One-dimensional Peierls phase separation in the dilute carrier density limit

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We use Density Matrix Renormalization Group to study a one-dimensional chain with Peierls electron-phonon coupling describing the modulation of the electron hopping due to lattice distortion. We demonstrate the appearance of an exotic phase-separated state, which we call Peierls phase separation, in the limit of very dilute electron densities, for sufficiently large couplings and small phonon frequencies. This is unexpected, given that Peierls coupling mediates effective pair-hopping interactions that disfavor phase clustering. The Peierls phase separation consists of a homogenous, dimerized, electron-rich region surrounded by electron-poor regions, which we show to be energetically more favorable than a dilute liquid of bipolarons. This mechanism qualitatively differs from that of typical phase separation in conventional electron-phonon models that describe the modulation of the electron’s potential energy due to lattice distortions. Surprisingly, the electron-rich region always stabilizes a dimerized pattern at fractional densities, hinting at a non-perturbative correlation-driven mechanism behind phase separation.

Introduction.— A primary goal in condensed matter physics targets the discovery and understanding of unusual phases of matter that arise from strong correlations. Correlated electron-lattice systems, besides being fascinating in their own right, manifest in many experimentally relevant situations such as polaronic phenomena in the dilute electron density limit [1–4], and superconductivity and charge order at finite electron concentrations [5–7].

Recent work [4] demonstrates that the Peierls electron-phonon coupling [8–10] (describing the modulation of the electron hopping due to lattice distortions) gives rise to strongly bound but light bipolarons that could condense into a superconductor at high temperatures, opening a possible route to phonon-mediated high-\(T_c\) superconductivity, whose fingerprints may already manifest in certain materials [11, 12]. A natural concern lies in the issue of competing instabilities that might favor a different order. For example, for the much studied generalized Holstein [13, 14] and Fröhlich [15, 16] electron-phonon models, in which the lattice distortion modulates the electron’s onsite energy, a sufficiently strong coupling induces phase separation in the limit of low carrier concentrations [17–19], presenting a major obstacle to bipolaronic superconductivity. This is not surprising. In these models, bipolarons become increasingly heavy at stronger couplings [20, 22] and thus benefit from the phonon-mediated long-range electron-electron attraction to minimize their total energy by grouping into multi-polaron complexes.

In contrast, as stated earlier, Peierls coupling favors light bipolarons even at very large couplings because it mediates effective pair-hopping interactions that enhance the kinetic energy of bipolarons [4]. Indeed, in this Letter we verify that in one dimension (1D) a dilute gas of Peierls bipolarons remains stable for moderate-to-strong coupling strengths (see Fig. 1), thus reinforcing the scenario of Peierls phonon-mediated high-\(T_c\) superconductivity in the dilute carrier limit. Surprisingly, at stronger couplings, the dilute bipolaron liquid does become unstable to phase separation. This, however, happens through a mechanism totally different from that in the standard

![FIG. 1. (color online) Phase diagrams of the 1D Peierls and extended Holstein (EH) models in the limit of very dilute electron density. The latter represents a lattice model that mimics the physics of the Fröhlich coupling, see Ref. [17], and for which \(\lambda = g^2/(2\Omega t)\). Solid (dotted) lines show the critical values \(\lambda_c(\Omega)\) separating a stable liquid of bipolarons for \(\lambda < \lambda_c\) from phase separation for \(\lambda > \lambda_c\), for the Peierls (EH) couplings. Unlike for the EH coupling, in the Peierls model the dilute liquid of bipolarons remains stable up to much larger \(\lambda\), with a diverging \(\lambda_c \rightarrow \infty\) as \(\Omega \rightarrow \infty\). These results were obtained using DMRG for a system with \(L = 16\) sites and \(N = 6\) electrons (see text for details).](image-url)
models, and which we uncover below.

We use Density Matrix Renormalization Group (DMRG) \cite{9} (see also \cite{42, 38}) to show that in 1D a sufficiently strong Peierls coupling stabilizes a phase-separated state whereby the carriers congregate into a nearly homogenous, *dimerized*, high-density electron region surrounded by electron-poor undimerized regions – the Peierls phase separation.

The salient features of our results are as follows:

1. Unlike Holstein coupling, sufficiently strong Peierls coupling \( \lambda > \lambda_c \) favors large polaronic complexes leading to *Peierls phase separation*. For very dilute electron densities, phase separation does not occur in the local (zero-range) Holstein model \cite{19}. Strong local Holstein coupling mediates a strong on-site electron-electron attraction which stabilizes heavy S0 (on-site) singlet bipolarons \cite{22}. However, no effective phonon-mediated longer-range attraction between Holstein bipolarons exists and so phase separation does not occur. We note that phase separation occurring at or near half-filling in local electron-phonon models \cite{39, 42} – while interesting – has no relevance to polaronic phenomena in the Peierls model, see \cite{43, 44}.

