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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 the random phase approximation on the ground state with uniform Bose-Einstein condensates (BEC's) 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 π/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 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 Bose-Einstein condensates (BEC's) [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 ultracold atoms, a number of theoretical studies have been done to explain various experimental results done for Bose-Fermi mixtures [6–18].

Further experimental advances have led to the realization of BEC's in quasi-one-dimensional (Q1D) system [5,19,20], by putting atoms in cylindrical traps long enough that the one-particle energy-level spacing in the radial direction exceeds the interatomic-interaction energy, and the atoms can move effectively in the axial direction (see also Ref. [21]). Characteristic properties of the Q1D BEC's have been demonstrated in the formation experiments of matter-wave solitons in repulsively or attractively interacting systems [22,23]. Also several new phenomena, which are typical in the Q1D Bose system, have been proposed theoretically: quasi condensates with fluctuating phases [24] and a Tonks-Girardeau gas of impenetrable bosons [25] 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 [26]. One of the most fascinating phenomena in such a system is the "Peierls instability": a lattice distortion with a period of $2k_F$ [27]. 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 wave number $2k_F$, which give a 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 an atomic-gas Bose-Fermi mixture at $T=0$. Different from conductors that have the periodic structures by lattices, it has no periodic structures originally, and the instability and periodic structure in the ground state are 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 Sec. II, we introduce the model and derive the equations in the random phase approximation using the Green's function method to calculate the bosonic excitation spectra. In Sec. III, the equations obtained in Sec. II are applied for the system with a 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 Sec. IV, we show that the state with periodic BEC's and density-wave states for both bosons and fermions (with a period of π/k_F) is more stable than the uniform state. In Sec. V, we briefly discuss the Peierls instability in the finite Q1D system confined in a harmonic oscillator (HO) potential [28].

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 $U_{b,f} = \frac{1}{2}m_{b,f}\{\omega_r^2(x^2+y^2)+\omega_a^2 z^2\}$ where $\omega_r \gg \omega_a$. When atoms are confined tightly enough in the r direction that the radial (r)

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part of their wave functions can be approximated by that of the lowest-energy state in the 2D HO potential $\frac{1}{2}m_{b,f}\omega_r^2(x^2+y^2)$, then we call that the system is in the Q1D region. It should be realized when the following holds.

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

(ii) The r-HO quanta should also be higher than the Fermi energy obtained by $\epsilon_F^{3D}=\hbar^2(6\pi^2 n_f^{3D})^{2/3}/2m_f$ [17].

The atomic states for the axial (a) 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

$$H=\int dz\,\hat{\phi}^\dagger(z)\left[-\frac{\hbar^2}{2m_b}\frac{d^2}{dz^2}+U_b(z)-\mu_b\right]\hat{\phi}(z)+\int dz\,\hat{\psi}^\dagger(z)\left[-\frac{\hbar^2}{2m_f}\frac{d^2}{dz^2}+U_f(z)-\mu_f\right]\hat{\psi}(z)+\int dz\,\hat{\phi}^\dagger(z)\left[\frac{g_{bb}}{2}\hat{\phi}^\dagger(z)\hat{\phi}(z)+g_{bf}\hat{\psi}^\dagger(z)\hat{\psi}(z)\right]\hat{\phi}(z), \tag{1}$$

where the $\mu_{b,f}$ are the 1D chemical potentials for bosons and fermions. The effective 1D coupling constants g_{bb} (boson and boson) and g_{bf} (boson and fermion) in Eq. (1) 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 [17,29]. It should be noted that, in the limit $\omega_a\to 0$, we obtain a 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 $\varphi_0(z)$ at $T=0$ and the expectation value of the boson field operator (order parameter for BEC), $\Phi(z)=\langle\hat{\phi}(z)\rangle=\sqrt{N_b}\varphi_0(z)$, satisfies 1D Gross-Pitaevskii equation

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

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 ϵ_j^f below the 1D Fermi energy $\epsilon_F=\mu_f$, which are obtained from the Hartree equation

$$\left[-\frac{\hbar^2}{2m_f}\frac{d^2}{dz^2}+U_f(z)+g_{bf}n_b(z)\right]\psi_j(z)=\epsilon_j^f\psi_j(z). \tag{3}$$

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

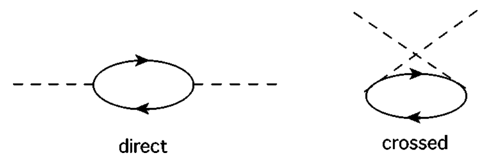

FIG. 1. Polarization potential induced by fermion particle-hole excitation. Dashed line: boson (noncondensate). Solid line: fermion.

