The recent realization of Bose-Fermi mixtures of ultracold atoms [1] is very promising for studying various strong correlation phenomena, with Bose fields replacing the lattice phonons of classic condensed-matter models. Virtual exchange of the Bose-field excitations were shown to induce fermion-fermion attractive interactions [2, 3], leading to Cooper-like pairing [4] and enhancing the transition to fermion superfluidity. Furthermore, completely novel phenomena were predicted, such as the formation of boson-fermion composite fermions [5, 6, 7, 8] and their subsequent pairing into quartets [9].

One particularly interesting direction is the possibility of mutual fermion-boson trapping in optical lattices [10, 11, 12, 13], opening the way to the realization of various discrete lattice models. For electrons confined to a quasi-one-dimensional electric conductor the coupling to bosonic phonons leads to the Peierls instability towards a charge density wave (CDW) with wave number equal to twice the Fermi wavelength $2k_F$. The corresponding instability for a Bose-Fermi mixture in an harmonic trap was recently predicted [14]. In this article we study the Peierls instability in a mixture of light fermionic and heavy bosonic atoms in a quasi-one-dimensional optical lattice, shown to be 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 wave length. Fermionic atoms and bosonic modulations will either position in alternate sites (Fig. 1a) or in the same sites (Fig. 1b) depending on the sign of the fermion-boson interactions.

We consider a mixture of $N_e$ spin polarized fermionic atoms and $N_a$ bosonic atoms confined to a quasi one-dimensional (Q1D) optical lattice with $M$ sites (see Fig. 4). For a strong optical field, one can expand boson- and fermion field operators in terms of the one-mode-per-site Wannier basis set [15], thus obtaining the lowest Bloch-band Hubbard model,

$$H = \sum_{jk} t c_j^\dagger c_k + g_{ac} \sum_j \hat{n}_j^c \hat{n}_j^a + \frac{g_{aa}}{2} \sum_j \hat{n}_j^a (\hat{n}_j^a - 1)$$

$$- \sum_{jk} t_a \hat{a}_j^\dagger \hat{a}_k + \frac{\omega_0^2 \ell^2}{2} \sum_j j^2 \left( m_e \hat{n}_j^c + m_a \hat{n}_j^a \right),$$

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 $\hat{n}_j^c = \hat{c}_j^\dagger \hat{c}_j$ 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 $m_e$, $t_e$ and $m_a$, $t_a$ respectively. The collisional terms $g_{ac}$ and $g_{aa}$ correspond to on-site boson-boson interaction which will be assumed positive (repulsive) throughout the paper, and onsite fermion-boson interaction, respectively. The last term on the r.h.s. of Eq. (1) is the harmonic trap potential where $\omega_0$ is the relevant oscillator frequency and $\ell$ is the lattice spacing.

In the weak-interaction limit the bosonic field in Eq. (1) may be treated in a mean-field approximation, replacing the bosonic density $\hat{n}_j^a$ by its $c$-number expectation value $n_j^a = \langle \hat{a}_j^\dagger \hat{a}_j \rangle$. We will further assume that the bosonic atoms are heavier than the fermionic atoms as for a $\text{Li}^{87}\text{Rb}$ mixture. Since the tunneling term depends exponentially on the atomic mass and since the dynamic polarizability of the larger boson atoms is greater than the polarizability of the fermions leading to effectively deeper traps for the bosons (see Fig. 1), we can neglect the bosonic hopping term and retain only fermion tunneling [21]. In this limit the system can be described by an adiabatic Holstein model, where its ground state is found

![fig1](image-url)
adiabatically by solving the ‘fast’ fermionic problem

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

(2)

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

$$H_{\text{eff}}^\varepsilon = \frac{g_{aa}}{2} \sum_j (n_j^a)^2 + \frac{m_c \omega^2 \ell^2}{2} \sum_j j^2 n_j^a .$$

(3)

For $\omega_0 = 0$, the adiabatic Holstein model is known to exhibit a Peierls instability [21], with respect to bosonic collective excitations with wave number equal to $N_c/M$, corresponding to twice the Fermi wave length $k_F = N_c/2M$ [22]. It is favorable for the system to reduce the 1D translation symmetry by enlarging the effective unit cell, thereby opening a gap in the fermionic spectrum. When the wavelength of the excitation is $2k_F$ this gap coincides with the discontinuity of the Fermi distribution, so that all fermions are on the side of the spectrum which lowers in energy. 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. It should be noted that in difference to the standard Su-Schrieffer-Heeger (SSH) model [22] used for quasi one-dimensional systems exhibiting a Peierls instability, the coupling to the bosonic degrees of freedom in our system is on-site whereas in the SSH model it effects the hopping probability.

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

$$n_j^a = \bar{n}_j^a + \delta n_j^a \cos \left( \frac{2\pi k_j}{M} \right) .$$

(4)

The density $\bar{n}_j^a = [\mu - (m_c \omega^2 \ell^2/2)]/g_{aa}$ with $\mu$ denoting the chemical potential of the bosons, is the Thomas-Fermi density profile which minimizes the fixed $N_a$ bosonic energy $H_{\text{eff}}^\varepsilon + \mu(\sum_j \bar{n}_j^a - N_a)$, 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 $j$, varying slowly compared to the modulation wavelength.