2. The *Peierls phase separation differs qualitatively from the phase separation observed in the extended Holstein and Fröhlich models at low densities*. As mentioned, finite-range electron-phonon models that describe the modulation of the electron’s potential energy due to (longer-wavelength) lattice distortions generally exhibit phase-separated regimes for sufficiently strong couplings \cite{19}. In these models, phonons mediate an effective electron-electron attraction whose range inherits that of the electron-lattice coupling. As a result, for a sufficiently large coupling, a small density of carriers will energetically favor sharing their clouds so as to lower their potential energy, thus giving way to phase separation rather than forming a gas of heavy bipolarons. Peierls coupling, however, mediates effective pair-hopping interactions that favor moving (and therefore light) bipolarons \cite{41}. Such interactions disfavor clustering of bipolarons since sharing their distortion clouds would sacrifice their kinetic energy. Indeed, in the strong anti-adiabatic limit \( \Omega \to \infty \) we have verified (not shown) that Peierls phase separation does not occur. DMRG shows that the Peierls phase separation becomes increasingly relevant on approach to the adiabatic limit, and that it congregate the electrons within a nearly homogenous, dimerized region reminiscent of the Su-Schrieffer-Heeger (SSH) ground state of polyacetylene \cite{47, 18}, however at a *fractional filling* different from half \cite{40, 50}. The Peierls phase separation is therefore not due to a polaronic effect in which heavy bipolarons congregate because of remnant longer-range attraction, as in standard models. Instead, it signals the instability of a dilute liquid of appreciably light bipolarons into a qualitatively different, dimerized phase stabilized by the Peierls coupling at a large, fractional effective electron density.

**Model.**— The 1D Hamiltonian including the Peierls electron-phonon coupling is given by \( \mathcal{H} = \mathcal{H}_e + \mathcal{H}_{\text{ph}} + V_{e-\text{ph}} \). \( \mathcal{H}_e = -t \sum_{i, \sigma} c_{i, \sigma}^{\dagger} c_{i+1, \sigma} + \text{H.c.} \) describes nearest-neighbor (NN) hopping of electrons of spin \( \sigma = \{ \uparrow, \downarrow \} \) in a single electronic band, with creation operator \( c_{i, \sigma}^{\dagger} \) at site \( i = 1, ..., L \), and number operator \( n_i = \sum_{\sigma} c_{i, \sigma}^{\dagger} c_{i, \sigma} \). The Peierls coupling describes, to linear order, the modulation of the hopping integral due to lattice distortions:

\[
V_{e-\text{ph}} = g \sum_{i, \sigma} (c_{i, \sigma}^{\dagger} c_{i+1, \sigma} + \text{H.c.})(b_i^\dagger + b_i - b_{i+1}^\dagger - b_{i+1}).
\]

Phonons belong to an optical Einstein mode of frequency \( \Omega \) (we set \( \hbar = 1 \)), \( \mathcal{H}_{\text{ph}} = \Omega \sum_i b_i^\dagger b_i \), with the boson creation operator \( b_i^\dagger \) at site \( i = 1, ..., L \). We characterize the strength of Peierls electron-phonon coupling via the dimensionless coupling \( \lambda = 2g^2/\Omega \).

**Methods.**— We study \( N \leq 16 \) electrons in the zero magnetization sector \( S_{\text{Tot}}^z = 0 \) of the Peierls model on chains of lengths \( L \leq 32 \). We use DMRG to compute the ground state, utilizing up to \( n_{\text{ph max}} = 1 + 20 \) phonon states to represent the local phonon Hilbert space. Numerical results were converged with respect to the bond dimension \( m \). A maximum \( m = 600 \) provides convergence with a truncation error smaller than \( 5 \times 10^{-7} \) for open boundary conditions (OBC) and \( 5 \times 10^{-6} \) for periodic boundary conditions (PBC), see the Supplementary Material for more information \cite{31}.