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

$$iG(x_1,x_2)=\begin{pmatrix}\langle T[\hat{\varphi}(x_1)\hat{\varphi}^\dagger(x_2)]\rangle & \langle T[\hat{\varphi}(x_1)\hat{\varphi}(x_2)]\rangle\\ \langle T[\hat{\varphi}^\dagger(x_1)\hat{\varphi}^\dagger(x_2)]\rangle & \langle T[\hat{\varphi}^\dagger(x_1)\hat{\varphi}(x_2)]\rangle\end{pmatrix}, \tag{4}$$

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

$$\left[i\hbar\frac{\partial}{\partial t}\tau_3-K_b^0(z_1)1\right]\cdot G(x_1,x_2)=\hbar\,\delta(x_1-x_2)1+\int d^2x_3\hbar\Sigma(x_1,x_3)\cdot G(x_3,x_2), \tag{5}$$

where $K_b^0(z)=-(\hbar^2/2m_b)d^2/dz^2+U_b(z)-\mu_b$ is a single-particle operator and the matrices τ_3 and 1 are defined by

$$\tau_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad 1=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{6}$$

The boson self-energy in Eq. (5) is in the 2×2 matrix form and separated into static and 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

$$\hbar\Sigma_0=g_{bb}\begin{pmatrix}2n_b+\dfrac{g_{bf}}{g_{bb}}n_f & \Phi\Phi\\ \Phi^*\Phi^* & 2n_b+\dfrac{g_{bf}}{g_{bb}}n_f\end{pmatrix}\delta(x_1-x_2). \tag{7}$$

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

$$\hbar\Pi(x_1,x_2)=-\frac{i}{\hbar}g_{bf}^2\begin{pmatrix}\Phi(z_1)\Phi^*(z_2) & \Phi(z_1)\Phi(z_2)\\ \Phi^*(z_1)\Phi^*(z_2) & \Phi^*(z_1)\Phi(z_2)\end{pmatrix}\times G^f(x_1,x_2)G^f(x_2,x_1), \tag{8}$$

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. (3):

$$iG^f(x_1,x_2)=\sum_j\psi_j(z_1)\psi_j(z_2)^*e^{-i\epsilon_j^f(t_1-t_2)}[\theta(t_1-t_2)\theta(\epsilon_j^f-\epsilon_F)-\theta(t_2-t_1)\theta(\epsilon_F-\epsilon_j^f)]. \tag{9}$$

To advance the calculation, we expand the boson field operators $\hat{\varphi}$ and $\hat{\varphi}^\dagger$ by boson creation and annihilation operators $\hat{\beta}_\lambda$ and $\hat{\beta}_\lambda^\dagger$ for the quasiparticle 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 quasiparticle 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

$$\mathcal{L}u_\lambda(z_1) + \int dz_2\{n_b g_{bb}\delta(z_1-z_2) + \hbar\Pi(z_1,z_2;\Omega_\lambda)\}\{u_\lambda(z_2) - v_\lambda(z_2)\} = \hbar\Omega_\lambda u_\lambda(z_1), \tag{10}$$

$$\mathcal{L}v_\lambda(z_1) + \int dz_2\{n_b g_{bb}\delta(z_1-z_2) + \hbar\Pi(z_1,z_2;\Omega_\lambda)\}\{v_\lambda(z_2) - u_\lambda(z_2)\} = -\hbar\Omega_\lambda v_\lambda(z_1), \tag{11}$$

where $\mathcal{L}=K_b^0+g_{bb}n_b+g_{bf}n_f$. The $\hbar\Pi$ denotes the energy representation of the polarization potential in Eq. (8):

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

where the index p (h) represents a state with energy above (below) the Fermi energy. Since we consider the stationary condensates, the order parameter Φ is assumed to be real [30].

