

Polarization-Driven Charge Frustration and Emergent Phases in the One-Dimensional Extended Hubbard Model

Sourabh Saha,¹ Jeroen van den Brink^{2,3,4}, Manoranjan Kumar^{1,*}, and Satoshi Nishimoto^{2,4,†,‡}

¹*Department of Condensed Matter and Materials Physics, S. N. Bose National Centre for Basic Sciences, JD Block, Sector III, Salt Lake, Kolkata 700106, India*

²*Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany*

³*Würzburg-Dresden Cluster of Excellence ct.qmat, 97074 Würzburg, Germany*

⁴*Department of Physics, Technical University Dresden, 01069 Dresden, Germany*



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Frustration is a key driver of exotic quantum phases, yet its role in charge dynamics remains largely unexplored. We show that charge frustration—induced by electronic polarization effects—stabilizes unconventional insulating states in the one-dimensional extended Hubbard model. Using exact diagonalization and density-matrix renormalization group, we uncover a charge-disordered phase that remains insulating despite lacking long-range order and possessing an effectively attractive on-site interaction—a behavior reminiscent of gapful spin liquids in frustrated spin systems. We also identify a fragile ferroelectric phase and a charge-density-wave state with emergent eight-site periodicity. These findings establish charge frustration, driven by charge-dipole interactions, as a robust mechanism for realizing exotic phases in low-dimensional correlated systems, with implications for organic conductors, transition-metal oxides, and ultracold polar molecules.

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Introduction—Strongly correlated electron systems exhibit a wide range of quantum phenomena, including superconductivity, magnetism, and charge ordering [1,2]. The Hubbard model and its extended variants have long served as fundamental theoretical frameworks for capturing these phenomena in correlated systems [3,4]. While the effects of Coulomb interactions—both short-range and long-range—are well studied, the role of polarization effects, particularly charge-dipole interactions, remains relatively underexplored despite their relevance in real materials and experimental systems.

Charge-dipole interactions, which couple mobile charges to induced dipoles, introduce qualitatively new effects distinct from purely Coulombic interactions. These interactions become especially important in low-dimensional systems such as organic conductors, transition-metal oxides, and ultracold polar molecules [5–7]. Recent experiments with dipolar Fermi gases, including ¹⁶¹Dy [8] and polar molecules like ²³Na⁴⁰K and ⁴⁰K⁸⁷Rb [9–11], further

underscore the need for a systematic theoretical understanding of polarization-driven phenomena.

One-dimensional (1D) systems strongly enhance quantum fluctuations, making them highly sensitive to competing interactions. Such competition frequently gives rise to exotic ground states, including charge-density waves (CDW), bond-order waves (BOW), spin-density waves (SDW), superconductivity, and phase separation [12–21]. Despite extensive studies of spin frustration, charge frustration explicitly induced by charge-dipole couplings has remained largely unexplored, apart from some pioneering works [22–24]. This gap poses fundamental questions about the nature and stability of emergent phases in low-dimensional correlated electron systems.

In this Letter, we present a systematic study of the ground-state properties of the 1D extended Hubbard model, explicitly incorporating charge-dipole interactions. Using exact diagonalization (ED) and density-matrix renormalization group (DMRG) methods [25], we reveal rich phase diagrams featuring unconventional insulating phases. Notably, we demonstrate that charge frustration driven by the competition between Coulomb and charge-dipole interactions stabilizes novel states: a fragile ferroelectric (FE) phase, a previously unreported charge-disordered insulating (CDI) phase, and a remarkable CDW phase with an emergent eight-site periodicity. Our results highlight charge frustration, driven by polarization effects, as a new route to exotic insulating and charge-ordered phases in low-dimensional correlated systems, with relevance to

*Contact author: manoranjan.kumar@bose.res.in

†These authors contributed equally to this work.

‡Contact author: s.nishimoto@ifw-dresden.de

organic conductors, transition-metal oxides, and ultracold polar molecules.

Model—We consider the 1D extended Hubbard model incorporating charge-dipole interactions to account for polarization effects. The Hamiltonian is

$$H = -t \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) + (U - 4P) \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_i n_i n_{i+1} + 2P \sum_i n_i n_{i+2} - 2P \sum_i n_i, \quad (1)$$

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (annihilates) an electron with spin σ at site i , and $n_i = n_{i,\uparrow} + n_{i,\downarrow}$. We focus on the half-filled case. The parameters t , U , and V represent the nearest-neighbor hopping amplitude, on-site Coulomb repulsion, and nearest-neighbor Coulomb interaction, respectively. The polarization energy P modifies the interactions in two distinct ways: it reduces the on-site repulsion by $4P$ and introduces a next-nearest-neighbor repulsion of strength $2P$. A detailed derivation of the charge-dipole interaction is provided in Supplemental Material [26].

