Peierls instability, periodic Bose-Einstein condensates and density waves in quasi-one-dimensional boson-fermion mixtures of atomic gases

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We study the quasi-one-dimensional (Q1D) spin-polarized bose-fermi mixture of atomic gases at zero temperature. Bosonic excitation spectra are calculated in random phase approximation on the ground state with the uniform BEC, and the Peierls instabilities are shown to appear in bosonic collective excitation modes with wave-number $2k_F$ by the coupling between the Bogoliubov-phonon mode of bosonic atoms and the fermion particle-hole excitations. The ground-state properties are calculated in the variational method, and, corresponding to the Peierls instability, the state with a periodic BEC and fermionic density waves with the period $\pi/k_F$ are shown to have a lower energy than the uniform one. We also briefly discuss the Q1D system confined in a harmonic oscillator (HO) potential and derive the Peierls instability condition for it.

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I. INTRODUCTION

The cooling and trapping techniques of atoms, used in the realization of BEC [1, 2] and degenerate fermi gases [3], have recently produced quantum bose-fermi mixtures of dilute atomic gases [4, 5]. Motivated by the controllability of various experimental parameters such as trap geometries, particle numbers, and interaction strengths in experiments of the ultra-cold atoms, a number of theoretical studies have been done to explain various experimental results done for bose-fermi mixtures [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17].

Further experimental advances have led to the realization of BEC in quasi-one-dimensional (Q1D) system [8, 15, 16]. Also several new phenomena, which are typical in the Q1D bose system, have been proposed theoretically: quasi-condensates with fluctuating phases [22] and a Tonks-Girardeau gas of impenetrable bosons [23] and so on.

In electric conductors, the Q1D systems have been realized in systems where electric currents can flow easier in one specific crystal direction than in the vertical directions [24]. One of the most fascinating phenomena in such a system is the “Peierls instability”: a lattice distortion with the period of $2k_F$ [25]. This instability gives rise to a charge-density wave in the ground state, a collective state of electrons, which is caused by the strong correlations among electrons due to the phonon-electron interaction. The origin of the effect is the divergence in phonon spectrum by the low-energy particle-hole (p-h) excitations near fermi surface with the wave-number $2k_F$, which give large contribution in phonon self-energy because of a phase-space reduction in Q1D systems.

In the present paper, we investigate the occurrence of the Peierls instability in the Q1D uniform system of atomic-gas bose-fermi mixture at $T = 0$. Different from conductors that have the periodic structures by lattices, it have no periodic structures originally, and the instability and the periodic structure in the ground state is brought purely by the coupling between the Bogoliubov-phonon mode of bosonic atoms and fermion p-h excitations.

This paper is organized as follows. In Section II, we introduce the model and derive the equations in random phase approximation using the Green’s function method to calculate the bosonic excitation spectra. In Section III, the equations obtained in Section II are applied for the system with the uniform ground state, and solved numerically. We show the calculated bosonic excitation spectra and that the Peierls instability appears in collective excitation modes around the wave-number $2k_F$. The analytical estimations are also given for the collective excitation spectra. In Section IV, we show that the state with periodic BEC and the density-wave states for both boson and fermion (with the period of $\pi/k_F$) is more stable than the uniform state. In Section V, we briefly discuss the Peierls instability in the finite Q1D system confined in a HO potential [26].

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II. MODEL, GREEN’S FUNCTIONS AND MEAN-FIELD BASIS

We consider a system of spin-polarized atoms at $T = 0$: $N_b$ bosons and $N_f$ fermions with masses $m_{b,f}$ each other, confined in an axially-symmetric HO potential $U_{b,f} = \frac{1}{2}m_{b,f} \left\{ \omega^2_r (x^2 + y^2) + \omega^2_z z^2 \right\}$ where $\omega_r \gg \omega_z$. When atoms are confined tightly enough in the $r$-direction that the radial ($r$) part of their wave functions can be approximated by that of the lowest-energy state in the 2D HO potential $\frac{1}{2}m_{b,f} \omega^2_r (x^2 + y^2)$, then we call that the system is in the $\text{QD}$ region. It should be realized when,

- The $r$-HO quanta $\hbar \omega_r$ should be higher than the boson-boson/boson-fermion interaction energies: $\epsilon^{3D}_{b,b} = 4\pi \hbar^2 a_{bb} N_b^{3D}/m_b$ and $\epsilon^{3D}_{b,f} = 2\pi \hbar^2 a_{bf} N_f^{3D}/m_r$, where $N^{3D}_b$ are the boson/fermion 3D-number densities and $a_{bb, bf}$ are the boson-boson/boson-fermion $s$-wave scattering lengths. The $m_r$ in $\epsilon^{3D}_{b,f}$ is a reduced mass: $m_r = m_b m_f/(m_b + m_f)$.

- The $r$-HO quanta should also be higher than the fermi energy obtained by $\epsilon^{3D}_{f} = \hbar^2 (6\pi^2 n_f^{3D})^{2/3}/2m_f$.