We should note that the number of eigenvalues Ω_λ obtained from Eqs. (10) and (11) may exceed the dimension of the bosonic quasiparticle space because these equations are not linear for the eigenvalue Ω_λ (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 quasiparticle wave functions, we take

$$\int dz_1[|u_\lambda(z_1)|^2 - |v_\lambda(z_1)|^2] - \int dz_1 dz_2\{u_\lambda^*(z_1) - v_\lambda^*(z_1)\} \times \left.\frac{d\Pi(z_1,z_2;\Omega)}{d\Omega}\right|_{\Omega_\lambda}\{u_\lambda(z_2) - v_\lambda(z_2)\} = 1. \tag{13}$$

III. PEIERLS INSTABILITY OF THE HOMOGENEOUS STATE

A. Dispersion equation for excitation energies

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

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

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 wave number $k=\pi n/L$ (n=integer) and mean-field single-particle energy $\epsilon_k^f=\hbar^2k^2/2m_f+g_{bb}n_b$. The Fermi wave number and energy, k_F and ϵ_F, becomes $k_F=\pi n_f$ and $\epsilon_F=\hbar^2\pi^2 n_f^2/(2m_f)+g_{bb}n_b$.

The boson quasiparticle wave functions u_λ and v_λ also become plane waves: $u_{\lambda,k}(z)=u_{\lambda,k}e^{ikz}$ and $v_{\lambda,k}(z)=v_{\lambda,k}e^{ikz}$. Substituting them into Eqs. (10) and (11), we obtain

$$(\epsilon_k^b - \mu_b)u_{\lambda,k} + \{g_{bb}n_b + \hbar\Pi_k(\Omega_\lambda)\}\{u_{\lambda,k} - v_{\lambda,k}\} = \hbar\Omega_\lambda u_{\lambda,k}, \tag{15}$$

$$(\epsilon_k^b - \mu_b)v_{\lambda,k} + \{g_{bb}n_b + \hbar\Pi_k(\Omega_\lambda)\}\{v_{\lambda,k} - u_{\lambda,k}\} = -\hbar\Omega_\lambda v_{\lambda,k}, \tag{16}$$

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

$$\hbar\Pi_k(\Omega_\lambda) = g_{bf}^2 n_b\int_{-k_F}^{k_F}\frac{dq}{2\pi}\left[\frac{1}{\hbar\Omega_\lambda - \epsilon_{q+k}^f + \epsilon_q^f + i\eta} - \frac{1}{\hbar\Omega_\lambda - \epsilon_q^f + \epsilon_{q+k}^f + i\eta}\right]. \tag{17}$$

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 Ω_λ:

$$(\hbar\Omega_\lambda)^2 = (e_k^b)^2 + 2e_k^b\{g_{bb}n_b + \hbar\Pi_k(\Omega_\lambda)\}, \tag{18}$$

where $e_k^b=\hbar^2k^2/2m_b$.

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

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

After execution of the q integration in Eq. (17), they become [31]

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

$$\hbar\Pi_k^{\rm Im}(\omega_\lambda,\gamma_\lambda) = -A_k\Bigg[\pi\theta\left(2k_F - \left|k - \frac{2m_f\omega_\lambda}{\hbar k}\right|\right) - \pi\theta\left(2k_F - \left|k + \frac{2m_f\omega_\lambda}{\hbar k}\right|\right) + \arctan\left(\frac{2\left(\frac{2m_f}{\hbar k}\right)^2\omega_\lambda\gamma_\lambda}{(k+2k_F)^2 + \left(\frac{2m_f}{\hbar k}\right)^2(\gamma_\lambda^2 - \omega_\lambda^2)}\right) - \arctan\left(\frac{2\left(\frac{2m_f}{\hbar k}\right)^2\omega_\lambda\gamma_\lambda}{(k-2k_F)^2 + \left(\frac{2m_f}{\hbar k}\right)^2(\gamma_\lambda^2 - \omega_\lambda^2)}\right)\Bigg], \tag{20}$$

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

$$\hbar^2(\omega_\lambda^2 - \gamma_\lambda^2) = (e_k^b)^2 + 2e_k^b\{g_{bb}n_b + \hbar\Pi_k^{\rm Re}\}, \tag{21}$$

$$\hbar^2\omega_\lambda\gamma_\lambda = e_k^b\hbar\Pi_k^{\rm Im}. \tag{22}$$

Now, in order to analyze the dispersion equations (21) and (22) qualitatively, we discriminate two cases. First, when $\hbar\Pi_k^{\rm Im}(\omega_\lambda) \neq 0$ and ω_λ, $k > 0$, 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:

$$\hbar\Pi_k^{\rm Re}(\omega_\lambda) = -A_k \ln\left|\frac{(k+2k_F)^2 - (2m_f\omega_\lambda/\hbar k)^2}{(k-2k_F)^2 - (2m_f\omega_\lambda/\hbar k)^2}\right|. \tag{23}$$

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

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

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

$$\zeta = \frac{g_{bf}^2}{\pi g_{bb}\hbar v_F}. \tag{25}$$

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 ζ.