Phases in the atomic limit—To gain initial insight into the ground-state properties of the model, we consider the atomic limit ($t = 0$). The phase diagram in this limit, shown in Fig. 1, reveals one Mott insulating phase and three distinct CDW phases, each characterized by long-range charge order. The Mott insulator corresponds to a SDW state without long-range magnetic order; finite hopping introduces antiferromagnetic (AFM) fluctuations via an effective exchange interaction $\propto t^2/(U - P)$.

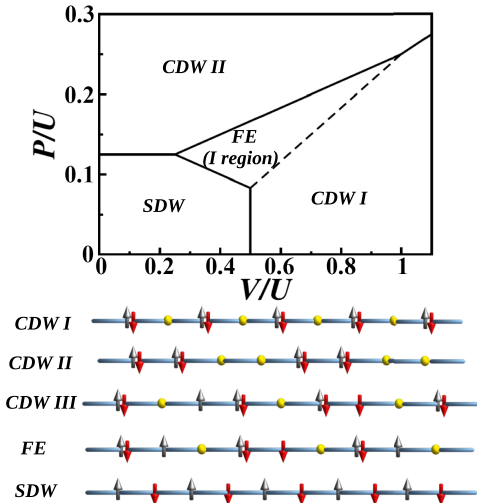


FIG. 1. Phase diagram of the system (1) in the atomic limit ($t = 0$) within the $(V/U, P/U)$ parameter space. The schematic electron configurations for each phase are illustrated, assuming an infinitesimally small t to indicate the corresponding spin configurations. The FE, CDW I, and CDW III states are energetically degenerate along the dashed line.

The three CDW phases exhibit twofold, threefold, and fourfold periodicities, denoted CDW I, FE, and CDW II, respectively, in line with previous studies [22–24]. In addition, at the FE-CDW I phase boundary, an eightfold periodic CDW state—labeled CDW III—becomes degenerate (see Supplemental Material [26]). This reflects a high degree of charge frustration near the phase boundaries, particularly in the region occupied by the FE phase.

This frustrated region is especially sensitive to quantum fluctuations when t is finite. As we show below, hopping destabilizes the classical charge orders and gives rise to exotic quantum states. We refer to this fluctuation-prone sector as the *intermediate region* (I region) in the remainder of this Letter.

Methods—We determine the phase boundaries using a level-crossing analysis [37,38] based on ED for several values of U/t . To refine these boundaries and explore regions inaccessible to the level-crossing approach, we perform large-scale DMRG simulations. Additional details are provided in Supplemental Material [26].

Phase boundaries via level-crossing approach—We estimate phase boundaries by analyzing level crossings in the excitation spectra. Each excitation is classified by discrete quantum numbers: inversion symmetry ($\sigma = \pm 1$), electron-hole symmetry ($J = \pm 1$), and total spin S . Transitions are identified by the crossing of energy levels with different symmetry labels, as summarized in Table I. In addition to the four insulating phases in Fig. 1, this approach also captures the BOW phase, known to appear at weak to intermediate U/t [12,13].

We thus distinguish five distinct phases: SDW, CDW I, CDW II, the I region, and BOW. The resulting phase diagrams for $U/t = 2, 4, 10$, and 20 , obtained from ED on a periodic $N = 12$ site cluster, are shown in Fig. 2. The system size accommodates both the six-site periodicity of the FE state and the four-site periodicity of CDW II. Remarkably, the overall phase structure in the $(V/U, P/U)$ plane remains qualitatively similar down to $U = 4t$. At $U = 2t$, however, the I region narrows significantly. Notably, the BOW phase persists even in the presence of

TABLE I. Sets of discrete symmetries used to classify excitation spectra at each phase transition in the level-crossing analysis.

Transition Phase A–Phase B	Symmetry quantum numbers	
	$A: (\sigma, J, S)$	$B: (\sigma, J, S)$
SDW–CDW I	$(+1, +1, 1)$	$(+1, -1, 0)$
SDW–CDW II	$(+1, +1, 1)$	$(+1, +1, 0)$
SDW–I region	$(-1, +1, 0)$	$(+1, -1, 0)$
SDW–BOW	$(+1, +1, 1)$	$(+1, +1, 0)$
CDW I–BOW	$(+1, -1, 0)$	$(-1, +1, 0)$
CDW I–I region	$(+1, +1, 0)$	$(+1, +1, 1)$
CDW II–I region	$(+1, +1, 0)$	$(+1, +1, 1)$

