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 \( \Delta \) 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 \( N_f \) spin-polarized fermionic atoms and \( N_b \) 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.

\[
H = - \sum_{\langle jk \rangle} t_{jk} \hat{c}_j^\dagger \hat{c}_k + g_{\text{ff}} \sum_j n_{fj}^2 \hat{n}_{fj}^2 + \frac{g_{\text{bb}}}{2} \sum_j n_{bj}^2 (\hat{a}_{bj}^\dagger \hat{a}_{bj} - 1) - \sum_{\langle jk \rangle} t_{jk} \hat{a}_j^\dagger \hat{a}_k + \frac{\omega_0 \ell^2}{2} \sum_j \hat{j}_j^2 (m_{bj} \hat{n}_{bj}^2 + m_{bf} \hat{n}_{bf}^2),
\]

where the operators \( \hat{c}_j \) and \( \hat{a}_j \) annihilate a spin-polarized fermion and a boson, respectively, in the \( j \)th site. The density operators \( \hat{n}_{bf}^j = \hat{c}_j^\dagger \hat{c}_j \) and \( \hat{n}_{bj} = \hat{a}_j^\dagger \hat{a}_j \) are the fermionic and bosonic densities, respectively. The fermion and boson atomic masses and hopping amplitudes are \( m_{\xi} \), \( t_{\xi} \) and \( m_{\alpha} \), \( t_{\alpha} \), respectively. The collisional terms \( g_{\text{ff}} \) and \( g_{\text{bb}} \) 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 \( \omega_0 \) is the relevant oscillator frequency and \( \ell \) is the lattice spacing.

We will consider the case where the bosonic atoms are heavier than the fermionic atoms—e.g., \(^6\text{Li}–^8\text{Rb} \) 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.](image-url)
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 \( t_e, g_{aa} \gg t_a \) [23]. For a 1D gas, boson-number fluctuations at the limit of small \( t_a \) scale linearly with \( t_a / g_{aa} \). Therefore, we replace the bosonic density \( n_{ij}^b \) in Eq. (1) by its c-number expectation value \( n_{ij}^b = \langle \hat{a}_i^\dagger \hat{a}_j \rangle \). The obtained results will thus be subject to the self-consistent condition that the predicted CDW be larger than boson density fluctuations.

When \( t_a \gg t_e \), the system can be described by an adiabatic Holstein model, wherein its ground state is found by solving the “fast” fermionic problem

\[
H_{eff}^f (\{ n_{ij}^f \}) = - \sum_{\langle ij \rangle} t_e c_i^\dagger c_j + \sum_j \left( \frac{m_e \omega_c^2 j^2}{2} + g_{ac} n_j^f \right) n_j^f, \tag{2}
\]

treating the bosonic densities \( n_{ij}^a \) as fixed parameters and then adding the resulting fermion energy (parametrically dependent on \( \{ n_{ij}^f \} \)) as an effective potential to the “slow” bosonic Hamiltonian,

\[
H_{eff}^a = - \sum_{\langle ij \rangle} t_a \hat{a}_i^\dagger \hat{a}_j + \frac{g_{aa}}{2} \sum_j (n_j^a)^2 + \frac{m_a \omega_c^2}{2} \sum_j j^2 n_j^a, \tag{3}
\]

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 \( \omega_c = 0 \), 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

\[
n_{ij}^f = n_{ij}^f + \Delta n_{ij}^f \cos(kj), \tag{4}
\]

with \( k = 2 \pi k / M \) and \( k \) integer. The density \( n_{ij}^f = \left[ \mu - (m_e \omega_c^2 j^2 / 2) \right] / g_{aa} \), with \( \mu \) denoting the chemical potential of the bosons, is the Thomas-Fermi density profile which minimizes the fixed \( N_c \) bosonic energy \( H_{eff}^a + \mu (\sum_j n_{ij}^a - N_a) \), in the absence of fermion-boson interactions. The density modulation depth \( \Delta n_{ij}^f = \bar{n}_{ij}^f \) is generally a function of \( j \), varying slowly compared to the modulation wavelength. Under this ansatz, the fermion Hamiltonian (2) takes the form

\[
H_{eff} = - \sum_{\langle ij \rangle} t_e \hat{c}_i^\dagger \hat{c}_j + \frac{g_{aa}}{g_{ac}} \sum_j n_{ij}^b + \sum_j \left[ Kj^2 + \Delta_j \cos(kj) \right] n_{ij}^f, \tag{5}
\]

where \( K = \bar{m}_e (\omega_c \ell^2 / 2) \) with \( \bar{m}_e = m_e \omega_c / g_{ac} m_a \) and \( \Delta_j = g_{ac} \Delta n_{ij}^f \). The mutual trapping of fermions and bosons can only take place when \( g_{ac} / g_{aa} = m_a / m_e \) 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 \( e_q \) as a function of the fermionic wave number \( q \), obtained from direct diagonalization of the Hamiltonian (5) for constant \( \Delta = \Delta_0 \). In Fig. 2(a) we set \( \omega_c = 0 \), 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 \( \omega_c \). 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 \( q = k / 2 \). For \( k = 2 k_F \) the gap coincides with the Fermi momentum, so that all the states with \( \left| q / M \right| < k / 2M = k_F / 2 \pi \) whose energy is lowered are full and all the states with \( \left| q / M \right| > k / 2M = k_F / 2 \pi \) which increase in energy are empty. Consequently, the fermionic energy is minimized for \( k = 2 \pi k / M = 2 k_F \), 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 \( k = 2 \pi N_c / M = 2 k_F \). Further local minima of the energy,
corresponding to smaller gaps opening at the Fermi momentum, also appear for $k = 2k_F/k$ with $j$ integer.