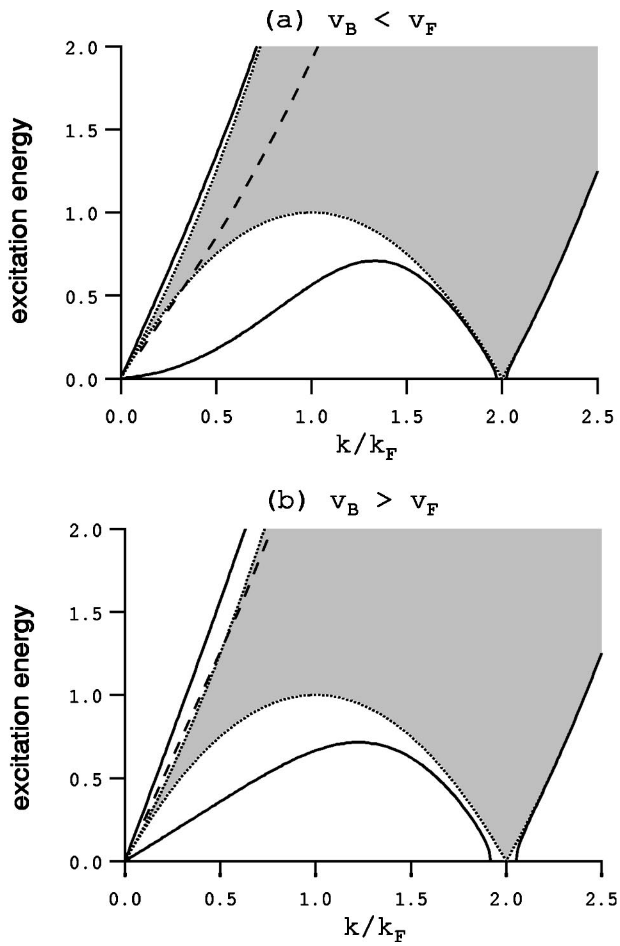

FIG. 2. Excitation spectrum (in units of $\hbar v_F k_F$) of Bose-Fermi mixtures. Solid lines: collective modes of *p-h* pairs and bosonic modes. Dashed line: free boson. Shaded area: continuum *p-h* pair excitation spectra.

B. Excitation spectra and Peierls instabilities

Let us study the bosonic excitation spectra on the homogeneous ground state (14) with solving the dispersion relations (21) and (22). To understand general features, we show numerical results for two typical cases 2(a) $v_B < v_F$ and 2(b) $v_B > v_F$ in Fig. 2: 2(a) $(v_B/v_F)^2 = 0.67$, $\zeta = 0.99$ and 2(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 Fig. 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 a 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 Fig. 2, and we can find that it runs between two collective spectra in the interacting ones.

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

In the 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 2(a)]. In the case that $v_B > v_F$ [case 2(b)], the corresponding modes are above the continuum. It suggests that the low-lying collective mode in 2(a) is mainly a Bogoliubov-phonon mode from bosonic atoms but the corresponding mode in 2(b) is mainly the fermion *p-h* one, and the high-lying modes have opposite characters. In Fig. 2, the bosonic excitation modes are found to be influenced by the interaction with the fermion *p-h* excitation modes and pushed downward or upward in the case 2(a) or 2(b).

Around $k \simeq 2k_F$, 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 $|q|/k_F$ ($q = k - 2k_F$):

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

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. (21):

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

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

Analyzing the eigenvalues of Eq. (21) in 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 the Q1D system, which suggests that the homogeneous state is unstable against fluctuations with a 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 ω_λ/k = const, the real part of the polarization potential becomes

$$\hbar\Pi_k^{\mathrm{Re}}(\omega_\lambda) = \frac{(g_{bf})^2 n_b}{\pi\hbar v_F} \frac{(v_F k)^2}{\omega_\lambda^2 - (v_F k)^2} \tag{28}$$

and the imaginary part Π_k^{Im} vanishes except at $v_B = v_F$. Substituting Eq. (28) into Eq. (21), we obtain two branches of excitations:

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

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 the stability condition for the $k \simeq 0$ mode:

$$\frac{\pi^2\hbar^2}{m_f} n_f \geqslant \frac{(g_{bf})^2}{g_{bb}}, \tag{30}$$

where we have used the relation $n_f = k_F/\pi$. This $k \simeq 0$ instability is considered to cause the phase-separated states to become 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 and competition between these states (for 2D Bose-Fermi mixtures in an optical lattice, see [18]).