The atomic states for the axial ($z$) degree of freedom are described by the $z$-dependent field operators for bosons and fermions, $\hat{\phi}(z)$ and $\hat{\psi}(z)$; the effective Hamiltonian for them is modeled by

$$
H = \int dz \left[ \frac{-\hbar^2}{2m_b} \frac{d^2}{dz^2} + U_b(z) - \mu_b \right] \hat{\phi}(z) + \int dz \left[ \frac{-\hbar^2}{2m_f} \frac{d^2}{dz^2} + U_f(z) - \mu_f \right] \hat{\psi}(z) + \int dz \left[ \frac{g_{bb}}{2} \hat{\phi}^\dagger(z) \hat{\phi}(z) + g_{bf} \hat{\phi}^\dagger(z) \hat{\psi}(z) \right] \hat{\phi}(z),
$$

where the $\mu_{b,f}$ are the 1D chemical potentials for bosons and fermions. The effective 1D coupling constants $g_{bb}$ (boson-boson) and $g_{bf}$ (boson-fermion) in $\Sigma$ are related to the $s$-wave scattering lengths: $g_{bb} = 2\hbar \omega_r a_{bb}$, $g_{bf} = 2\hbar \omega_r a_{bf}$, which can be obtained from the 3D interaction by integrating out the radial parts of the wave functions $\bar{\phi}(r)$ and $\bar{\phi}(r)$. It should be noted that, in the limit $\omega_z \to 0$, we obtain the uniform system in the axial dimension.

In weak interacting systems, the mean field approximation should give a good starting point for further calculations, where bosons are assumed to occupy the lowest single-particle state $\phi_0(z)$ at $T = 0$, and the expectation value of the boson field-operator (order parameter for BEC), $\Phi(x) = \langle \hat{\phi}(z) \rangle = \sqrt{N_b} \phi_0(z)$, satisfies 1D Gross-Pitaevskii equation:

$$
\left[ \frac{-\hbar^2}{2m_b} \frac{d^2}{dz^2} + U_b(z) + g_{bb} n_b + g_{bf} n_f \right] \Phi = \mu_b \Phi,
$$

where the (axial) 1D boson density $n_b$ is defined by $n_b(z) = |\Phi(z)|^2$.

For fermions, the ground state is obtained by a Slater determinant of fermion single-particle wave functions $\psi_j(z)$ for the mean-field energies $\epsilon^f_j$ below the 1D fermi energy $\epsilon_F = \mu_f$, which are obtained from the Hartree equation:

$$
\left[ \frac{-\hbar^2}{2m_f} \frac{d^2}{dz^2} + U_f(z) + g_{bf} n_b(z) \right] \psi_j(z) = \epsilon^f_j \psi_j(z).
$$

In this state, the fermion density is obtained by $n_f(z) = \sum_{\epsilon^f_j \leq \epsilon_F} |\psi_j(z)|^2$.

We are interested in the bosonic excitation modes of the system, which can be obtained by the bosonic Green’s functions

$$
iG(x_1, x_2) = \left( \langle T[\hat{\phi}(x_1) \hat{\phi}^\dagger(x_2)] \rangle \right) \left( \langle T[\hat{\phi}^\dagger(x_1) \hat{\phi}(x_2)] \rangle \right).
$$

where $x = (z, t)$ and $\hat{\phi}(x) = \hat{\phi}(z, t) - \Phi(z)$. They satisfy the Dyson equation:

$$
i\hbar \frac{\partial}{\partial t} \tau_3 - K_0^b(z_1)|1\rangle \cdot G(x_1, x_2) = \hbar \delta(x_1 - x_2)|1\rangle
$$

$$
+ \int d^2 x_3 \hbar \Sigma(x_1, x_3) \cdot G(x_3, x_2),
$$

where $K_0^b(z) = -(\hbar^2/2m_b) d^2/dz^2 + U_b(z) - \mu_b$ is a single-particle operator and the matrices $\tau_3$ and $|1\rangle$ are defined by

$$
\tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad 1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}.
$$

The boson self-energy in Eq. (11) is in the $2 \times 2$-matrix form, and separated into the static and the dynamical parts: $\Sigma(x_1, x_2) = \Sigma_0(x_1, x_2) + \Pi(x_1, x_2)$. In the mean-field approximation, the static part is given by

$$
\hbar \Sigma_0 = g_{bb} \left( \begin{array}{cc} 2n_b + \frac{a_{bf}}{\epsilon^f} n_f & \Phi^* \Phi \\ \Phi \Phi^* & 2n_b + \frac{a_{bf}}{\epsilon^f} n_f \end{array} \right) \delta(x_1 - x_2),
$$

In the dynamical part, we take the contributions from the fermion particle-hole ($p$-$h$) pair-excitations (Figure. 1):

$$
\hbar \Pi(x_1, x_2) = \frac{i}{\hbar} g_{bf} \left( \begin{array}{ccc} \Phi(z_1) \Phi^*(z_2) & \Phi(z_1) \Phi(z_2) \\ \Phi^*(z_1) \Phi(z_2) & \Phi^*(z_1) \Phi^*(z_2) \end{array} \right) \times G^f(x_1, x_2) G^f(x_2, x_1),
$$

which is just a polarization potential for pair-excitations. It should be noted that this approximation is equivalent to the random phase approximation, and gives the strong correlation effects, especially in the bosonic collective modes (Bogoliubov-phonon mode).
For the fermion Green’s function in Eq. (8), we use that for the unperturbed fermion single-particle state obtained from Eq. (6):

$$iG_f(x_1, x_2) = \sum_j \psi_j(z_1)\psi_j(z_2)^* e^{-i\epsilon_f^j(t_1-t_2)}$$

$$\times [\theta(t_1-t_2)\theta(\epsilon_f^j - \epsilon_F) - \theta(t_2-t_1)\theta(\epsilon_F - \epsilon_f^j)].$$  (9)

