Peierls instability for confined ultracold boson-fermion lattice gases

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Abstract

We study an ultracold Bose-Fermi 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. We demonstrate the formation of a density wave numerically and via a continuum analytical model.

The Model

We consider a mixture of N_c spin polarized fermionic atoms and N_a bosonic atoms confined to a quasi one dimensional (Q1D) optical lattice with M sites (see Fig. bellow). For a strong optical field, one can expand boson- and fermion field operators in terms of the one-mode-per-site Wannier basis set [1], thus obtaining the lowest Bloch-band Hubbard model

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

- $\hat{c}_j$ is a spin polarized fermion annihilation operator which annihilates a fermion at the j-th site
- $\hat{a}_j$ is a boson annihilation operator which annihilates a fermion at the j-th site
- $\hat{n}_j^c = \hat{c}_j^+\hat{c}_j$ is the fermion density operator for the j-th site
- $\hat{n}_j^a = \hat{a}_j^+\hat{a}_j$ is the bosonic density operator
- t_c and t_a are the hopping amplitudes for fermions and bosons
- m_c and m_a are fermion and boson atomic masses
- g_{aa} is the onsite boson-boson interaction strength
- g_{ac} is the onsite fermion-boson interaction strength
- ω_0 in the last term on the r.h.s is the frequency of the trapping harmonic potential
- l is the lattice spacing

The Adiabatic Holstein Model

Approximations:

1. Replacing the bosonic density $\hat{n}_j^a$ by its c-number $\hat{n}_j^a = \langle \hat{a}_j^+\hat{a}_j\rangle$ expectation value
2. Bosonic atoms are heavier than the fermionic atoms, e.g. , ^{6}Li and ^{87}Rb mixture.

In his limit the system can be described by an adiabatic Holstein model.

Adiabatic Approximation

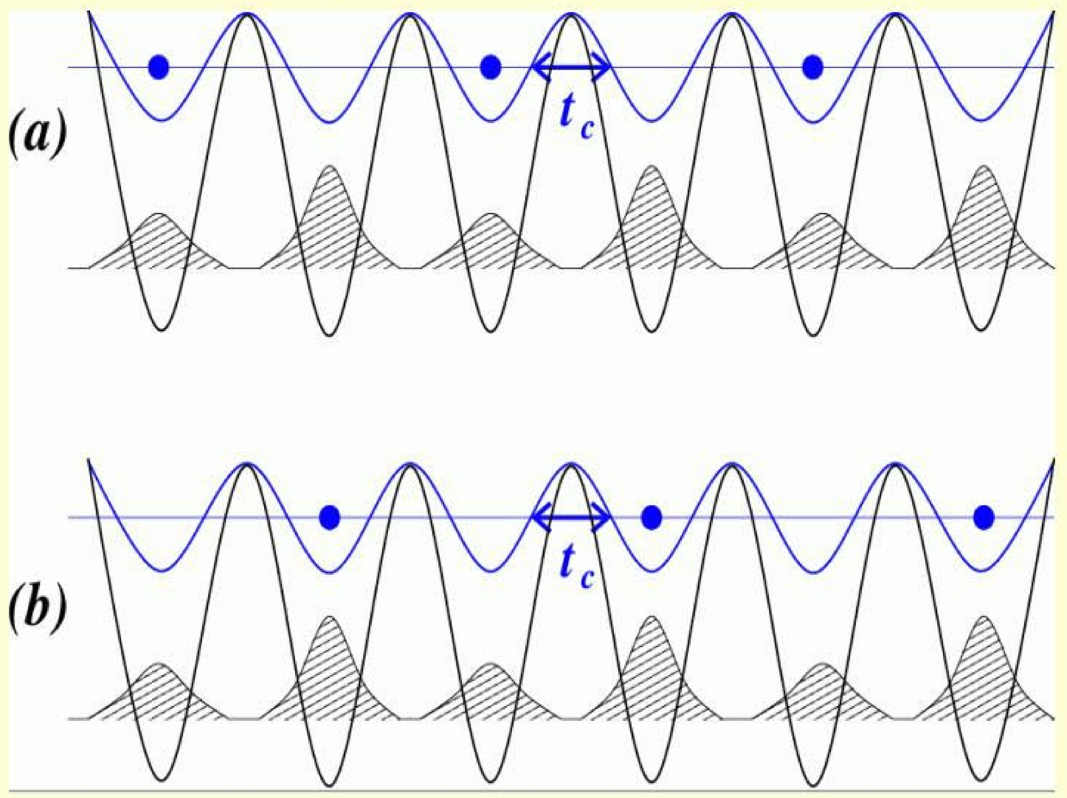
Fast fermionic degrees of freedom:

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

Slow bosonic degrees of freedom:

$$H_{eff}^a = \frac{g_{aa}}{2}\sum_j (n_j^a)^2 + \frac{m_a\omega_0^2\ell^2}{2}\sum_j j^2 n_j^a \, .$$

Static bosonic field is treated with the Thomas-Fermi approximation With respect to the trap



Peierls instability in a lattice Fermi-Bose mixture

FIG.: (a) repulsive fermion-boson interactions
(b) attractive fermion-boson interactions
The shaded part depicts the bosonic mean field density whereas filled circles denote fermionic atoms.

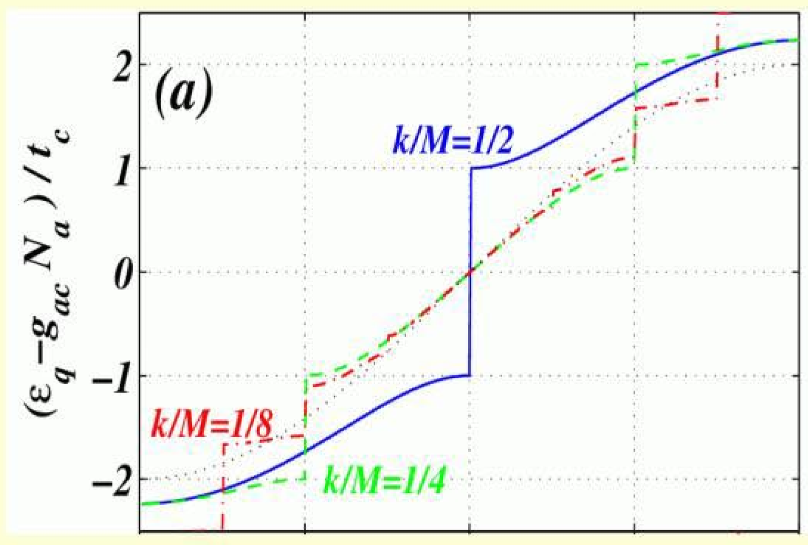
Peierls Instability

For $\omega_0 = 0$, the adiabatic Holstein model is known to exhibit a Peierls instability [2], with respect to bosonic collective excitations with wave number equal to N_c/M, corresponding to twice the Fermi wave length $k_F = N_c/2M$. 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 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 [3] 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 show bellow how the energy of the system is affected by spatial bosonic modulation of the form: $n_j^a = \bar{n}_j^a + \delta n_j^a \cos(\frac{2\pi k j}{M})$.

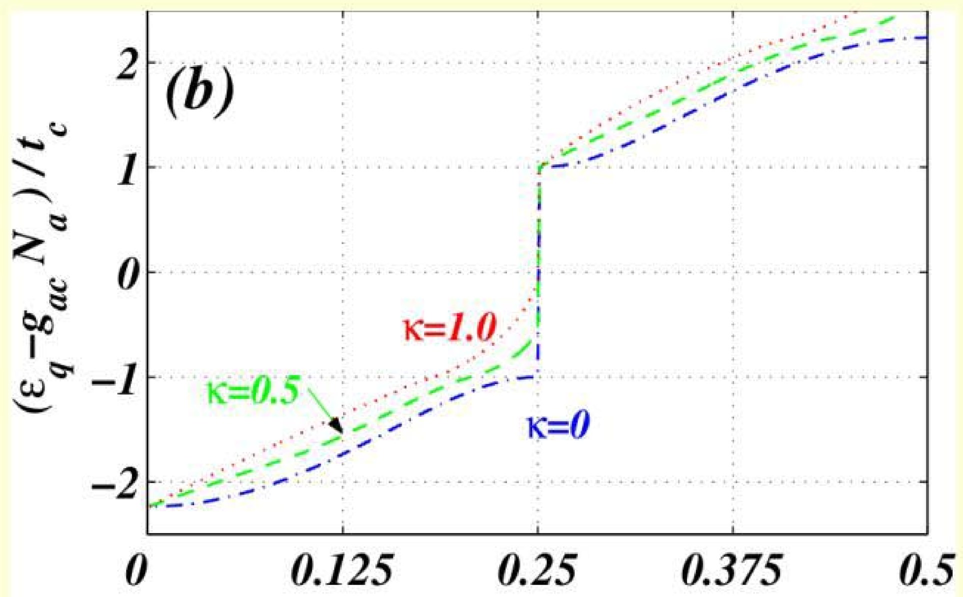
Numerics Demonstrating Peierls Instability