**Results.**— Previous work showed that Peierls bipolarons are stable against dissociation into single polarons for all \( \lambda \), unless an extremely large Hubbard repulsion is present (a possibility we ignore here) \cite{41}. We first analyze the stability of a dilute liquid of these Peierls bipolarons. We use DMRG to find the ground-state (GS) energies \( E_N \) for \( N = 1, 2, 4, 6 \) electrons on a chain with \( L = 32 \) sites. (We have performed finite-size scaling of the results confirming that \( L = 32 \) data is representative of the infinite chain limit.) We define \( \Delta_2 = 2E_1 - E_2, \Delta_4 = 2E_2 - E_4, \Delta_6 = E_2 + E_4 - E_6 \) and study their dependence on \( \lambda \) in Fig. 2 for \( \Omega = 2t \). In the thermodynamic limit, all \( \Delta_N \geq 0 \): \( \Delta_N = 0 \) signals that smaller complexes each composed of less than \( N \) particles are energetically favorable (e.g., \( \Delta_2 = 0 \) means that the \( N = 2 \) GS consists of two single polarons), while \( \Delta_N > 0 \) signals the stability of a bound state of the \( N \) carriers. We find \( \Delta_2 > 0 \) for all \( \lambda \), confirming that, the \( N = 2 \) GS always corresponds to a bipolaron, in agreement with \cite{41}. \( \Delta_4 \) and \( \Delta_6 \) both become positive above roughly the same \( \lambda_c \geq 0.8 \), showing the tendency of all carriers present in the system to coalesce if \( \lambda \geq \lambda_c \). We note that negative \( \Delta_2, \Delta_4 \) values for \( \lambda < \lambda_c \) are due to finite-size effects, as shown in the inset.

Evidence that coalescing at \( \lambda > \lambda_c \) represents a signature of true phase separation is presented in Fig. 3. Panel
(a) shows the average electron density $\langle \hat{n}_i \rangle$ against $i$ for a chain with OBC and $L = 32$ sites, for $N = 4, 8, 12, 16$ electrons (nominal densities 0.125 to 0.5; darker to lighter lines) at $\lambda = 1$ and $\Omega = 2t$. The electrons congregate into an electron-rich region whose core is homogeneous with $\langle n \rangle = 2/3$, while the ends of the chain are electron free. We emphasize that OBC centers the electron-rich region at $L/2$. We have verified (not shown) that PBC give identical results, except the electron-rich region can be centered anywhere. Panel (b) shows that the lattice dimerizes in the core of the electron-rich region: $(-1)^i (\hat{b}_i + \hat{b}_i^\dagger) > 0$. This is reminiscent of the SSH GS, but for a different electron density. Finally, panel (d) shows that double occupancy in the core of the electron-rich region is very small, $\langle \hat{n}_i \hat{n}_{i+1} \rangle \sim 0.125 \ll 1$. This is not so surprising since the average density is $2/3$. Importantly, however, this implies that turning on a moderate repulsive Hubbard $U$ will not affect these results significantly, see, e.g., [52]. In contrast, as shown in panel (c), for $\lambda < \lambda_c$, $\langle \hat{n}_i \rangle$ exhibits $N/2$ roughly equally spaced maxima, indicating $N/2$ bipolarons lined up along the chain because of the OBC. Moreover, here we find no dimerization: $\langle \hat{b}_i + \hat{b}_i^\dagger \rangle = 0$ (not shown).

These results prove that the dimerized electron-rich region stabilized for $\lambda > \lambda_c$ cannot be simply a “denser” liquid/crystal of bipolarons, like in the standard models, but must be a very different state.

To verify this, we use DMRG with PBC to study the homogeneous GS established at large electron concentrations $n$, for chains with $L = 16, 20, 24$ sites and with $N = 2 N_{\text{pair}}$ ranging from $L - 8$ to $L$. For $L = 16$, this corresponds to $n = N/L \in [0.5, 1]$, while for $L = 24$, $n \in [0.66, 1]$. We find that all these ground states exhibit dimerization. Their GS energies scaled with $N_{\text{pair}}$ are plotted against $\lambda$ in Fig. 3 (dark to lighter dashed lines as $n$ increases). In contrast, the full red line shows the GS energy of a single bipolaron $E_2$ in an otherwise empty chain, in the thermodynamic limit, corresponding to $n = 0$. It provides a very good estimate for the expected GS energy per pair, for a very dilute gas of bipolarons. Fig. 3 proves that at small $\lambda$, this energy lies well below the (appropriately scaled) GS energies of the high-density phases. However, at larger $\lambda$, some of the latter become energetically more favorable. In particular, the switch happens at $\lambda \approx 0.8 \approx \lambda_c$ for $n = 0 - 0.7$. This confirms that above $\lambda_c$, it is indeed energetically favorable for the very dilute gas of electrons to phase separate into a high-density, homogeneous (apart from its edges), electron-rich region surrounded by empty regions.