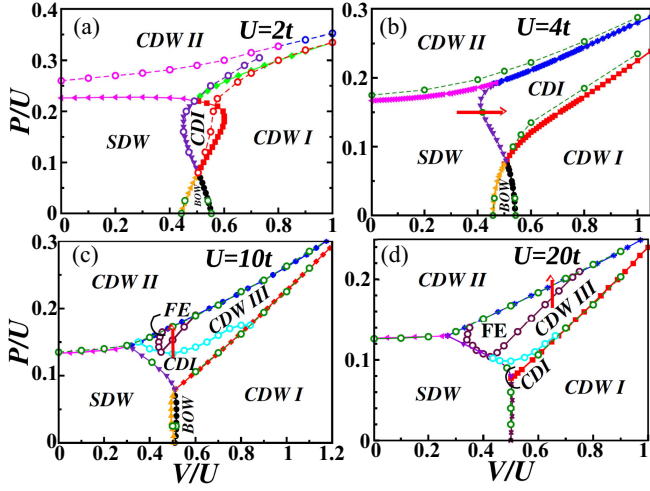


FIG. 2. Ground-state phase diagrams of the model in Eq. (1) for four values of U/t , plotted in the $(V/U, P/U)$ plane. Solid symbols denote phase boundaries determined via level-crossing analysis, while open symbols are obtained from DMRG. In (a), transitions of the same type are shown in the same color. Arrows in (b)–(d) indicate parameter paths used for analysis in subsequent sections.

finite polarization. Phase boundaries and the stability of the BOW region are further refined using DMRG; see Supplemental Material for details [26].

Beyond the FE phase found in the atomic limit, we identify two additional insulating states within the I region: a CDI phase, which is neither charge ordered nor Mott type, and a long-period CDW phase (CDW III) exhibiting eight-site periodicity. These phases are challenging to detect via level crossing due to symmetry constraints. We therefore perform a detailed analysis using DMRG, as described below.

Stability of FE state—As noted, the entire I region corresponds to the FE phase in the atomic limit. However, this state is highly fragile against finite hopping and difficult to detect numerically [24]. To probe its stability, we approach the FE state from large U/t . Figure 3(a) shows the charge density for $U/t = 50$ and 15, at fixed $V/U = 0.5$ and $P/U = 0.15$, chosen near the FE phase center in the atomic limit. The characteristic three-site pattern—doubly occupied, singly occupied, and empty—is evident, corresponding to a CDW with wave vector $q = 2\pi/3$. The modulation amplitude is reduced at $U/t = 15$, reflecting enhanced quantum fluctuations.

To quantify long-range FE order, we compute the order parameter $\langle \mathcal{O}_{\text{FE}} \rangle = \lim_{N \rightarrow \infty} \frac{1}{2} |\langle n_{N/2-2} \rangle - \langle n_{N/2} \rangle|$. Figure 3(b) shows its dependence on t/U at fixed $V/U = 0.5$ and $P/U = 0.15$. Starting from unity at $t/U = 0$, it decreases and vanishes abruptly only near $t/U \sim 0.08$, signaling a first-order transition. This highlights the extreme fragility of the FE phase, which occupies a wide region at $U/t = 20$ [Fig. 2(d)] but shrinks drastically at $U/t = 10$ [Fig. 2(c)].

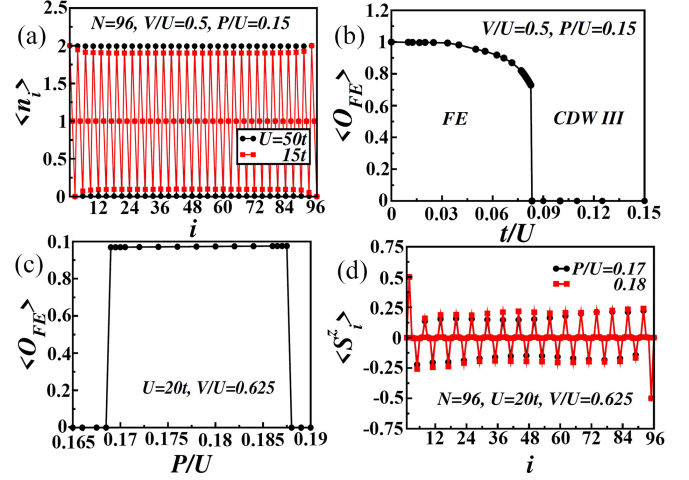


FIG. 3. DMRG results for the FE state. (a) Charge density distribution at large and moderate U/t . (b), (c) FE order parameter as a function of t/U and P/U , respectively; the parameter path for (c) is shown in Fig. 2(d). (d) Local spin profile $\langle S_i^z \rangle$ for representative parameters. All parameters are given in the figure.