Fermionic energy spectrum

(a)Various values of modulation wave-number $\omega_0 = 0$

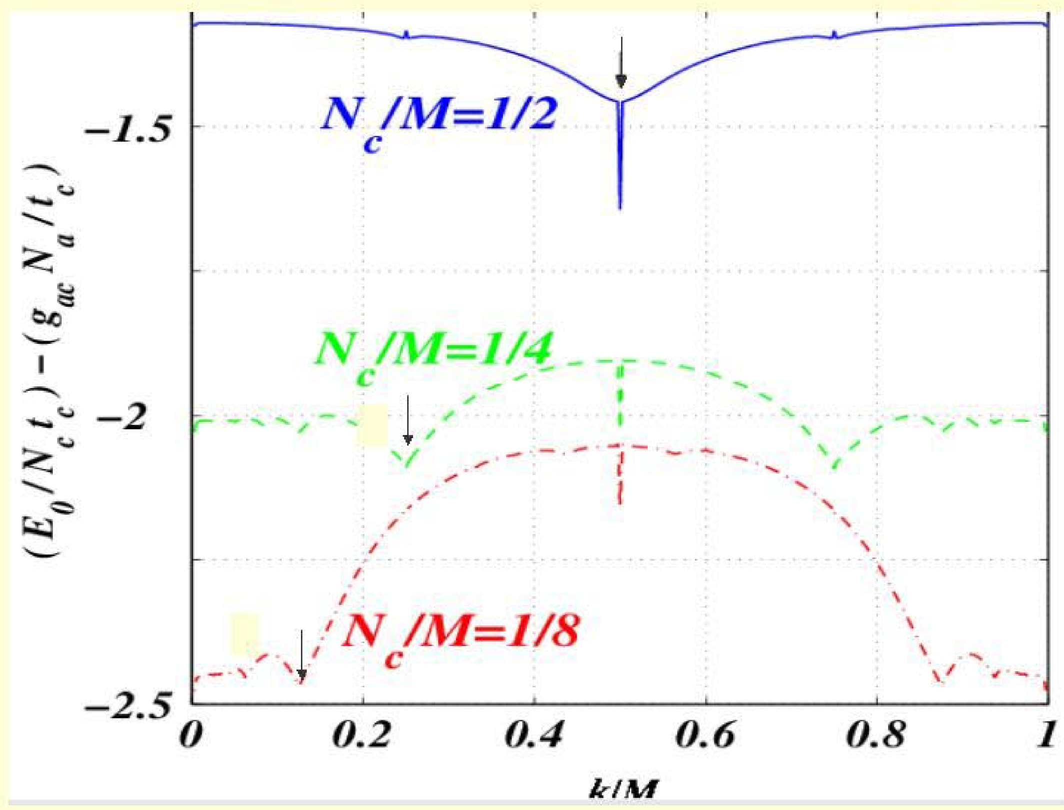


(b) As a function of ω_0 for fixed modulation wave number $k/M = 1/2$



Ground State Fermionic Energy:

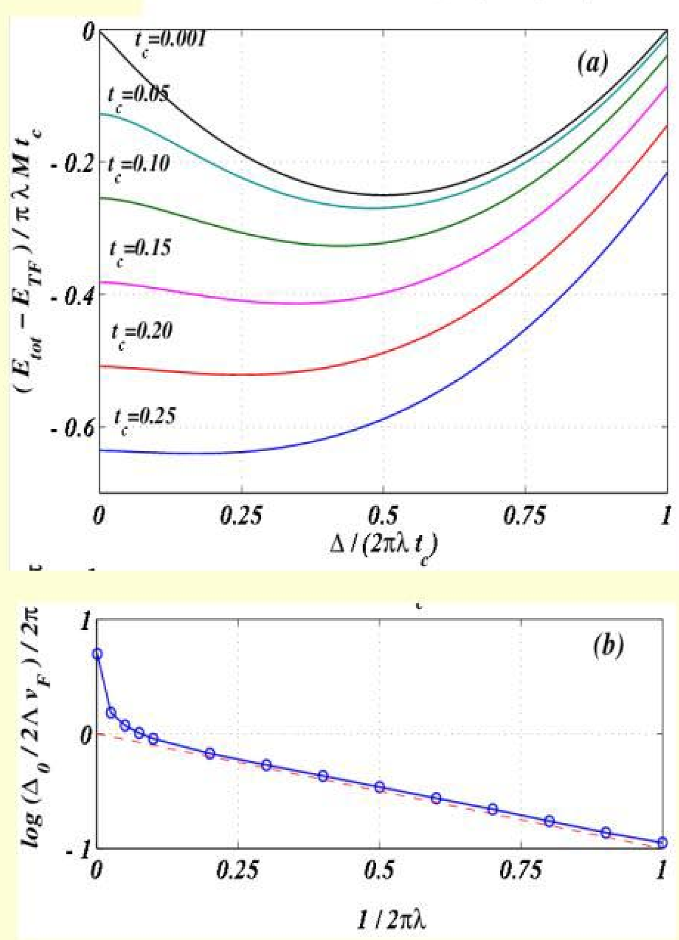
As a function of the modulation wave-number for various fermionic filling factors: $N_c/M = 1/2$ (solid), $N_c/M = 1/4$ (dashed), $N_c/M = 1/8$(dash-dotted). The external trap frequency is set to $\kappa = 0.1t_c$ and the bosonic amplitude modulation is set equal to t_c. Arrows indicate the bosonic modulation wave-number minimizing E_c .



$$\kappa = \bar{m}(\omega_0 l M)^2/2 \qquad \bar{m} = m_c - (g_{ac}/g_{aa})m_a$$

Harmonic trap effects:

FIG.: (a) Total energy of the system as a function of the gap for various values of t_c. (b) optimal gap values as a function of t_c. The dashed line depicts the predicted strong coupling behavior of the continuum model: $\Delta_0 = 2v_F\Lambda\exp(-1/\lambda)$.



$$\Delta_j = g_{ac}\delta n_j^a \qquad \lambda = g_{ac}^2/(2\pi g_{aa}t_c)$$

References

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Analytic (Continuum) Model

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

where $\Psi(x) \equiv \begin{pmatrix}\psi_1(x)\\ \psi_2(x)\end{pmatrix}$ is a spinor representation of the fermionic field in terms of right and left moving fermionic fields σ_i are Pauli matrices and σ_0 is the identity matrix. v_F Is the Fermi velocity. The trap potential: $V(x) = m\omega_0^2x^2/2$ .The gap parameter: $\Delta_j = g_{ac}\delta n_j^a \to \Delta(x)$

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 [5]. 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 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

we assume: $u_n(x) = \Phi_n(x)u_n \, , \; v_n(x) = \Phi_n(x)v_n$,

The resulting Bogoliubov-de Gennes(BdG) equations:

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

The local Fermion spectrum $\varepsilon_n = \sqrt{E_n^2 + \Delta^2}$

Is the oscillator energy $E_n = (n_F - n + 1/2)\omega_0$ measured with respect to the Fermi energy $E_{n_F} = (n_F + 1/2)\omega_0$

The fermionic ground state energy:

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

and self consistent gap equation :

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

Resulting in the following gap equation:

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

with the strong coupling limit solution:

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

$$v_F\Lambda >> \Delta_0$$

Where $\lambda = g_{ac}^2/(2\pi g_{aa}t_c)$ is a dimensionless coupling constant and Λ is a high momentum cut-off