Holstein model and Peierls instability in one-dimensional boson-fermion lattice gases

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We study an ultracold Bose-Fermi atomic mixture in a one-dimensional optical lattice. When boson atoms are heavier then fermion atoms the system is described by an adiabatic Holstein model, exhibiting a Peierls instability for commensurate fermion filling factors. A bosonic density wave with a wave number of twice the Fermi wave number will appear in the quasi-one-dimensional system, due to the opening of a gap at the Fermi energy in the fermion spectrum.

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The realization of Bose-Fermi mixtures (BFM's) of ultracold atoms [1–5] is very promising for studying strong correlation phenomena, with Bose fields replacing lattice phonons in condensed-matter models. Virtual exchange of boson excitations induces fermion-fermion attractive interactions [6–9], leading to Cooper-like pairing [10–12] and enhancing the transition to fermion superfluidity. Furthermore, novel phenomena are predicted, such as the formation of composite fermionic pairs [13–15] and their subsequent pairing into quartets [13].

BFM's in optical lattices [5,14–19] open the way to the realization of various discrete models. For electrons confined to a quasi-one-dimensional (Q1D) electric conductor, coupling to bosonic phonons leads to the Peierls instability towards a charge density wave (CDW) with twice the Fermi wave number k_F [20]. The instability originates in the breakdown of electronic translational symmetry and the consequent opening of a gap Δ in the electronic spectrum due to the CDW modulation of the phonon distribution. When the modulation wave number is $2k_F$, this gap opens precisely at the Fermi momentum and the Peierls theorem [20] states that a minimal value of the energy is always attained for some finite value of the gap parameter.

The corresponding instability for a BFM in an harmonic trap was recently predicted [21]. Whereas Ref. [21] considers a Bose-Fermi mixture in a Q1D configuration without explicit periodic confinement, here we study a system subject also to an optical lattice potential. The underlying physics of the two models is quite different. In our model the coupling to bosonic atoms modifies the on-site energy of the fermions. Therefore in our model the Peierls instability for the Q1D, heavy-boson–light-fermion lattice is well described by an adiabatic Holstein model. The resulting CDW, depicted schematically in Fig. 1, consists of both a fermionic density wave and a spatial modulation in the bosonic density, with twice the Fermi wavelength. Fermionic atoms and bosonic modulations will either be positioned in alternate sites [Fig. 1(a)] or in the same sites [Fig. 1(b)] depending on the sign of fermion-boson interactions.

We consider a mixture of N_c spin-polarized fermionic atoms and N_a bosonic atoms in a Q1D optical lattice with M sites (Fig. 1). For sufficiently tight traps, only the lowest Bloch band needs to be considered and one can expand boson- and fermion-field operators in terms of the one-mode-per-site Wannier basis set [22], thus obtaining the Hubbard model,

$$H = -\sum_{\langle jk\rangle} t_c \hat{c}_j^\dagger \hat{c}_k + g_{ac}\sum_j \hat{n}_j^c \hat{n}_j^a + \frac{g_{aa}}{2}\sum_j \hat{n}_j^a(\hat{n}_j^a - 1) - \sum_{\langle jk\rangle} t_a \hat{a}_j^\dagger \hat{a}_k + \frac{\omega_0^2 \ell^2}{2}\sum_j j^2 (m_c \hat{n}_j^c + m_a \hat{n}_j^a), \quad (1)$$

where the operators $\hat{c}_j$ and $\hat{a}_j$ annihilate a spin-polarized fermion and a boson, respectively, in the jth site. The density operators $\hat{n}_j^c = \hat{c}_j^\dagger \hat{c}_j$ and $\hat{n}_j^a = \hat{a}_j^\dagger \hat{a}_j$ are the fermionic and bosonic densities, respectively. The fermion and boson atomic masses and hopping amplitudes are m_c, t_c and m_a, t_a, respectively. The collisional terms g_{aa} and g_{ac} correspond to the on-site boson-boson interaction which will be assumed positive (repulsive) throughout the paper, and on-site fermion-boson interaction, respectively. The last term on the right-hand side (RHS) of Eq. (1) is the harmonic trap potential where ω_0 is the relevant oscillator frequency and ℓ is the lattice spacing.