Figure 3(c) further characterizes the transition by showing $\langle \mathcal{O}_{\text{FE}} \rangle$ versus P/U for $U/t = 20$ and $V/U = 0.625$. The system evolves from CDW II to FE to CDW III, with discontinuous jumps in $\langle \mathcal{O}_{\text{FE}} \rangle$ at both boundaries, providing clear evidence for first-order transitions. This is consistent with the FE phase (threefold) mediating between two CDWs with coprime periodicities—fourfold (CDW II) and eightfold (CDW III).

Additional insight comes from the spin structure. Assuming superexchange between singly occupied sites, the FE phase maps to an AFM Heisenberg chain. Figure 3(d) shows the z -component spin profile $\langle S_i^z \rangle$ for $P/U = 0.17$ and 0.18 at $U/t = 20$, $V/U = 0.625$. As expected, $\langle S_i^z \rangle \approx 0$ at doubly occupied and empty sites, with staggered spin moments on singly occupied ones, schematically: “ $\cdots \uparrow \downarrow \uparrow \circ \uparrow \downarrow \downarrow \circ \cdots$ ”. However, long-range magnetic order is absent due to the spin isotropy. This is confirmed by a vanishing spin gap. Note that the effective exchange interaction is extremely weak; for example, $J_{\text{eff}} \sim 9.4 \times 10^{-4}$ for $U/t = 20$, $V/U = 0.625$, and $P/U = 0.18$. Further details are provided in Supplemental Material [26].

Thus, we confirm that the I region hosts the FE phase at large U/t , but increasing hopping destabilizes it, giving rise to two novel phases (see below): a CDI without charge order and distinct from a Mott insulator, and a CDW III phase with long-range eight-site modulation ($q = 3\pi/4$).

Properties of CDI phase—We now examine the CDI phase in detail, focusing on its emergence from the SDW phase and its unconventional insulating character. Figure 4(a) shows the charge gap, defined as $\Delta_c = \lim_{N \rightarrow \infty} [E_0(N+2, 0) + E_0(N-2, 0) - 2E_0(N, 0)]/2$, where $E_0(N_e, S^z)$ is the ground-state energy of a system with N sites, N_e electrons, and total spin- z component S^z .

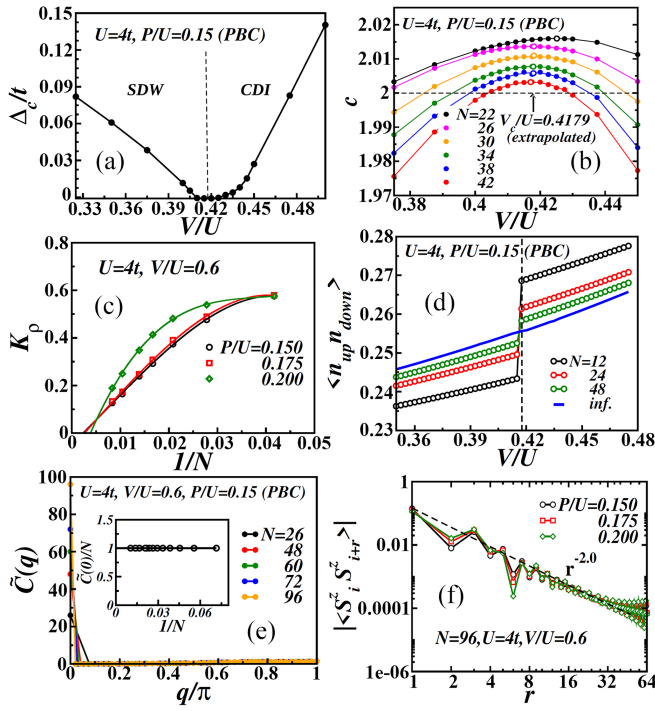


FIG. 4. DMRG results for the SDW and CDI phases. (a) Charge gap Δ_c/t as a function of V/U ; the parameter path for (a),(b),(d) is shown in Fig. 2(b). (b) Central charge c versus V/U , with open circles marking the peak positions used for finite-size extrapolation. (c) Finite-size scaling analysis of the Tomonaga-Luttinger parameter K_ρ within the CDI phase. (d) Double occupancy $\langle n_{i\uparrow}n_{i\downarrow} \rangle$ versus V/U , highlighting the transition from SDW to CDI phases. (e) Charge structure factor $\tilde{C}(q)$ computed in the CDI phase; inset shows $\tilde{C}(0)/N$ versus $1/N$. (f) Log-log plot of the spin-spin correlation function $|\langle S_i^z S_{i+r}^z \rangle|$ within the CDI phase. All parameters are given in the figure.

The data are presented as a function of V/U for $U/t = 4$ and $P/U = 0.15$. In the SDW phase, Δ_c is finite, as expected for a Mott insulator. As V/U increases, the gap decreases, closes at the transition point, and reopens in the CDI phase, indicating a continuous transition between two charge-gapped states. Meanwhile, the spin gap remains zero throughout, as confirmed in Supplemental Material [26].