To advance the calculation, we expand the boson field operators, $\hat{\varphi}$ and $\hat{\varphi}^\dagger$, by boson creation/annihilation operators, $\hat{\beta}_\lambda$ and $\hat{\beta}_\lambda^\dagger$ for the quasi-particle states:

$$\hat{\varphi}(z) = \sum_\lambda \{u_\lambda(z)\hat{\beta}_\lambda - v_\lambda^*(z)\hat{\beta}_\lambda^\dagger\},$$

$$\hat{\varphi}^\dagger(z) = \sum_\lambda \{u_\lambda^*(z)\hat{\beta}_\lambda^\dagger - v_\lambda(z)\hat{\beta}_\lambda\},$$

where the quasi-particle wave functions, $u_\lambda(z_1)$ and $v_\lambda(z_1)$, for the eigenenergies $\hbar\Omega_\lambda$ can be determined from the Bogoliubov-type eigenequations:

$$\mathcal{L}u_\lambda(z_1) + \int dz_2 \left\{n_bg_{bh}\delta(z_1-z_2) + \hbar\Pi(z_1, z_2; \Omega_\lambda)\right\} \{u_\lambda(z_2) - v_\lambda(z_2)\} = \hbar\Omega_\lambda u_\lambda(z_1),$$  (10)

$$\mathcal{L}v_\lambda(z_1) + \int dz_2 \left\{n_bg_{bh}\delta(z_1-z_2) + \hbar\Pi(z_1, z_2; \Omega_\lambda)\right\} \{v_\lambda(z_2) - u_\lambda(z_2)\} = -\hbar\Omega_\lambda v_\lambda(z_1),$$  (11)

where $\mathcal{L} = K_b^o + g_{bh}n_b + g_{bf}n_f$. The $\hbar\Pi$ denotes the energy-representation of the polarization potential in Eq. (5):

$$\hbar\Pi(z_1, z_2; \Omega_\lambda) = g_{bf}^2 \sum_{p,h} \Phi(z_1)\Phi(z_2)\times \left[\frac{\psi_p^*(z_1)\psi_p(z_1)\psi_p^*(z_2)\psi_p(z_2)}{\hbar\Omega_\lambda - \epsilon_f^p + \epsilon_f} - \frac{\psi_p^*(z_1)\psi_p(z_1)\psi_p^*(z_2)\psi_p(z_2)}{\hbar\Omega_\lambda - \epsilon_h^p + \epsilon_h}\right].$$  (12)

where the index $p(h)$ represents a state with energy above (below) the fermi energy. Since we consider the stationary condensates, the order parameter $\Phi$ is assumed to be real [28].

We should note that the number of eigenvalues $\Omega_\lambda$ obtained from Eqs. (10,11) may exceed the dimension of the bosonic quasi-particle space because these equations are not linear for the eigenvalue $\Omega_\lambda$ (The $\hbar\Pi$ depends on the eigenvalue). In this case, the eigenfunctions for different eigenvalues do not satisfy the orthogonality relations, but they are proved still to be a complete set.

For normalizations of the quasi-particle wave functions, we take

$$\int dz_1 \left[|u_\lambda(z_1)|^2 - |v_\lambda(z_1)|^2\right]$$

A. Dispersion equation for Excitation energies

Let’s consider the case of $\omega_n = 0$, and discuss the stability of the 1D homogeneous states in uniform mixtures, where the boson/fermion (1D) densities $n_{b,f}$ and the order parameter $\Phi$ take constant values:

$$\Phi = \sqrt{\frac{N_b}{L}}, \quad n_{b,f} = \frac{N_{b,f}}{L},$$  (14)

where $L$ is a quantization length for the box-potential regularization. In this case, the fermion single wave functions become plane waves, $\psi_k = e^{ikz}/\sqrt{L}$, with the wave number $k = \pi n/L$ ($n = \text{integer}$) and the mean-field single-particle energy $\epsilon_f^k = \hbar^2 k^2/(2m_f) + g_{bb}n_b$. The fermi wave-number and energy, $\epsilon_F$ and $\epsilon_F$, becomes $k_F = \pi n_f$ and $\epsilon_F = \hbar^2 \pi^2 n_f^2/(2m_f) + g_{bb}n_b$. 

III. PEIERLS INSTABILITY OF HOMOGENEOUS STATE

FIG. 1: Polarization potential induced by fermion particle-hole excitation. Dashed line: boson (non-condensate), solid line: fermion.
The boson quasi-particle wave functions $u_{\lambda,k}$ and $v_{\lambda}$ also become plane waves: $u_{\lambda,k}(z) = u_{\lambda,k}e^{ikz}$, $v_{\lambda,k}(z) = v_{\lambda,k}e^{ikz}$. Substituting them into Eqs. (10,11), we obtain

$$(\epsilon^b_k - \mu_b)u_{\lambda,k} + \{g_{bb}n_b + \hbar \Pi_k(\Omega_\lambda)\} \{u_{\lambda,k} - v_{\lambda,k}\} = \hbar \Omega u_{\lambda,k}, \quad (15)$$