IV. DENSITY WAVES IN THE BOSON-FERMION GROUND STATE

The results obtained in the previous section show 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 $\Phi(z) = b_u + b_p\cos(2k_F z)$. The constant bosonic density is given by $n_b = b_u^2 + b_p^2/2$. In the case of a 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

$$\frac{\hat{H}}{L} = \frac{g_{bb}}{2}(b_u^4 + b_u^2 b_p^2) + \epsilon_p^b b_p^2 + \sum_k \epsilon_k^f \hat{c}_k^\dagger \hat{c}_k + g_{bf} b_u b_p \sum_k (\hat{c}_{k-2k_F}^\dagger \hat{c}_k + \hat{c}_{k+2k_F}^\dagger \hat{c}_k), \tag{31}$$

where $\hat{c}_k$ and $\hat{c}_k^\dagger$ are the annihilation and creation operators for fermions with wave number k and energy $\epsilon_k^f = \hbar^2 k^2/2m_f + g_{bf}(b_u^2 + b_p^2/2)$. The ϵ_p^b in Eq. (31) is the energy generated from the periodic condensate: $\epsilon_p^b = e_{2k_F}^b/2 + g_{bb} b_u^2$. 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 states with $k \pm 2k_F$.

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

$$iF_{k,k'}(t-t') \equiv \langle T[\hat{c}_k(t)\hat{c}_{k'}^\dagger(t')] \rangle = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} F_{k,k'}(\omega), \tag{32}$$

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 nonvanishing off-diagonal matrix elements at $F_{k,k\pm 2k_F}$ 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 the case of $k_F \geqslant k > 0$, the Dyson equation for the Green's function can be approximated by

$$\begin{pmatrix} \hbar\omega - \epsilon_k^f & -\Delta \\ -\Delta & \hbar\omega - \epsilon_{k-2k_F}^f \end{pmatrix} \begin{pmatrix} F_{k,k} \\ F_{k,k-2k_F} \end{pmatrix} = \begin{pmatrix} \hbar \\ 0 \end{pmatrix}, \tag{33}$$

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:

$$F_{k,k} = \frac{U_k^2}{\omega - E_k^-/\hbar - i\eta} + \frac{V_k^2}{\omega - E_k^+/\hbar + i\eta}, \tag{34}$$

$$F_{k,k-2k_F} = \frac{-U_kV_k}{\omega - E_k^-/\hbar - i\eta} + \frac{U_kV_k}{\omega - E_k^+/\hbar + i\eta}, \tag{35}$$

where

$$U_k = \sqrt{\frac{1}{2}}\left\{1 - \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta^2}}\right\}^{1/2}, \tag{36}$$

$$V_k = \sqrt{\frac{1}{2}}\left\{1 + \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta^2}}\right\}^{1/2}, \tag{37}$$

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

$$E_k^{\pm} = \epsilon_k^f - \xi_k \pm \sqrt{\xi_k^2 + \Delta^2}, \tag{38}$$

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 Δ, we calculate the total energy of the system in the present approximation. The fermionic contributions to the energy are obtained by summing up the E_k^- in Eq. (38) up to the Fermi wave number k_F:

$$\begin{aligned} E_f &= \int dk E_k^- \theta(k_F - |k|) \\ &= \left(\frac{e_F}{3} + g_{bf}n_b\right)n_f + n_f\left[e_F - \sqrt{e_F^2 + \Delta^2} \right. \\ &\quad \left. - \frac{\Delta^2}{e_F}\ln\left(\frac{e_F + \sqrt{e_F^2 + \Delta^2}}{|\Delta|}\right)\right], \end{aligned} \tag{39}$$

where $e_F = \hbar v_F k_F/2$. For simplicity, we consider the weak-coupling limit $|\Delta| \ll e_F$; then, the total energy density of the system becomes

$$\begin{aligned} E_{\text{tot}}(|\Delta|) - E_{\text{tot}}(0) = \frac{n_f\Delta^2}{4e_F}\left[\frac{2}{\zeta}\left\{1 + \left(\frac{m_f v_F}{m_b v_B}\right)^2\right\} \right. \\ \left. - \frac{1}{2}\left\{1 + 2\ln\frac{4e_F}{|\Delta|}\right\}\right]. \end{aligned} \tag{40}$$

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

$$\frac{|\Delta|}{e_F} = 4\exp\left[-\frac{2}{\zeta}\left\{1 + \left(\frac{m_f v_F}{m_b v_B}\right)^2\right\}\right]. \tag{41}$$

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

$$E_{\text{tot}}(|\Delta|) - E_{\text{tot}}(0) = -\frac{\Delta^2}{4\pi\hbar v_F}, \tag{42}$$

which shows that the state with the "periodic condensate" $(b_p \neq 0)$ has lower energy than the uniform one.

