dependent electron-phonon interaction has been considered for a Fröhlich polaron by A. S. Alexandrov and P. E. Kornilovitch, Phys. Rev. Lett. 82, 807 (1999). Interestingly, their analytic approach (like our method) is also valid for \( t/\omega_0 \lesssim 1 \).
22. The many-polaron problem with infinite-range electron-phonon coupling was studied for the spinless Fröhlich model by A. S. Alexandrov and P. E. Kornilovitch, J. Phys.: Condens. Matter 14, 5337 (2002). The cooperative effect considered by these authors is long-ranged whereas our treatment of the breathing mode involves short-range EPI.
23. For a review of many-polaron effects for both Fröhlich polarons and Holstein polarons involving spin and spinless fermions, see A. S. Alexandrov and J. T. Devreese, Advances in Polaron Physics
(Springer, Berlin, 2009). However, this book does not cover the dominant NNN hopping due to cooperative EPI effects considered in our paper.