Under the ansatz [4] the fermion Hamiltonian [2] takes the form

$$H_{\text{eff}}^\varepsilon = -\sum \langle jk \rangle t_c \hat{c}_j^\dagger \hat{c}_k + \frac{g_{ac}}{g_{aa}} \mu \sum_j \hat{n}_j^c$$

$$+ \sum_j \left[ \kappa \left( \frac{j}{M} \right)^2 + \Delta_j \cos \left( 2\pi k \frac{j}{M} \right) \right] \hat{n}_j^c ,$$

(5)

where $\kappa = m_c(\omega_0 \ell^2)/2$ with $m_c = m - (g_{ac}/g_{aa})m_a$, and $\Delta_j = g_{ac}\delta n_j^a$. Evidently, the mutual trapping of both fermions and bosons can only take place when $g_{ac}/g_{aa} \leq m_c/m_a$ or fermion atoms will scatter out of the trap by the boson mean-field. In what follows we shall assume that this condition is satisfied. In Fig. 2 we plot the fermionic energy spectrum, $E_q$, as a function of the Fermionic wave number, $q$, obtained from direct diagonalization of the fermionic Hamiltonian [5] for constant $\Delta_j = \Delta$. In Fig. 2a the harmonic trap frequency is set equal to zero, whereas the effect of the trap is demonstrated in Fig. 2b by fixing the modulation frequency to $k = M/2$ and plotting the spectrum for various values of $\omega_0$. The bosonic modulation distorts the periodicity of the lattice, thereby opening a gap at $q = k/2$. For $k/M = 2k_F$ the gap coincides with the Fermi momentum, so that all the states with $|q|/M < k/2M = k_F$ whose energy is lowered are full and all the states with $|q|/M > k/2M = k_F$ which increase in energy are empty. Consequently, the fermionic energy is minimized for $k = 2k_F$, as depicted in Fig. 2, 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 wavenumber of the spatial modulation in the boson field. Sharp minima are attained as expected, for $k/M = N_c/M = 2k_F$. Further local minima of the energy, corresponding to smaller gaps opening at the Fermi momentum, also appear for integer multiples of $k/M$.

The total energy of a half-filled system with $k = M/2$ is plotted in Fig. 4, as a function of the modulation depth $\Delta$. As can be seen from the proceeding analysis, the reduction in $E_c$ due to the bosonic modula-
The fermionic Hamiltonian (5) is rewritten as minimizing

\[ \min \text{ (simplified, we will focus in what follows, on the half fill-} \]

by employing the commonly used continuum model. For excitation spectrum by means of Bragg spectroscopy \[24\].

Further insight into these numerical results is gained by means of atom interferometry where the formation of a CDW is indeed energetically favorable. At some finite modulation amplitude indicating that the minimum in the total energy of the system is the Thomas-Fermi energy. Thus, boson-boson repulsive interactions increase the energy quadratically with the modulation depth. Consequently there is always a minimum in the total energy of the system \( E_{tot} = E_c + E_a \) at some finite modulation amplitude indicating that the formation of a CDW is indeed energetically favorable. The optimal modulation depth decreases as \( \kappa \) increases since linear fermionic dispersion is attained at decreasingly small values of the gap. The resulting CDW can be detected by means of atom interferometry where the doubling of the unit cell will be manifested in the inverse lattice spacing or via the measurement of the collective excitation spectrum by means of Bragg spectroscopy \[23\].

Further insight into these numerical results is gained by employing the commonly used continuum model. For simplicity, we will focus in what follows, on the half filling case \( N_c/M = 1/2 \) where the bosonic order parameter minimizing \( E_c \) of the form \( n_q = a_q^\dagger a_q + \delta n_q \cos(\pi j) \). We note that similar treatment can be applied for other commensurate fermion filling factors. In the continuum limit, the fermionic Hamiltonian \[6\] is rewritten as

\[ H_c = \int dx \Psi^\dagger(x) \left[ -\frac{1}{2m} \frac{\partial^2}{\partial x^2} - V(x) \right] \Psi(x) , \]

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, \( \sigma_i \) are Pauli matrices \( \sigma_0 \) is the identity matrix, and \( m \) is the effective atomic mass. The continuum limit for the trap potential is \( V(x) = m\omega_0^2 x^2/2 \) and the gap parameter is \( \Delta_j \to \Delta(x) \). We note that in the Takayama-Liu-Liu-Maki (TLM) model \[22\] which is the continuum limit of the SSH model, there is no confining potential and the dispersion is linearized. Moreover \( \sigma_j \) 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. We follow a similar method to the one used by Anderson to calculate the excitation spectrum of a superconductor with local disorder \[20\]. 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

\[ \psi_1(x) = \sum_n u_n(x) \hat{d}_n , \psi_2(x) = \sum_n v_n(x) \hat{d}_n , \]

where \( \hat{d}_n \) are fermionic mode annihilation operators. The functions \( u_n(x), v_n(x) \) are assumed to take the form