We will consider the case where the bosonic atoms are heavier than the fermionic atoms—e.g., ^{6}Li-^{87}Rb mixture—to the extent that they are in an insulating Mott phase with a vanishingly small number fluctuations (i.e., site-number states). This should be contrasted with Ref. [21] which takes the bosons to be in the superfluid regime (i.e., in a coherent state) and the masses to be comparable. Since the

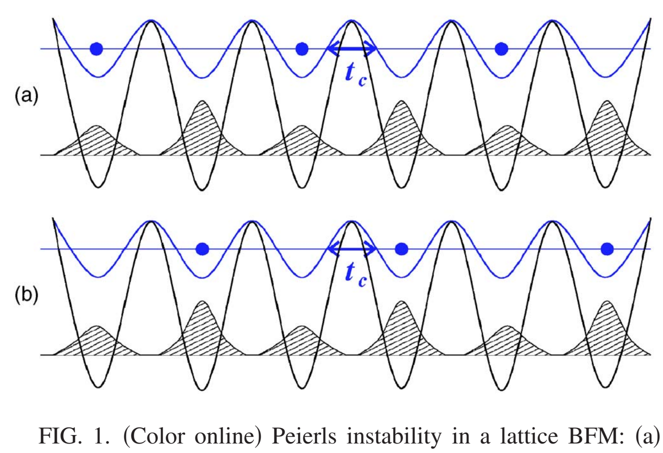

FIG. 1. (Color online) Peierls instability in a lattice BFM: (a) repulsive fermion-boson interactions and (b) attractive fermion-boson interactions. The shaded part depicts the bosonic mean-field density whereas solid circles denote fermionic atoms.

tunneling terms depend exponentially on the atomic mass and as the dynamic polarizability of the larger boson atoms is greater than the polarizability of the fermions leading to effectively deeper traps for the bosons (Fig. 1), we have t_c, $g_{aa} \gg t_a$ [23]. For a Q1D gas, boson-number fluctuations at the limit of small t_a scale linearly with t_a/g_{aa}. Therefore, we replace the bosonic density $\hat{n}_j^a$ in Eq. (1) by its c-number expectation value $n_j^a = \langle \hat{a}_j^\dagger \hat{a}_j \rangle$. The obtained results will thus be subject to the self-consistent condition that the predicted CDW be larger than boson density fluctuations.

When $t_c \gg t_a$ the system can be described by an adiabatic Holstein model, wherein its ground state is found by solving the "fast" fermionic problem

$$H_{eff}^c(\{n_i^a\}) = -\sum_{\langle jk \rangle} t_c \hat{c}_j^\dagger \hat{c}_k + \sum_j \left(\frac{m_c \omega_0^2 \ell^2}{2} j^2 + g_{ac} n_j^a \right) \hat{n}_j^c, \quad (2)$$

treating the bosonic densities n_j^a as fixed parameters and then adding the resulting fermion energy (parametrically dependent on $\{n_j^a\}$) as an effective potential to the "slow" bosonic Hamiltonian,

$$H_{eff}^a = -\sum_{\langle jk \rangle} t_a \hat{a}_j^\dagger \hat{a}_k + \frac{g_{aa}}{2} \sum_j (n_j^a)^2 + \frac{m_a \omega_0^2 \ell^2}{2} \sum_j j^2 n_j^a. \quad (3)$$

Boson hopping in Eq. (3) can be neglected provided that $t_a/\Delta < 1$ [24]. In what follows, we shall assume that $t_a = 0$ and impose self-consistency by restricting our results to the case where the CDW modulation is larger than the boson hopping energy.

For $\omega_0 = 0$, the adiabatic Holstein model is known to exhibit a Peierls instability [20], with respect to bosonic collective excitations with wave number $k = 2\pi N_c/M$, corresponding to twice the Fermi wave number $k_F = \pi N_c/M$ [25].

The 1D translation symmetry is reduced by enlarging the effective unit cell. For example, for $N_c/M = 1/2$ the unit cell doubles, opening a gap in the fermionic spectrum at the zone boundary of the folded Brillouin zone. We note that unlike the standard Su-Schrieffer-Heeger (SSH) model [26] wherein the coupling to the bosonic degrees of freedom affects the hopping probability, the bosonic CDW in our system couples to the fermions through on-site interactions.