To further support these findings, we calculate the central charge, $c = 3[S_N(N/2 - 1) - S_N(N/2)] / \ln[\cos(\pi/N)]$, where $S_N(l)$ is the von Neumann entanglement entropy of a subsystem of length l in a periodic chain of length N [39,40]. Figure 4(b) shows c as a function of V/U for several system sizes at fixed $U/t = 4$ and $P/U = 0.15$. Each curve exhibits a single peak, and extrapolating these peaks to the thermodynamic limit locates the transition at $V/U = 0.4179$, in excellent agreement with both the gap-closing point (0.4175) and the level-crossing estimate (0.4171). Notably, $c = 2$ appears only at the critical point, where both spin and charge excitations are gapless, while $c = 1$ holds in both the SDW and CDI phases due to a single gapless spin mode.

The insulating character of the CDI phase is further confirmed through the Tomonaga-Luttinger parameter K_ρ , defined via the slope of the charge structure factor $C(q) = \sum_r e^{iqr} (\langle n_i n_{i+r} \rangle - \langle n_i \rangle \langle n_{i+r} \rangle)$ in the limit of small momentum, $K_\rho = \pi \lim_{q \rightarrow 0} C(q)/q$ [41]. As shown in Fig. 4(c), K_ρ extrapolates to zero throughout the CDI phase, confirming its incompressibility.

The CDI phase also exhibits unique local characteristics. Figure 4(d) shows the double occupancy $\langle n_{i\uparrow}n_{i\downarrow} \rangle$, which remains below 0.25 in the SDW phase, consistent with repulsive interactions. However, it exceeds 0.25 in the CDI phase, indicating an effective on-site attraction. This distinguishes CDI from a conventional Mott insulator.

To examine the possibility of charge ordering or phase separation, we evaluate the structure factor without subtracting the mean density: $\tilde{C}(q) = \sum_r e^{iqr} \langle n_i n_{i+r} \rangle$. Figure 4(e) shows $\tilde{C}(q)$ for $U/t = 4$, $V/U = 0.6$, and $P/U = 0.15$. A single peak appears at $q = 0$, with $\tilde{C}(0) = N$, consistent with a uniform charge distribution. The absence of significant peaks at finite q confirms that the system lacks long-range charge order, and the fact that $\tilde{C}(0)$ does not exceed N rules out phase separation. The charge profile thus remains spatially uniform, resembling that of a Mott insulator, though distinct in microscopic character.

Remarkably, despite the absence of long-range order, the CDI phase remains insulating. Its origin lies in the proximity to several competing charge-ordered phases—CDW I, CDW II, FE, and CDW III—which induce short-range patterns in the ground-state wave function. These local configurations act as effective double occupancy barriers, suppressing charge transport and localizing carriers. This mechanism is also reflected in the collapse of the charge dispersion in the single-particle excitation spectrum. Moreover, as shown in Fig. 4(f) the spin-spin correlation function $|\langle S_i^z S_{i+r}^z \rangle|$ decays as $1/r^2$, indicating the absence of magnetic interactions. This rapid decay does not arise from conventional spin dynamics, but rather from the lack of effective spin couplings imposed by the underlying charge disorder. Additional supporting data are provided in Supplemental Material [26].

The CDI phase thus represents a novel type of insulating state—uniform, non-Mott, and stabilized by frustration—induced local correlations. A deeper theoretical understanding of its nature remains an open question for future investigation.

CDW state with eight-fold periodicity—We now turn to the CDW III phase, which emerges within the I region at large U/t [see Fig. 2]. Figure 5(a) shows the charge structure factor $C(q)$, computed at $U/t = 10$, $V/U = 0.8$, and $P/U = 0.2$. A pronounced peak appears at $q = 3\pi/4$, whose divergence with system size confirms long-range order with eight-site periodicity [Fig. 5(b)].

To identify the charge alignment, we plot the density-density correlations in Fig. 5(c), which reveal a