Based on the results of Fig. 3 alone, it is not possible to pinpoint the density of this electron-rich region, only that $0.5 < n < 0.8$. Clearly this $n$ must be special in order to yield the lowest ratio $E_{GS}/N$. The celebrated SSH GS with $n = 1$ is found to be energetically more expensive than $N/2 E_2$ at all $\lambda$, so this is not a candidate for this $\Omega$. At small $\lambda$, this is because the half-filled electron band is energetically expensive compared to a very dilute electron gas. The energy of the SSH GS decreases fast as...
The bigger puzzle is: (ii) that according to Fig. 3 and consistent with all our other results, these electron-rich states with the lowest \( E_{GS}/N \) are dimerized. They seem to exhibit little on-site correlations, consistent with the rather low core densities \( n < 1 \). If correlations can be ignored, then textbook arguments mandate an instability with \( Q = 2k_F \) \[^{[53]}\]. For the \( n = 2/3 \) state illustrated in Fig. 3, this corresponds to three-site periodicity, not the two-site dimerization clearly seen in Fig. 3(b), and confirmed when studying the homogeneous states of Fig. 4. Other \( n \) values favored at other \( \Omega \) values should have other superlattice constants, and yet we always find dimerization with \( Q = \pi \), as if \( n = 1 \).

**Conclusion.** — We studied the Peierls electron-phonon coupling on a 1D chain and proved that a dilute bipolaron gas is stable against phase separation up to fairly large couplings \( \lambda < \lambda_c \), unlike in standard models where \( \lambda_c \) turns out to be rather small. This reinforces the possibility of high-temperature superconductivity in models with Peierls-like coupling in the dilute electron density limit. For \( \lambda > \lambda_c \) we presented evidence for a new type of phase segregation, the Peierls phase separation, which has a number of fascinating properties including dimerization of electron-rich regions at all stabilized \( n \) values. More work is needed to understand the mechanism behind the breakdown of the \( Q = 2k_F \) rule.

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**Further remarks.** — More work is needed to fully understand the nature of the phase-separated state, a task we will undertake in the future. Our results highlight two puzzles: (i) if the density in the core region is always commensurate (as indicated by our results), does this occur as a result of a general feature of phase separation or is it specific to the Peierls phase separation? In this regard, it would be interesting to explore how does the mechanism behind the breakdown of the \( Q = 2k_F \) rule.

\[ \text{FIG. 4. (color online) GS energy } E_{GS}/N_{\text{pair}} \text{ against } \lambda, \text{ for chains of lengths } L = 16, 20, 24 \text{ with increasing number of electrons } N = L-8, L-4, L-2, L \text{ (dark to light dashed lines), and } N_{\text{pair}} = N/2. \text{ These are DMRG results for PBC, so these finite-density phases are homogeneous and dimerized (not shown). The full red line is the bipolaron energy } E_2. \text{ The condition } E_2 < E_{GS}/N_{\text{pair}} \text{ suggests that at low concentrations } n = N/L, \text{ a diluted gas of bipolarons is energetically favorable. In contrast, } E_2 > E_{GS}/N_{\text{pair}} \text{ signals instability towards phase separation.} \]
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Here we discuss additional computational details about the DMRG simulations performed in this work.

Fig. S1(a)-(c) shows the ground-state energy as a function of the number of states kept in the local phonon Hilbert space for a $L = 16$ sites chain, with $\lambda = 1$ and $\Omega = 2t$. The data shows that within the Peierls phase-separated regime the ground-state energy converges for $n_{ph\text{max}} + 1 \approx 12$ with a precision of $10^{-4}$ for OBC and $10^{-3}$ for PBC. As already mentioned in the main text, a bond dimension $m = 600$ suffices to obtain convergence with a truncation error smaller than $5 \times 10^{-7}$ for OBC and $5 \times 10^{-6}$ for PBC for chains with length $L \leq 32$ and with $N \leq 16$ electrons.

Fig S1(b)-(d) confirms a known result to DMRG practitioners: numerical convergence proves to be much harder for PBC than for OBC. The data shows that even for a small system ($L = 16$ sites) up to 40 DMRG sweeps (with $L - 1$ iterations per sweep) are needed to numerically converge to the precision set above. For the $L = 32$ data shown in the main text, we performed up to 100 DMRG sweeps.

We finally note that a precise determination of the spatial electronic density profile in the Peierls phase-separated regime would be generally numerically challenging for the following reasons. Many almost-degenerate states very close to the ground state connected by translation of the electron-rich region with respect to the electron-poor region exist. This is compounded by the difficulty associated with the study of very large systems with sufficiently large number of electrons (whilst keeping the density $n$ extremely small but finite) needed to accurately represent a phase in the thermodynamical limit [54].

FIG. S1. (color online) Convergence of the ground-state energy obtained using DMRG with respect to the local Hilbert space dimension $n_{ph\text{max}} + 1$ (top) and number of iterations (bottom) for the 1D Peierls model with open (OBC) (left) and periodic (PBC) (right) boundary conditions. In this figure, we study a $L = 16$ chain for $\lambda = 1$ and $\Omega = 2t$. 