$$(\epsilon^b_k - \mu_b)v_{\lambda,k} + \{g_{bb}n_b + \hbar \Pi_k(\Omega_\lambda)\} \{v_{\lambda,k} - u_{\lambda,k}\} = -\hbar \Omega v_{\lambda,k}, \quad (16)$$

where $\epsilon^b_k = \hbar^2 k^2 / 2m_b + g_{bb}n_b + g_{bf}n_f$, and the polarization potential $\hbar \Pi_k(\Omega_\lambda)$ for plane waves is given by

$$\hbar \Pi_k(\Omega_\lambda) = g_{bf}^2 n_b \int_{-k_F}^{k_F} dq \left[ \frac{1}{\hbar \Omega - \epsilon^b_{q+k} + \epsilon^b_q + i\eta} \right. \left. - \frac{1}{\hbar \Omega - \epsilon^b_q + \epsilon^b_{q+k} + i\eta} \right], \quad (17)$$

Using the equality of the bosonic chemical potential and the interaction energy in the mean-field approximation, $\mu_b = g_{bb}n_b + g_{bf}n_f$, we obtain the dispersion equation for $\Omega_\lambda$:

$$(\hbar \Omega)^2 = (\epsilon^b_k)^2 + 2\epsilon^b_k \{g_{bb}n_b + \hbar \Pi_k(\Omega_\lambda)\}, \quad (18)$$

where $\epsilon^b_k = \hbar^2 k^2 / 2m_b$.

Introducing the complex energy $\Omega_\lambda = \omega_\lambda - i\gamma_\lambda$, we separate the polarization potential into the real and the imaginary parts

$$\hbar \Pi_k(\omega_\lambda, \gamma_\lambda) = \hbar \Pi_k^{Re}(\omega_\lambda, \gamma_\lambda) + i\hbar \Pi_k^{Im}(\omega_\lambda, \gamma_\lambda). \quad (19)$$

After execution of the $q$-integration in Eq. (17), they become

$$\hbar \Pi_k^{Re}(\omega_\lambda, \gamma_\lambda) = -\frac{A_k}{2} \left[ \ln \left\{ \frac{(k + 2k_F)^2}{(k - 2k_F)^2} \right\} \right] + \frac{2m_f \omega_\lambda}{h_k} \left( \frac{(k + 2k_F)^2}{(k - 2k_F)^2} \right) \right] - \frac{\pi \theta \left( k - \frac{2m_f \omega_\lambda}{h_k} \right)}{\pi \theta \left( k + \frac{2m_f \omega_\lambda}{h_k} \right)} \right] - \frac{\arctan \left( \frac{2m_f \omega_\lambda}{(k + 2k_F)^2 + \left( \frac{2m_f \omega_\lambda}{h_k} \right)^2} \right)}{\arctan \left( \frac{2m_f \omega_\lambda}{(k - 2k_F)^2 + \left( \frac{2m_f \omega_\lambda}{h_k} \right)^2} \right)} \right], \quad (20)$$

where $A_k = \frac{g_{bf}^2 n_b m_f}{2\pi \hbar k_F}$, and the principal values should be taken for the arctangent function: $-\frac{\pi}{2} \leq \arctan x \leq \frac{\pi}{2}$. Using these results, Eq. (18) can be separated into the coupled equations

$$\hbar^2 (\omega_\lambda^2 - \gamma_\lambda^2) = (\epsilon^b_k)^2 + 2\epsilon^b_k \{g_{bb}n_b + \hbar \Pi_k^{Re}\}, \quad (21)$$

$$\hbar^2 \omega_\lambda \gamma_\lambda = \epsilon^b_k \cdot \hbar \Pi_k^{Im}. \quad (22)$$

Now, in order to analyze the dispersion equations (21,22) qualitatively, we discriminate two cases. First, when $\hbar \Pi_k^{Im}(\omega_\lambda) \neq 0$ and $\omega_\lambda, k > 0$, Eqs. (21) and (22) have solutions with complex energies ($\gamma_\lambda > 0$), which correspond to the continuum p-h excitations in the continuum.

Second, in the region where any p-h pair excitations are prohibited ($\gamma_\lambda = 0$), the polarization potential becomes real:

$$\hbar \Pi_k^{Re}(\omega_\lambda) = -\frac{A_k}{2} \ln \left\{ \frac{(k + 2k_F)^2}{(k - 2k_F)^2} \right\} \left[ \frac{(2m_f \omega_\lambda/h_k)^2}{(k + 2k_F)^2 + (2m_f \omega_\lambda/h_k)^2} \right] \left[ \frac{(2m_f \omega_\lambda/h_k)^2}{(k - 2k_F)^2 + (2m_f \omega_\lambda/h_k)^2} \right]. \quad (23)$$

In this case, introducing the dimensionless variables $\tilde{\omega}_\lambda = 2\omega_\lambda / (v_F k_F)$ and $\tilde{k} = k/k_F$ ($v_F = h k_F / m_f$: the fermi velocity), the dispersion relation, eq. (21), becomes

$$\tilde{\omega}_\lambda^2 = \frac{m_f^2}{m_b^2} \tilde{k}^4 + \frac{2k^2 v_B^2}{v_F^2} \left\{ 2 - \frac{\zeta}{k} \ln \left( \frac{k^2 (k + 2)^2 - \omega_\lambda^2}{k^2 (k - 2)^2 - \omega_\lambda^2} \right) \right\}, \quad (24)$$

where $v_B = \sqrt{g_{bb}n_b / m_b}$ and $\zeta$ is the dimensionless boson-fermion coupling constant defined by

$$\zeta = \frac{g_{bf}^2}{\pi g_{bb} h v_F}. \quad (25)$$

The solutions of Eq. (24) correspond to the bosonic excitation energies, which we are interested in, and $v_B$ is just the Bogoliubov-phonon sound velocity. It should be noted that the scaled equation (24), depends on three dimensionless parameters, $m_f / m_b$, $v_B / v_F$, and $\zeta$.