In order to demonstrate the Peierls instability we will study how the energy of the system is affected by spatial bosonic modulations of the form

$$n_j^a = \bar{n}_j^a + \delta n_j^a \cos(kj), \quad (4)$$

with $k = 2\pi\tilde{k}/M$ and $\tilde{k}$ integer. The density $\bar{n}_j^a = [\mu - (m_a \omega_0^2 j^2/2)]/g_{aa}$, with μ denoting the chemical potential of the bosons, is the Thomas-Fermi density profile which minimizes the fixed N_a bosonic energy $H_{eff}^a + \mu(\sum_j \hat{n}_j^a - N_a)$, in the absence of fermion-boson interactions. The density modulation depth $\delta n_j^a \ll \bar{n}_j^a$ is generally a function of j,

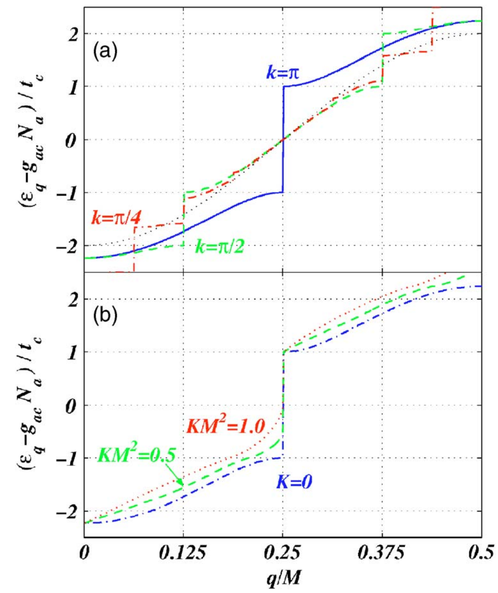

FIG. 2. (Color online) Fermionic spectrum for various bosonic modulations with $\omega_0 = 0$ (a) and as a function of ω_0 for a fixed modulation with $k = \pi$ (b).

varying slowly compared to the modulation wavelength. Under this ansatz, the fermion Hamiltonian (2) takes the form

$$H_{eff}^c = -\sum_{\langle jk \rangle} t_c \hat{c}_j^\dagger \hat{c}_k + \frac{g_{ac}}{g_{aa}} \mu \sum_j \hat{n}_j^c + \sum_j [K j^2 + \Delta_j \cos(kj)] \hat{n}_j^c, \quad (5)$$

where $K = \bar{m}(\omega_0 \ell)^2/2$ with $\bar{m} = m_c - (g_{ac}/g_{aa}) m_a$ and $\Delta_j = g_{ac} \delta n_j^a$. The mutual trapping of fermions and bosons can only take place when $g_{ac}/g_{aa} < m_c/m_a$ or fermion atoms will scatter out of the trap by the Bose mean field. In what follows we shall assume that this condition is satisfied. In Fig. 2 we plot the fermion spectrum ε_q as a function of the fermionic wave number q, obtained from direct diagonalization of the Hamiltonian (5) for constant $\Delta_j = \Delta$. In Fig. 2(a) we set $\omega_0 = 0$, whereas the effect of the trap is demonstrated in Fig. 2(b) by fixing the modulation frequency to $k = \pi$ and plotting the spectrum for various values of ω_0. It is evident that the effect of the trap is to modify the fermion dispersion away from the gap from quadratic to linear. The bosonic modulation distorts the periodicity of the lattice, thereby opening a gap at $q = \tilde{k}/2$. For $k = 2k_F(\tilde{k} = N_c)$ the gap coincides with the Fermi momentum, so that all the states with $|q|/M < \tilde{k}/2M = k_F/2\pi$ whose energy is lowered are full and all the states with $|q|/M > \tilde{k}/2M = k_F/2\pi$ which increase in energy are empty. Consequently, the fermionic energy is minimized for $k \equiv 2\pi\tilde{k}/M = 2k_F$, as depicted in Fig. 3 where we plot the fermionic ground-state energy E_c obtained by integration over the fermion spectrum up to the Fermi energy, as a function of the wave number of the spatial modulation in the boson field. Sharp minima are attained, as expected, for $k = 2\pi N_c/M = 2k_F$. Further local minima of the energy,