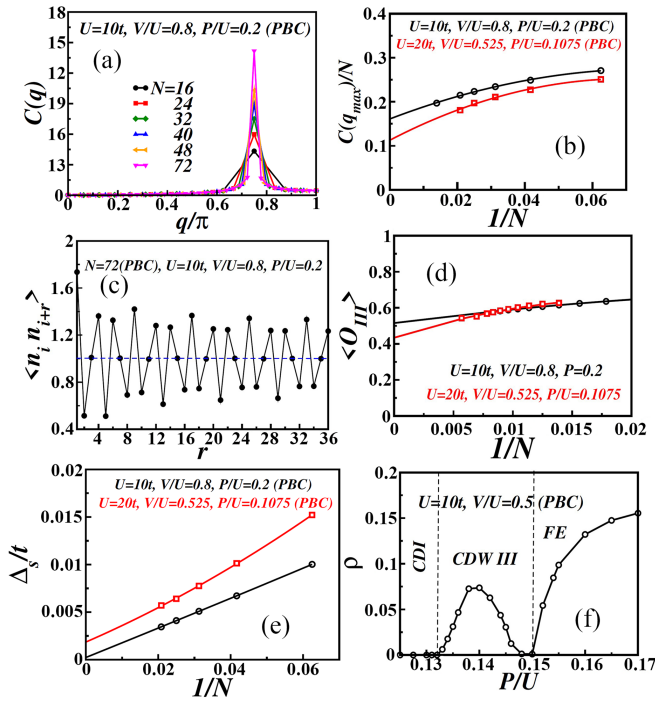


FIG. 5. DMRG results for the CDW III phase. (a) Charge structure factor $C(q)$ and (b) finite-size scaling of the normalized peak height at $q = 3\pi/4$. (c) Density-density correlations. (d) Finite-size scaling of the CDW III order parameter. (e) Finite-size scaling of the spin gap. (f) Charge order parameter ρ versus P/U ; the parameter path for (f) is shown in Fig. 2(c). All parameters are given in the figure.

characteristic pattern: “ $\cdots \uparrow\downarrow \circ \uparrow\downarrow \circ \uparrow\downarrow \downarrow \circ \cdots$.” Each period contains three charge-rich, three charge-poor, and two intermediate sites. To quantify this order, we define the CDW III order parameter as $\langle O_{\text{III}} \rangle = \frac{1}{6} \sum_{i=N/2-3}^{N/2+4} \gamma_i \langle n_i \rangle$, where $\gamma_i = 1$ for charge-rich sites, -1 for charge-poor sites, and 0 otherwise. Finite-size scaling confirms a nonzero value in the thermodynamic limit [Fig. 5(d)], establishing the stability of the CDW III phase.

In the spin sector, this configuration localizes spin-1/2 moments on singly occupied sites, where charge patterns such as “ $\uparrow\downarrow \circ \uparrow\downarrow$ ” and “ $\circ \uparrow\downarrow \circ$ ” appear alternately between them. This maps the system onto a spin-Peierls Heisenberg chain with alternating exchange couplings. In fact, from a small-cluster analysis, we estimate the effective couplings to be $J_1^{\text{eff}} = 0.01604t$ and $J_2^{\text{eff}} = 0.01422t$ for $U/t = 20$, $V/U = 0.525$, and $P/U = 0.1075$, yielding a spin gap $\Delta_s/t \approx 0.0036$. This is in good agreement with the spin gap obtained directly from the original model, $\Delta_s = \lim_{N \rightarrow \infty} [E_0(N, 1) - E_0(N, 0)]$, which gives $\Delta_s \sim 0.0019t$ [Fig. 5(e)]. Further details are provided in Supplemental Material [26].

To delineate the CDW III region, we compute the scaled structure factor $\rho = \lim_{N \rightarrow \infty} C(q_{\text{max}})/N$ along a path from the CDI phase through CDW III into the FE phase at $U = 10t$ and $V/U = 0.5$ [Fig. 5(f)]. In the CDI phase,

$\rho = 0$; it becomes finite in the CDW III phase at $q_{\text{max}} = 3\pi/4$, and vanishes again as the system transitions into the FE phase. There, a new peak emerges at $q_{\text{max}} = 2\pi/3$, signaling the onset of threefold FE charge order.

The CDW III phase originates near the CDW I–FE boundary at large U/t . In the atomic limit, its configuration is energetically degenerate with those of CDW I and FE on the boundary. Finite hopping lifts this degeneracy, and the gain in spin-Peierls energy can stabilize CDW III over FE. This mechanism explains why, in the $U/t = 20$ phase diagram [Fig. 2(d)], the region adjacent to CDW I—classically part of the FE phase—is replaced by CDW III.

Summary—We have investigated the ground-state properties of the 1D extended Hubbard model with charge-dipole interactions, using ED and DMRG calculations. The inclusion of polarization effects introduces competing interactions that drive strong charge frustration. Within this frustrated regime, we uncover a novel charge-disordered insulating phase that is charge gapped yet non Mott in character—lacking both charge order and magnetic interactions, and stabilized by local short-range correlations induced by nearby CDW states. We also identify the extreme fragility of the FE phase under quantum fluctuations, and a CDW phase with emergent eight-site periodicity. These phases arise from the interplay between charge frustration and hopping-induced quantum fluctuations. Our results shed light on fundamental mechanisms governing charge transport and coherence in low-dimensional systems, and offer insights relevant to the design of correlated materials and dipolar quantum platforms.

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Data availability—The data that support the findings of this Letter are openly available [42].