### B. Excitation Spectra and Peierls Instabilities

Let’s study the bosonic excitation spectra on the homogeneous ground state with solving the dispersion relations (21,22). To understand general features, we show numerical results for two typical cases, (a) $v_B < v_F$ and...
FIG. 2: Excitation spectrum (in units of $\hbar v_F k_F$) of boson-fermion mixtures. Solid lines: collective modes of p-h pairs and bosonic modes, dashed line: free boson, shaded area: continuum p-h pair excitation spectra.

(b) $v_B > v_F$, in Figure 2: (a) $(v_B/v_F)^2 = 0.67$, $\zeta = 0.99$ and (b) $(v_B/v_F)^2 = 1.50$, $\zeta = 0.80$. The same values have been taken for boson and fermion masses, $m_b = m_f$, for all cases. The shaded areas in Figure 2 correspond to the continuum spectra corresponding to the fermionic p-h excitation states, and the solid lines are to the isolated modes, corresponding to the collective excitations. It should be noted that two collective modes (low- and high-lying) exist with the same wave number $k$ (except narrow regions around $2k_F$): they can be interpreted to be coherent superposition of the Bogoliubov-phonon mode from bosonic atoms and the fermion p-h collective mode. For comparison, the Bogoliubov-phonon spectra in boson-fermion noninteracting systems ($g_{bf} = 0$) have been plotted in Figure 2, and we can find that it runs between two collective spectra in the interacting ones.

Let’s discuss the specific features of the collective modes, especially in small $k$ and $k \approx 2k_F$ regions.

In small wave-number region, $k < k_F |1 - (v_B/v_F)^2|$, the Bogoliubov-phonon modes (dashed line) in the boson-fermion noninteracting limit are located below the fermion p-h excitation modes in energy and absorbed into the fermion p-h continuum when $v_B < v_F$ (case (a)). In case that $v_B > v_F$ (case (b)), the corresponding modes are above the continuum. It suggests that the low-lying collective mode in (a) is mainly a Bogoliubov-phonon mode from bosonic atoms but the corresponding mode in (b) is mainly the fermion p-h one, and the high-lying modes have opposite characters. In Figure 2, the bosonic excitation modes are found to be influenced by the interaction with the fermion p-h excitation modes, and pushed downward/upward in case (a)/(b).

Around $k \approx 2k_F$, the low-lying collective modes become very soft and, between two critical wave-numbers $k_− < k < k_+$, they are found to be zero-modes in both cases. To calculate the energy of these modes analytically, we expand Eq. (22) to the leading order of $|q|/k_F$ ($q = k - 2k_F$):

$$\hbar^2 \omega_{\lambda} \gamma_\lambda = A_{2k_F} e^k_{k_F} \left[ \pi \theta(\omega_\lambda - v_F |q|) - \arctan \left( \frac{2\omega_\lambda \gamma_\lambda}{\gamma_\lambda^2 + \omega_\lambda^2} \right) \right].$$  (26)

When $\omega_\lambda < v_F |q|$, the above equation reduces to $\omega_\lambda \gamma_\lambda = 0$. In the case of $\omega_\lambda = \gamma_\lambda = 0$, two critical wave-numbers are obtained from Eq. (24):

$$\frac{k_+}{k_F} = 2 \pm 4 \exp \left[ -\frac{2}{\zeta} \left\{ 1 + \left( \frac{m_f v_F}{m_b v_B} \right)^2 \right\} \right],$$  (27)

which gives ($k_- = 1.97k_F$, $k_+ = 2.02k_F$) for (a) in Figure 2, and ($k_- = 1.92k_F$, $k_+ = 2.05k_F$) for (b) in the same figure.

Analyzing the eigenvalues of Eq. (24) more detail, we find that they become purely imaginary ($\omega_\lambda = 0$, $\gamma_\lambda \neq 0$) in the region between the two critical wave-numbers, $k_- < k < k_+$; it is just the “Peierls instability” in Q1D system, which suggests that the homogeneous state is unstable against the fluctuations with the wave-number around $2k_F$.