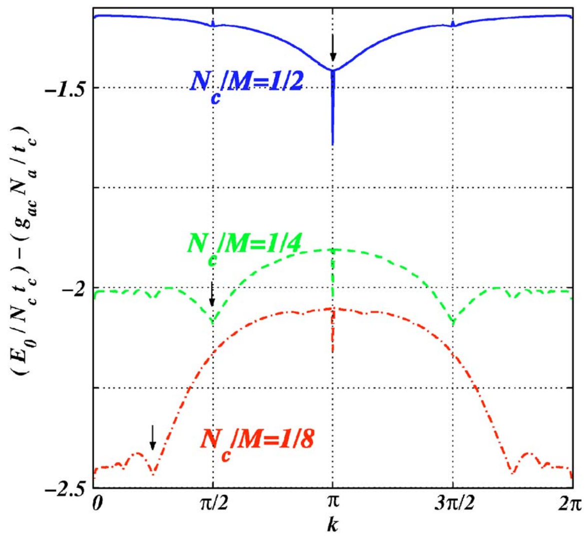

FIG. 3. (Color online) Ground-state fermionic energy as a function of the modulation wave number for various fermion filling factors: $N_c/M=1/2$ (solid line), $N_c/M=1/4$ (dashed line), and $N_c/M=1/8$ (dash-dotted line). The external trap force constant is $KM^2=0.1t_c$, and the bosonic amplitude modulation is set equal to t_c. Arrows indicate bosonic modulation wave numbers minimizing E_c.

corresponding to smaller gaps opening at the Fermi momentum, also appear for $k=2k_F/j$ with j integer.

The total energy of a half-filled system with $k=\pi(\tilde{k}=M/2)$ is plotted in Fig. 4(a), as a function of the modulation depth Δ. The boson contribution to the total energy, $E_a=E_{TF}+(g_{aa}/2g_{ac})\Sigma_j\Delta_j^2\cos^2(kj)$ [where $E_{TF}=(5/7)\mu N_a$ is the Thomas-Fermi energy], increases quadratically with the modulation depth. Hence, minimal total energy $E_{tot}=E_c+E_a$ will be attained at some finite modulation amplitude, indicating the formation of a CDW. The optimal modulation depth decreases as t_c increases since linear fermionic dispersion is attained at decreasingly small values of the gap.

The resulting CDW can be detected by means of Bragg spectroscopy [27] which probes the dynamic structure factor $S(q,\omega)$ of the system. For a periodic system $S(q,\omega)$ is maximized for q corresponding to the periodicity of the system. Since the Peierls instability involves a density modulation with wave number equal to $2k_F$, there should be a strong $q=\pi/\ell$ signature in the Bragg spectrum for bosonic as well as fermionic atoms, though the maximum will appear for different ω.

Further insight is gained by employing the commonly used continuum model [28]. For simplicity, we will focus, in what follows, on the half-filling case $N_c/M=1/2$ where the bosonic order parameter minimizing E_c is of the form $n_j^a=\bar{n}_j^a+\delta n_j^a\cos(\pi j)$. A similar treatment can be applied for other commensurate fermion filling factors. In the continuum limit, applicable when the lattice correlation length $\xi=2lt_c/\Delta$ is greater than the lattice constant l, the fermionic Hamiltonian (5) is rewritten as