The total energy of a half-filled system with $k = \pi/k = M/2$ is plotted in Fig. 4(a), as a function of the modulation depth $\Delta$. The boson contribution to the total energy, $E_a = E_{TF} + \langle g_{so}/2g_{sc} \rangle \Sigma \Delta_j^2 \cos^2(k_j)$ [where $E_{TF} = (5/7)\mu N_a$ is the Thomas-Fermi energy], increases quadratically with the modulation depth. Hence, minimal total energy $E_{tot} = E_a + E_c$ 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, 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 $\omega$.

Further insight is gained by employing the commonly used continuum model. For simplicity, we will focus, in what follows, on the half-filling case $N_f/M = 1/2$ where the bosonic order parameter minimizing $E_c$ is of the form $n_j^b = n_j^0 + \delta n_j^b \cos(\pi j)$. A similar treatment can be applied for other commensurate fermion filling factors. In the continuum limit, applicable when the lattice correlation length $\xi = 2l_t/\Delta$ is greater than the lattice constant $l$, the fermionic Hamiltonian (5) is rewritten as

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

where

\[
\Psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}
\]

is the spinor representation of the fermionic field in terms of right- and left-moving atoms, $\sigma_2$ are Pauli matrices, $\sigma_0$ is the identity matrix, and $m$ is the effective atomic mass. The continuum limit for the trap potential is $V(x) = \hbar_0 x^2/2$, and the gap parameter is $\Delta_c - \Delta(x)$. We note that the Takayama-Lin-Liu-Maki (TLM) model is the continuum limit of the SSH model, there is no confining potential and the dispersion is linearized. Moreover, $\sigma_1$ 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 boson 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, 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 \( \psi_l(x) \) as

\[
\psi_l(x) = \sum_n \Phi_n(x) \hat{d}_n, \quad \psi_\uparrow(x) = \sum_n \Phi_n(x) \hat{d}^\dagger_n,
\]

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 \( H_c = \sum_n \epsilon_n \hat{d}_n \hat{d}^\dagger_n \), 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 the fermionic local spectrum, the total energy functional of the system is given as the sum

\[
E_{\text{tot}} = \sum F_q + \Delta_{\text{tot}} = \frac{1}{2} \int dx |\Phi_n(x)|^2 \sqrt{E_n^2 + \Delta(x)^2},
\]

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

\[
E_a = \frac{1}{2} \frac{\lambda}{2\pi v_F} \int dx (\Delta(x))^2 dx,
\]

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

\[
\Delta(x) = \frac{\lambda_{\text{loc}} N_c}{2} \sum_{q=1}^{N_c} |\Phi_n(x)|^2 \sqrt{E_n^2 + \Delta_0^2},
\]

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

\[
1 = v_F \int dx (\sqrt{v_F^2 q^2 + \Delta_0^2})^{-1},
\]

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 \( \xi \gg \ell \) [32].

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

\[
\Delta_0 = 2v_F \Lambda \exp(-1/\lambda).
\]

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 \( \Delta_0 = \pi \Lambda t_c = v_F \Lambda \). The strong-coupling behavior is depicted in Fig. 4(b) where the minimum-energy gap \( \Delta_0 \) 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 \( T < \Delta_0 \). The fermionic excitation spectrum depends exponentially on the ratio \( T/\Delta_0 \) 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 \( T_c \) for observing 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 \( \Delta > t_c \) the ground state of the system is a Peierls CDW state.

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[23] A rough estimate for the mass difference at which bosonic hopping $t_a$ is negligible with respect to fermionic hopping $t_c$ is obtained by assuming the same polarizability for fermions and bosons and approximating the lowest-band Wannier functions as Gaussians. This leads to the expression $\ln(t_d/t_c) = \frac{\sigma_c^2}{\sigma_a^2}$ where $\sigma_{a,c} = \sqrt{\hbar/m_{a,c} \omega_{a,c}}$ is the characteristic size of the (Gaussian) ground state for bosons and fermions, respectively. Since in order to allow tunneling characteristic experimental values have $t_c \sim \sigma_c$ and since $\omega_{a,c} \propto m_{a,c}^{-1/2}$, we find $\ln(t_d/t_c) = \alpha (\sqrt{m_c} - \sqrt{m_a})$ where $\alpha$ is of order $1$. It is therefore evident that the mass of the atoms should only differ by a few atomic mass units for $t_d$ to be exponentially small with respect to $t_c$.
[27] A. M. Rey et al., e-print cond-mat/0406552.
[29] The same effect can also be viewed as the smearing the Fermi surface [21].
[31] It should be noted that the continuum criterion is a necessary and sufficient condition for our analytic treatment starting with Eq. (6).