Finally, we should comment on a different kind of instability that may occur in the small wave-number fluctuation [17]. When we take the $k \to 0$ limit with keeping $\omega_\lambda/k = \text{constant}$, the real part of the polarization potential becomes

$$\hbar \Pi^R_k (\omega_\lambda) = \frac{(g_{bf})^2 m_b (v_F k)^2}{\pi \hbar v_F} \frac{\omega_\lambda^2 - (v_F k)^2}{\omega_\lambda^2}.$$  (28)

and the imaginary part $\Pi^I_k$ vanishes except at $v_B = v_F$. Substituting Eq. (25) into Eq. (24), we obtain two branches of excitations:

$$\hbar \omega_{\pm} = \hbar k \left[ \frac{v_B^2 + v_F^2}{2} \pm \frac{1}{2} \sqrt{(v_F^2 - v_B^2)^2 + 4 \zeta v_F^2 v_B^2} \right]^{1/2}.$$  (29)

In the strong boson-fermion interacting case ($\zeta > 1$), the energy of the low-lying mode becomes purely imaginary, and it suggests an instability of the system. We find that the stability condition for the $k \approx 0$ mode:

$$\frac{\pi^2 \hbar^2}{m_f} n_f \geq \frac{(g_{bf})^2}{g_{bb}},$$  (30)
where we have used the relation \( n_f = k_F / \pi \). This \( k \approx 0 \) instability is considered to cause the phase-separated states more stable. In the present paper, we do not discuss this instability and concentrate only on the density-wave states caused by the Peierls instability, which is discussed in the next section. It should be a very interesting problem to study the cooperation/competition between these states.

IV. DENSITY WAVES IN BOSON-FERMION GROUND STATE

The results obtained in the previous section shows that the homogeneous state is not the true ground state of the system and a lower energy can be obtained for the state with a spatially-periodic condensate characterized by the \( 2k_F \)-periodic order parameter: \( \Phi(z) = b_u + b_p \cos(2k_Fz) \). The constant bosonic density is given by \( n_b = b_u^2 + b_p^2 / 2 \). In the case of weakly-periodic variation \( b_p \ll b_u \), up to second order in \( b_p \), the mean-field Hamiltonian for the Bose-Fermi system becomes

\[
\hat{H} = \frac{g_{bf}}{2} (b_u^2 + b_b^2) + \epsilon_b b_b^2 + \sum_k \epsilon_k c_k^\dagger c_k + g_{bf} \sum_k (\hat{c}_k + \hat{c}_{k+2k_F})^{\dagger} \hat{c}_k,
\]

where \( \epsilon_k \) is the energy generated from the periodic condensate: \( \epsilon_b = \epsilon_b^{2k_F} / 2 + g_{bf} b_u^2 \). The last term in Eq. (31) is for the processes that the fermion with a wave-number \( k \) feeling periodic- and uniform-bosonic condensates scatters into the states with \( k \pm 2k_F \).

In order to obtain a single-particle energy, we calculate the fermion Green’s function:

\[
iF_{k,k'}(t-t') \equiv \langle T[\hat{c}_k(t)\hat{c}_k^{\dagger}(t')] \rangle = \frac{2}{\pi} \int_0^{\infty} e^{-i\omega(t-t')} F_{k,k'}(\omega)
\]

(32)

where \( \hat{c}_k(t) = e^{i\hat{H}t/\hbar} \hat{c}_k e^{-i\hat{H}t/\hbar} \). For a fixed wave-number \( k \), the Green’s function \( F_{k,k'}(\omega) \) has non-vanishing off-diagonal matrix elements at \( F_{k,k+2k_F} \) in the Hamiltonian (31). In the limit \( k \to +k_F \), fermion states with wave-numbers \( k \) and \( k-2k_F \) are almost degenerate in energy, but that with \( k+2k_F \) is separated. Consequently, in case of \( k_F \geq k > 0 \), the Dyson equation for the Green’s function can be approximated by

\[
\begin{pmatrix}
\hbar \omega - \epsilon_k^F \\
-\Delta & \hbar \omega - \epsilon_{k-2k_F}^F
\end{pmatrix}
\begin{pmatrix}
F_{k,k} \\
F_{k,k-2k_F}
\end{pmatrix} = \begin{pmatrix}
\hbar \\
0
\end{pmatrix},
\]

(33)

where \( F_{k,k} \) is a diagonal part of the Green’s function, and \( \Delta = g_{bf} b_u b_p \). They can be solved easily:

\[
F_{k,k} = \frac{U_k^2}{\omega - E_k^c / \hbar - i\eta} + \frac{V_k^2}{\omega - E_k^c / \hbar + i\eta},
\]

(34)

where

\[
F_{k,k-2k_F} = \frac{-U_k V_k}{\omega - E_k^c / \hbar - i\eta} + \frac{U_k V_k}{\omega - E_k^c / \hbar + i\eta},
\]

(35)

where

\[
U_k = \sqrt{\frac{1}{2}} \left( 1 - \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta^2}} \right)^{1/2},
\]

(36)

\[
V_k = \sqrt{\frac{1}{2}} \left( 1 + \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta^2}} \right)^{1/2},
\]

(37)

with \( \xi_k = \hbar v_F (k - k_F) \). The single-particle energy with wave-number \( k \) is obtained from the pole of \( F_{k,k}(\omega) \):

\[
E_k^c = \epsilon_k^F - \xi_k \pm \sqrt{\xi_k^2 + \Delta^2},
\]

(38)

from which we can understand that the \( 2|\Delta| \) is the energy gap at the Fermi surface. It is clear that the periodic condensate has produced an energy gap \( 2|\Delta| \) near the Fermi surface.