- [1] E. Dagotto, Complexity in strongly correlated electronic systems, *Science* **309**, 257 (2005).
- [2] P. A. Lee, N. Nagaosa, and X.-G. Wen, Doping a Mott insulator: Physics of high-temperature superconductivity, *Rev. Mod. Phys.* **78**, 17 (2006).

- [3] M. Qin, T. Schäfer, S. Andergassen, P. Corboz, and E. Gull, The Hubbard model: A computational perspective, *Annu. Rev. Condens. Matter Phys.* **13**, 275 (2022).
- [4] D. P. Arovas, E. Berg, S. A. Kivelson, and S. Raghu, The Hubbard model, *Annu. Rev. Condens. Matter Phys.* **13**, 239 (2022).
- [5] H. Mosadeq and R. Asgari, Quantum phases of a one-dimensional dipolar Fermi gas, *Phys. Rev. B* **91**, 085126 (2015).
- [6] A. H. Talebi and B. Davoudi, Spin and charge fluctuations in a one-dimensional lattice with long-range interactions, *Physica (Amsterdam)* **571B**, 204 (2019).
- [7] Y.-P. Huang and D.-W. Wang, Quantum phase diagrams of fermionic dipolar gases in a planar array of one-dimensional tubes, *Phys. Rev. A* **80**, 053610 (2009).
- [8] M. Lu, N. Q. Burdick, and B. L. Lev, Quantum degenerate dipolar Fermi gas, *Phys. Rev. Lett.* **108**, 215301 (2012).
- [9] C.-H. Wu, J. W. Park, P. Ahmadi, S. Will, and M. W. Zwierlein, Ultracold fermionic Feshbach molecules of $^{23}\text{Na}^{40}\text{K}$, *Phys. Rev. Lett.* **109**, 085301 (2012).
- [10] A. Chotia, B. Neyenhuis, S. A. Moses, B. Yan, J. P. Covey, M. Foss-Feig, A. M. Rey, D. S. Jin, and J. Ye, Long-lived dipolar molecules and Feshbach molecules in a 3D optical lattice, *Phys. Rev. Lett.* **108**, 080405 (2012).
- [11] K.-K. Ni, S. Ospelkaus, M. De Miranda, A. Pe'er, B. Neyenhuis, J. Zirbel, S. Kotochigova, P. Julienne, D. Jin, and J. Ye, A high phase-space-density gas of polar molecules, *Science* **322**, 231 (2008).
- [12] M. Nakamura, Mechanism of CDW-SDW transition in one dimension, *J. Phys. Soc. Jpn.* **68**, 3123 (1999).
- [13] M. Nakamura, Tricritical behavior in the extended Hubbard chains, *Phys. Rev. B* **61**, 16377 (2000).
- [14] P. Sengupta, A. W. Sandvik, and D. K. Campbell, Bond-order-wave phase and quantum phase transitions in the one-dimensional extended Hubbard model, *Phys. Rev. B* **65**, 155113 (2002).
- [15] E. Jeckelmann, Ground-state phase diagram of a half-filled one-dimensional extended Hubbard model, *Phys. Rev. Lett.* **89**, 236401 (2002).
- [16] M. Tsuchiizu and A. Furusaki, Phase diagram of the one-dimensional extended Hubbard model at half filling, *Phys. Rev. Lett.* **88**, 056402 (2002).
- [17] A. Dhar, J. J. Kinnunen, and P. Törmä, Population imbalance in the extended Fermi-Hubbard model, *Phys. Rev. B* **94**, 075116 (2016).
- [18] M. Kumar, S. Ramasesha, and Z. G. Soos, Tuning the bond-order wave phase in the half-filled extended Hubbard model, *Phys. Rev. B* **79**, 035102 (2009).
- [19] M. Kumar and Z. G. Soos, Bond-order wave phase of the extended Hubbard model: Electronic solitons, paramagnetism, and coupling to Peierls and Holstein phonons, *Phys. Rev. B* **82**, 155144 (2010).
- [20] S. Ejima and S. Nishimoto, Phase diagram of the one-dimensional half-filled extended Hubbard model, *Phys. Rev. Lett.* **99**, 216403 (2007).
- [21] D.-W. Qu, B.-B. Chen, H.-C. Jiang, Y. Wang, and W. Li, Spin-triplet pairing induced by near-neighbor attraction in the extended Hubbard model for cuprate chain, *Commun. Phys.* **5**, 257 (2022).
- [22] J. van den Brink, M. B. J. Meinders, J. Lorenzana, R. Eder, and G. A. Sawatzky, New phases in an extended Hubbard model explicitly including atomic polarizabilities, *Phys. Rev. Lett.* **75**, 4658 (1995).
- [23] M. B. J. Meinders, J. van den Brink, J. Lorenzana, and G. A. Sawatzky, Atomic screening and intersite Coulomb repulsion in strongly correlated systems, *Phys. Rev. B* **52**, 2484 (1995).
- [24] M. E. Torio, A. A. Aligia, K. Hallberg, and H. A. Ceccatto, Phase diagram of the extended Hubbard chain with charge-dipole interactions, *Phys. Rev. B* **62**, 6991 (2000).
- [25] S. R. White, Density matrix formulation for quantum renormalization groups, *Phys. Rev. Lett.* **69**, 2863 (1992).
- [26] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/d5sw-qdfp> for I. Derivation of the polarization term in the Extended Hubbard model. II. Ground-state degeneracy at the atomic limit ($t = 0$). III. Demonstration of level-crossing method. IV. Details of DMRG technique. V. Order parameters for the CDW I and CDW II states. VI. Spin gap in the CDW I and CDW II phases. VII. Properties of the SDW state. VIII. Finite-size effects appearing near the SDW-CDI transition. IX. Additional central-charge analysis of the CDI phase. X. Absence of charge and spin orders in the CDI state. XI. Mixed short-range charge orders in CDI states. XII. Confirmation of insulating behavior in the CDI phase via single-particle spectral analysis. XIII. Mapping of FE and CDW III states onto effective spin models. XIV. Order parameter for the BOW phase. XV. Additional information for the FE phase. XVI. Additional information for the CDW III phase. Supplemental Material includes Refs. [27–36].
- [27] J. F. Annett, R. M. Martin, A. K. McMahan, and S. Satpathy, Electronic Hamiltonian and antiferromagnetic interactions in La_2CuO_4 , *Phys. Rev. B* **40**, 2620(R) (1989).
- [28] M. S. Hybertsen, E. B. Stechel, M. Schluter, and D. R. Jennison, Renormalization from density-functional theory to strong-coupling models for electronic states in Cu-O materials, *Phys. Rev. B* **41**, 11068 (1990).
- [29] J. B. Grant and A. K. McMahan, Realistic electronic structure calculations for magnetic insulators like La_2CuO_4 , *Phys. Rev. Lett.* **66**, 488 (1991).
- [30] C. Varma, Missing valence states, diamagnetic insulators, and superconductors, *Phys. Rev. Lett.* **61**, 2713 (1988).
- [31] E. Lieb, T. Schultz, and D. Mattis, Two soluble models of an antiferromagnetic chain, *Ann. Phys. (N.Y.)* **16**, 407 (1961).
- [32] M. Oshikawa, Commensurability, excitation gap, and topology in quantum many-particle systems on a periodic lattice, *Phys. Rev. Lett.* **84**, 1535 (2000).
- [33] B. Nachtergaele and R. Sims, A multi-dimensional Lieb-Schultz-Mattis theorem, *Commun. Math. Phys.* **276**, 437 (2007).
- [34] S. Ramasesha and Z. Soos, Diagrammatic valence-bond theory for finite model Hamiltonians, *Int. J. Quantum Chem.* **25**, 1003 (1984).
- [35] Z. G. Soos and S. Ramasesha, Valence-bond theory of linear Hubbard and Pariser-Parr-Pople models, *Phys. Rev. B* **29**, 5410 (1984).