\[ u_n(x) = \Phi_n(x) u_n , \quad v_n(x) = \Phi_n(x) v_n , \]

where \( \Phi_n(x) \) are harmonic oscillator eigenfunctions. Substituting Eq. \[7\] and Eq. \[8\] into Eq. \[6\] and requiring that \( H_c = \sum_n \varepsilon_n \hat{d}_n^\dagger \hat{d}_n \), we obtain two coupled BdG equations. In the framework of the LDA, we diagonalize the BdG equations for a local order parameter \( \Delta \). The functions \( \Phi_n(x) \) diagonalize the spatial part of the BdG equations which simplify to

\[ \begin{align*}
\langle \varepsilon - E_n \rangle u_n &= -i \Delta v_n \\
\langle \varepsilon + E_n \rangle v_n &= i \Delta u_n .
\end{align*} \]

Diagonalization of \[[1]1\] 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 2b at the continuum limit. In the limit \( \omega_0 \to 0 \), we have \( n_F \omega_0 = v_F q \), where \( v_F = 2t_c \ell \) is the Fermi velocity (with \( \hbar \) set equal to 1) and \( q \) is the wave number for the plain wave solution of the non-confined problem, so that the well known spectrum for a \( \cos(\pi j) \) modulation \( \varepsilon_q = \pm \sqrt{(qv_F)^2 + \Delta^2} \) 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

\[ \begin{array}{c}
\text{FIG. 3: Ground-state fermionic energy as a function of the modulation wavenumber for various fermion filling factors:} \\
N_c/M = 1/2 \text{ (solid), } N_c/M = 1/4 \text{ (dashed), } N_c/M = 1/8 \text{ (dash-dotted). The external trap frequency is set to } \kappa = 0.1t_c \text{ and the bosonic amplitude modulation is set equal to } \kappa_c. \text{ Arrows indicate the bosonic modulation wavenumber minimizing } E_c.
\end{array} \]
as

\[ E_c = \sum_{n=1}^{N_c} \int dx |\Phi_n(x)|^2 \sqrt{E_n^2 + \Delta(x)^2} \simeq \sum_{n=1}^{N_c} \sqrt{E_n^2 + \Delta_0^2}, \tag{10} \]

where \( \Delta_0 \) is a constant order parameter whose value is the spatial average of \( \Delta(x) \). The boson contribution \( E_a \) is given by

\[ E_a = \frac{1}{2\pi \lambda v_F} \int \Delta(x)^2 dx, \tag{11} \]

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 \( E_a = (g_{aa}/2g_{ac}) M \Delta_0^2 \). Minimizing \( E_{tot} \) by setting its variation with respect to \( \Delta(x) \) to zero, we obtain a self-consistent gap equation for \( \Delta(x) \),

\[ \Delta(x) = \frac{\lambda \Delta_0}{2} \sum_{n=1}^{N_c} |\Phi_n(x)|^2 \frac{\Delta_0}{\sqrt{E_n^2 + \Delta_0^2}} \tag{12} \]

which is similar in form to the gap equation obtained by Anderson \[26\].

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

\[ 1 = v_F \lambda \int_0^\Lambda dq \left( \sqrt{(v_F q^2 + \Delta_0^2)} \right)^{-1}, \tag{13} \]

where \( \Lambda = \pi/2\ell \) is a momentum cut-off of the order of the fermionic band width. In the weak coupling regime \( v_F \Lambda \ll \Delta_0 \), Eq. \[13\] 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

\[ \Delta_0 = 2v_F \Lambda \exp(-1/\lambda). \tag{14} \]

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. 4a, which attain a minimum at \( \Delta_0 = \pi \lambda t_c = v_F \Lambda \). The strong coupling behavior is depicted in Fig. 4b where the minimum energy gap \( \Delta_0 \) is shown to precisely follow Eq. \[14\] (dashed line) for sufficiently large \( t_c \).

The formation of a CDW in the Fermi-Bose mixture will be affected by finite temperature effects. To observe Peierls instability the temperature should be lower than the gap \( T \ll \Delta_0 \). The fermionic excitation spectrum depends exponentially on the ratio \( T/\Delta_0 \) so that the number of excited fermionic atoms should be exponentially small. However the density of thermal bosonic excitations has a power-law behavior \( n_{ex} = (N_a/V)(T/T_c)^{1/2} \), where \( V \) is the volume and \( T_c \) is the critical temperature. This leads to a more restrictive constraint \( T/T_c \ll (\Delta_0/g_{ac}\bar{n})^2 \), where \( \bar{n} \) is the bosonic density.

FIG. 4: Total energy of the system as a function of the gap \( \Delta \) for various values of \( t_c \) (a) and optimal gap values as a function of \( t_c \) (b). The dashed line depicts the predicted strong coupling behavior of Eq. \[14\].

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To certain extent, the adiabatic limit in our case is even better justified than in the original Holstein model which relies on the fixed electron/atom mass-ratio, since $t_a/t_b$ is determined by the overlap of the Wannier functions, decaying exponentially with mass-ratio and relative trap depths.

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