To evaluate the value of \( \Delta \), we calculate the total energy of the system in the present approximation. The fermionic contributions to the energy is obtained by summing-up the \( E_k^c \) in Eq. (38) up to the fermi wave-number \( k_F \):

\[
E_f = \frac{1}{2} \sum_k \left( \epsilon_k^F - \xi_k \pm \sqrt{\xi_k^2 + \Delta^2} \right),
\]

(39)

where \( \epsilon_F = \hbar v_F k_F / 2 \). For simplicity, we consider the weak coupling limit, \( \Delta \ll \epsilon_F \), then the total energy density of the system becomes

\[
E_{tot}(|\Delta|) - E_{tot}(0) = \frac{n_f \Delta^2}{4 \epsilon_F}
\]

\[
\times \left[ 2 \frac{\left( \frac{m_F v_F}{m_B v_B} \right)^2}{2 \left( 1 + \frac{m_F v_F}{m_B v_B} \right)^2} - \frac{1}{2} \left( 1 + 2 \ln \frac{4\epsilon_F}{|\Delta|} \right) \right].
\]

(40)

Minimizing Eq. (40) with respect to \( |\Delta| \), we obtain the stationary value of the gap parameter

\[
|\Delta| = 4 \epsilon_F \left[ 2 \frac{\left( \frac{m_F v_F}{m_B v_B} \right)^2}{2 \left( 1 + \frac{m_F v_F}{m_B v_B} \right)^2} - \frac{1}{2} \left( 1 + 2 \ln \frac{4\epsilon_F}{|\Delta|} \right) \right].
\]

(41)

Using the above result, the energy difference between the ground and the uniform (\( \Delta = 0 \)) states is

\[
E_{tot}(|\Delta|) - E_{tot}(0) = -\frac{\Delta^2}{4 \epsilon_F \hbar v_F},
\]

(42)

which shows that the state with the “periodic condensate” \( (b_p \neq 0) \) has lower energy than the uniform one.
FIG. 3: Gap energy as function of $m_f v_F/m_b v_B$ (in units of $v_F$) for $\zeta = 0.99$.

Next, we discuss the fermionic density, which is obtained from the Green’s function:

$$n_f(z) = \lim_{\nu \to 0^+} \sum_k \int \frac{d\omega}{2\pi i} e^{i\nu \omega} \left[ F_{k,k} + F_{k,k-2k_F} e^{2i k_F z} + F_{k-2k_F,k} e^{-2i k_F z} + F_{k-2k_F,k-2k_F} \right].$$

Using Eqs. (45, 46, 47, 49), it becomes

$$n_f(z) = \sum_k \left[ U_k^2 + V_k^2 - 2U_k V_k \cos(2k_F z) \right]$$

$$= n_f \left[ 1 - \frac{\Delta}{v_F \zeta} \cos(2k_F z) \right].$$

which shows that, for finite $\Delta$, the fermion state is in the density-wave one where the fermionic density has a periodicity $2k_F$. Corresponding to Eq. (49), the direct calculation shows that the bosonic density $n_b(z)$ has the similar density-wave structure:

$$n_b(z) = n_b \left[ 1 + \frac{\Delta}{\sqrt{\omega} \rho_0} \cos(2k_F z) \right].$$

It should be noted that, different from $n_f(z)$, the periodic part in $n_b(z)$ is proportional to the absolute value of the gap parameter $|\Delta|$. That means that the boson and fermion density-waves are out of phase for the boson-fermion repulsive system, but in phase for the attractive one.

As seen in Eq. (49), the gap energy $\Delta$ essentially depends on two combinations of parameters, $m_f v_F/m_b v_B$ and the dimensionless coupling constant $\zeta$. In Figure 3, we just plotted the gap energy as a function of $m_f v_F/m_b v_B$ for $\zeta = 0.99$, from which we can read off that the boson-fermion density-wave state can be observed in increasing the 1D density of condensate and/or using heavier bosons than fermions.

V. PEIERLS INSTABILITY OF SYSTEM IN HARMONIC OSCILLATOR POTENTIAL

In this section, we briefly discuss the non-uniform boson-fermion mixtures confined in a HO potential with the finite axial dimension ($\omega_a \neq 0$), and the condition for its Peierls instability.

Using the eigenenergy $\epsilon^h_{mn} = \hbar \omega_n (n + \frac{1}{2})$ ($n = 0, 1, 2, \cdots$) and the wave function $\phi^h_{mn}$ for the 1D HO potential, the quasiparticle amplitudes $u_\lambda$ and $v_\lambda$ are expanded by

$$u_\lambda(z) = \sum_n u_\lambda^n \phi^h_{mn}(z), \quad v_\lambda(z) = \sum_n v_\lambda^n \phi^h_{mn}(z).$$

Substituting them into Eqs. (10, 11), we can obtain the eigenequations for the excitation energies $\hbar \omega_\lambda$:

$$\sum_n \left[ (\epsilon^h_{mn} - \hbar \omega_\lambda) \delta_{m,n} u_\lambda^n + \hbar \Pi_{mn}(\omega_\lambda) (v_\lambda^n - u_\lambda^n) \right] = 0, (47)$$

$$\sum_n \left[ (\epsilon^h_{mn} + \hbar \omega_\lambda) \delta_{m,n} v_\lambda^n + \hbar \Pi_{mn}(\omega_\lambda) (v_\lambda^n - u_\lambda^n) \right] = 0, (48)$$

where, to concentrate on the role of the polarization potential effects in finite systems, we have neglected the Hartree potential. The polarization potential $\hbar \Pi_{mn}$ in Eqs. (47, 48), is given by

$$\hbar \Pi_{mn}(\omega_\lambda) = (g_{fy})^2 N_b$$

$$\times \sum_{ph} \left[ \frac{\langle mh|p0 \rangle \langle 0|ph \rangle \hbar \Pi_{mn}(\omega_\lambda)}{\hbar \omega_\lambda - \epsilon^h_p + \epsilon^h_\lambda - \epsilon^h_\rho + \epsilon^h_{ho} \rho_0} \right].$$