- [36] U. Schollwöck, The density-matrix renormalization group, *Rev. Mod. Phys.* **77**, 259 (2005).
- [37] R. Jullien and F. Haldane, Finite-size scaling study of dimerisation in the frustrated 1D $S = \frac{1}{2}$ antiferromagnet, *Bull. Am. Phys. Soc.* **28**, 344 (1983).
- [38] K. Okamoto and K. Nomura, Fluid-dimer critical point in $S = \frac{1}{2}$ antiferromagnetic Heisenberg chain with next nearest neighbor interactions, *Phys. Lett. A* **169**, 433 (1992).
- [39] P. Calabrese and J. Cardy, Entanglement entropy and quantum field theory, *J. Stat. Mech.* (2004) P06002.
- [40] S. Nishimoto, Tomonaga-luttinger-liquid criticality: Numerical entanglement entropy approach, *Phys. Rev. B* **84**, 195108 (2011).
- [41] S. Ejima, F. Gebhard, and S. Nishimoto, Tomonaga-Luttinger parameters for doped Mott insulators, *Europhys. Lett.* **70**, 492 (2005).
- [42] S. Saha, J. van den Brink, M. Kumar, and S. Nishimoto, Dataset of “polarization-driven charge frustration and emergent phases in the one-dimensional extended Hubbard model,” [10.5281/zenodo.17283260](https://zenodo.org/record/17283260) (2025).

Correction: A project number in the Acknowledgments contained a typographical error and has been fixed.