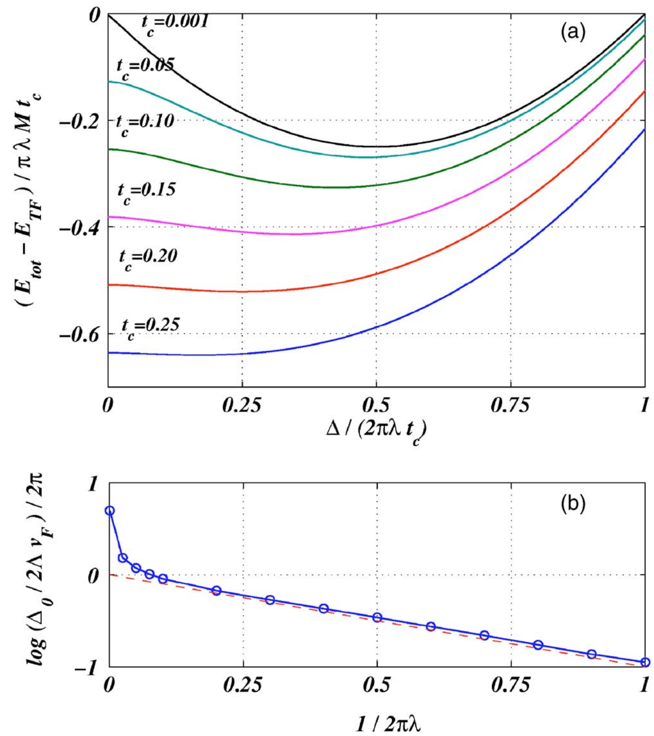

FIG. 4. (Color online) Total system energy as a function of Δ for various values of t_c (a) and optimal gap values as a function of t_c (b). The dashed line depicts the strong-coupling behavior of Eq. (13).

$$H_c=\int dx\Psi^{\dagger}(x)\left[-\frac{1}{2m}\sigma_0\frac{\partial^2}{\partial x^2}-\imath\hbar v_F\sigma_3\frac{\partial}{\partial x}+\Delta(x)\sigma_2+\sigma_0V(x)\right]\Psi(x), \tag{6}$$

where

$$\Psi(x)\equiv\begin{pmatrix}\psi_1(x)\\ \psi_2(x)\end{pmatrix}$$

is the spinor representation of the fermionic field in terms of right- and left-moving atoms, σ_i are Pauli matrices, σ_0 is the identity matrix, and m is the effective atomic mass. The continuum limit for the trap potential is $V(x)=m\omega_0^2x^2/2$, and the gap parameter is $\Delta_j\rightarrow\Delta(x)$. We note that in the Takayama-Lin-Liu-Maki (TLM) model [28] which is the continuum limit of the SSH model, there is no confining potential and the dispersion is linearized. Moreover σ_1 appears for the coupling between left and right movers because the TLM coupling to phonons modifies the off-diagonal hopping rate, whereas in our case the coupling to the bose field modifies the diagonal self-energy terms.

The fermion spectrum is obtained by Bogoliubov–de Gennes (BdG) diagonalization of the fermionic Hamiltonian. It may appear that due to the harmonic trapping potential the 1D translation symmetry for the fermionic atoms is lost [29], thereby inhibiting the Peierls instability. To demonstrate that the Peierls instability will appear even in systems with reduced translation symmetry, we follow a similar method to the one used by Anderson to calculate the excitation spectrum of a superconductor with local disorder [30]. In this technique, which is essentially equivalent to a local density approximation (LDA), the fermionic spectrum is calculated by spatial averaging over spectra with different local order parameters. We expand the field operators $\psi_{1,2}(x)$ as

$$\psi_1(x) = \sum_n \Phi_n(x) u_n \hat{d}_n, \quad \psi_2(x) = \sum_n \Phi_n(x) v_n \hat{d}_n, \qquad (7)$$

where $\hat{d}_n$ are fermionic mode annihilation operators and $\Phi_n(x)$ are harmonic oscillator eigenfunctions. Substituting Eq. (7) into Eq. (6) and requiring that $H_c = \Sigma_n \varepsilon_n \hat{d}_n^\dagger \hat{d}_n$, we obtain two coupled BdG equations.

The above expansion in harmonic oscillator eigenfunctions eliminates the trapping potential from the BdG equations. One can now proceed by calculating the off-diagonal matrix elements—i.e., expand Δ in terms of the asymptotic expansion of the harmonic oscillator functions [21]. Below we use a more general approach which is useful for any arbitrary trapping potential and can be equally applied to treat local potential fluctuations. In the framework of the LDA, we diagonalize the BdG equations for a local order parameter Δ. The functions $\Phi_n(x)$ diagonalize the spatial part of the BdG equations which simplify to

$$(\varepsilon_n - E_n) u_n = - \imath \Delta v_n, \quad (\varepsilon_n + E_n) v_n = \imath \Delta u_n. \qquad (8)$$

Diagonalization of Eqs. (8) results in the local fermionic spectrum $\varepsilon_n = \sqrt{E_n^2 + \Delta^2}$ in terms of the oscillator's energy $E_n = (n_F - n + 1/2)\omega_0$ measured with respect to the Fermi energy $E_{n_F} = (n_F + 1/2)\omega_0$. This spectrum compares well with the numerical spectra of Fig. 2(b) at the continuum limit. In the limit $\omega_0 \to 0$, we have $n\omega_0 \to v_F q$, where $v_F = 2t_c \ell$ is the Fermi velocity (with $\hbar$ set equal to 1) and q is the wave number for the plane-wave solution of the nonconfined problem, so that the well-known spectrum for a $\cos(\pi j)$ modulation $\varepsilon_q = \pm \sqrt{(q v_F)^2 + \Delta^2}$ is reproduced.