The matrix elements in Eq. (50) are defined by

$$\langle mh|p0 \rangle = \int d\varphi^h_{mn} \phi^h_{mn} \phi^h_{o} \varphi_0.$$
where $\beta = m g_{bb} a_{ho} / h^2$ with $a_{ho} = \sqrt{\hbar / m \omega_a}$ (the HO length in the axial direction).

As we have seen in chapter III, Peierls instability comes from the coupling between the boson mode with wave-number near $2k_F$ and the fermion p-h excitations near $k_F$. Although the wave-number is not strictly conserved in a HO potential, the instability mode would have 'wavenumber': $k_n = \sqrt{2n^2/\alpha_{ho}} \sim 2k_F$. Since the higher nodal modes $n \sim N_f$ have a broader spatial extension ($L_n = \sqrt{2n a_{ho}}$) than a condensate one, the asymptotic expansions can be used for the $\phi_n^{ho}$ in the middle of the trap $|z| < z_{TF} < L_n$.

$$\phi_n^{ho}(z) \propto \cos \left( k_n z - \frac{n \pi}{2} \right). \quad (53)$$

For a bosonic eigenstate with higher nodal mode, the negative energy amplitude $v_n^a = 0$ of Eq. (17) can be neglected.

Using these approximations, the matrix elements like $\langle 0 p | h n \rangle$ become linear combinations of the form $J_1(z_{TF} K) / z_{TF} K$, where $J_1(x)$ is the 1st-order Bessel function and the $K$ is a wave-number difference between the initial and the finial states: $K = k_n + k_h - k_p$. In the case of $|x| \gg 1$, using the asymptotic expansion of the Bessel function, $J_1(x)/x \sim |x|^{-3/2}$, the terms of $|x| \leq O(1)$ can contribute to the matrix elements. Under the restriction of wave-numbers $k_h \leq k_F$ and $k_p > k_F$ with $k_n \sim 2k_F$ ($k_F = \sqrt{2N_f / a_{ho}}$), the main contributions of matrix element are from the scattering processes: $k_n \rightarrow k_p + k_h$ and $k_n + k_h \rightarrow k_p$. To make an estimate, we replace a product of Bessel functions as

$$J_1(x_1) J_1(x_2) \approx \frac{1}{x_1 x_2} \theta(1 - |x_1|) \theta(1 - |x_1 - x_2|), \quad (54)$$

and take the continuum-limit for the wave-number sums: $\sum_{p,h} \rightarrow \int dp \int dh$.

Finally, the eigenenergy for a collective state with the wave number $k_n = 2k_F$ can be obtained

$$\hbar \omega_\lambda = 4 \epsilon_F - \frac{g_{bf}^2 n_b(0)}{2 \pi h v_F} \ln |4k_F z_{TF}|. \quad (55)$$

Contrary to the uniform system, the static polarization potential, the second term of right hand side of Eq. (55), is not divergent at $2k_F$. This is because the scattering of trapped atoms without wave-number conservation smears a singularity due to a sharp fermi sea. The Peierls instability occurs where the polarization energy is overcome by the kinetic energy $4 \epsilon_F$:

$$1 < \frac{\zeta v_B^2(0)^2}{4 v_F^2} \ln |4k_F z_{TF}| \quad (56)$$

As a possible candidate for the Peierls instability, we take the rubidium isotope system: $^{87}$Rb--$^{85}$Rb mixtures. Taking the scattering lengths in $^{87}$Rb, $a_{bb} = 5.3 \text{nm}$ and $a_{bf} = 29.1 \text{nm}$ and the typical trapping frequencies, $\omega_a = 2\pi \times 10 \text{Hz}$ and $\omega_r = 2\pi \times 15 \text{kHz}$, Eq. (56) gives $N_f = 10^3$ and $N_b = 2 \times 10^4$ for the realization of the Peierls instability.

**VI. SUMMARY**

In the present paper, we studied the occurrence of Peierls instability in Q1D boson-fermi mixtures at zero temperature. We analyzed the bosonic collective-excitation spectra in random phase approximation. It shows that the mixtures of uniform BEC and a fermi gas are unstable against a spontaneous formation of a collective mode of wave-number $2k_F$; this type of instability is known as Peierls instability. This result suggests that the ground state of bosons is a periodic condensate with the period $\pi / k_F$. In the variational method, the boson-fermion density wave state have been shown to have a lower energy than the uniform state. We also expanded our analysis for systems in an axial harmonic oscillator potential and derived Peierls instability condition.

It is well known that density waves in Q1D conductors lead to generations of a Lee-Rice-Anderson and a phase soliton modes. Thus, studies of the dynamical properties of boson-fermion density waves should be interesting problems in future.

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