Having found the fermionic local spectrum, the total energy functional of the system is given as the sum $E_{tot} = E_c + E_a$. The fermion energy E_c is given within the LDA as

$$E_c = \sum_{n=1}^{N_c} \int dx |\Phi_n(x)|^2 \sqrt{E_n^2 + \Delta(x)^2} \simeq \sum_{n=1}^{N_c} \sqrt{E_n^2 + \Delta_0^2}, \qquad (9)$$

where Δ_0 is a constant order parameter whose value is the spatial average of $\Delta(x)$. The boson contribution E_a is given by

$$E_a = \frac{1}{2\pi \lambda v_F} \int \Delta(x)^2 dx, \qquad (10)$$

where $\lambda = g_{ac}^2/(2\pi g_{aa} t_c)$ is the dimensionless fermion-boson coupling constant. For a constant $\Delta(x) = \Delta_0$ we have $E_a = (g_{aa}/2g_{ac}^2) M \Delta_0^2$. Minimizing E_{tot} by setting its variation with respect to $\Delta(x)$ to zero, we obtain a self-consistent gap equation for $\Delta(x)$,

$$\Delta(x) = \frac{\lambda \omega_0}{2} \sum_{n=1}^{N_c} |\Phi_n(x)|^2 \frac{\Delta_0}{\sqrt{E_n^2 + \Delta_0^2}}, \qquad (11)$$

similar to the gap equation obtained by Anderson [30].

For sufficiently wide traps, $|\Phi_n(x)|^2$ can be replaced by its average value, thus restoring the familiar gap equation

$$1 = v_F \lambda \int_0^\Lambda dq (\sqrt{v_F q^2 + \Delta_0^2})^{-1}, \qquad (12)$$

where $\Lambda = \pi/2\ell$ is a momentum cutoff of the order of the fermionic bandwidth. Equation (12) is valid as long as one can replace the fermionic density of states by its average value. This criterion, which also applies to the Anderson theorem, is satisfied in the continuum limit [31], where the coherence length is much greater than the lattice spacing $\xi \gg l$ [32].

In the weak-coupling regime $v_F \Lambda \ll \Delta_0$, Eq. (12) is solved by $\Delta_0 = v_F \lambda \Lambda = g_{ac}^2 / 2g_{aa}$, whereas in the strong-coupling regime $v_F \Lambda \gg \Delta_0$ we have the well-known solution

$$\Delta_0 = 2 v_F \Lambda \exp(-1/\lambda). \qquad (13)$$

Our numerical results agree well with these continuum predictions as demonstrated in Fig. 4. The weak-coupling limit is confirmed by the low t_c curves in Fig. 4(a), which attain a minimum at $\Delta_0 = \pi \lambda t_c = v_F \lambda \Lambda$. The strong-coupling behavior is depicted in Fig. 4(b) where the minimum-energy gap Δ_0 is shown to precisely follow Eq. (13) (dashed line) for sufficiently large t_c.

To conclude, we have shown that a lattice BFM with heavy bosons and light fermions can be described by an adiabatic Holstein model. The ground state of the system at $T=0$ is a Peierls CDW. At finite T, the CDW could only be observed provided that $T \ll \Delta_0$. The fermionic excitation spectrum depends exponentially on the ratio T/Δ_0 so that the number of excited fermionic atoms is exponentially small. However, since the bosonic spectrum does not contain a finite gap, the considerations on the critical temperature T_p for obserbving a Peierls CDW due to the bosonic site-number fluctuations are much more elaborate. It should also be mentioned that for the realistic case of finite bosonic hopping one should expect, for a strong enough interaction between the fermionic and bosonic atoms, a fermionic polaron phase [18]. As for quantum fluctuations, it has been shown [24,25] that for a critical fermion-boson coupling strength above which $\Delta > t_a$ the ground state of the system is a Peierls CDW state.

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