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

$$\begin{aligned} n_f(z) = \lim_{\eta\to 0_+}\sum_k \int \frac{d\omega}{2\pi i} e^{i\eta\omega}[F_{k,k} + F_{k,k-2k_F}e^{i2k_Fz} \\ + F_{k-2k_F,k}e^{-i2k_Fz} + F_{k-2k_F,k-2k_F}]. \end{aligned} \tag{43}$$

Using Eqs. (34)–(37), it becomes

$$\begin{aligned} n_f(z) &= \sum_k [U_k^2 + V_k^2 - 2U_kV_k\cos(2k_Fz)] \\ &= n_f\left[1 - \frac{\Delta}{e_F\zeta}\cos(2k_Fz)\right], \end{aligned} \tag{44}$$

which shows that, for finite Δ, the fermion state is in the density-wave one where the fermionic density has a periodicity $2k_F$. Corresponding to Eq. (44), the direct calculation shows that the bosonic density $n_b(z)$ has a similar density-wave structure:

$$n_b(z) = n_b\left[1 + \frac{|\Delta|}{|g_{bf}|n_b}\cos(2k_Fz)\right]. \tag{45}$$

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. (41), the gap energy Δ essentially depends on two combinations of parameters: $m_f v_F/m_b v_B$ and the dimensionless coupling constant ζ. In Fig. 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 by increasing the 1D density of condensate and/or using heavier bosons than fermions.

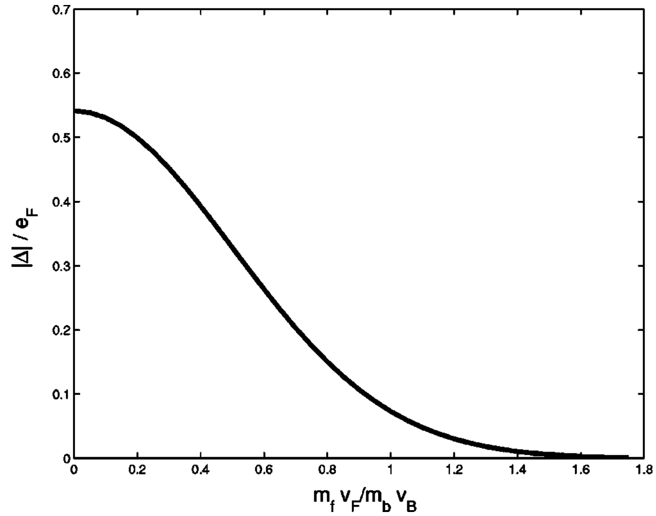

FIG. 3. Gap energy as function of $m_f v_F/m_b v_B$ (in units of e_F) for $\zeta=0.99$.

V. PEIERLS INSTABILITY OF THE SYSTEM IN THE HARMONIC OSCILLATOR POTENTIAL

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

Using the eigenenergy $\epsilon_n^{ho} = \hbar\omega_a\left(n+\frac{1}{2}\right)$ ($n=0,1,2,\ldots$) and the wave function ϕ_n^{ho} for the 1D HO potential, the quasiparticle amplitudes u_λ and v_λ are expanded by

$$u_\lambda(z) = \sum_n u_n^\lambda \phi_n^{ho}(z), \quad v_\lambda(z) = \sum_n v_n^\lambda \phi_n^{ho}(z). \tag{46}$$

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

$$\sum_n [(\epsilon_n^{ho} - \hbar\omega_\lambda)\delta_{m,n}u_n^\lambda + \hbar\Pi_{mn}(\omega_\lambda)(u_n^\lambda - v_n^\lambda)] = 0, \tag{47}$$

$$\sum_n [(\varepsilon_n^{ho} + \hbar\omega_\lambda)\delta_{m,n}v_n^\lambda + \hbar\Pi_{mn}(\omega_\lambda)(v_n^\lambda - u_n^\lambda)] = 0, \tag{48}$$

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) and (48), is given by

$$\hbar\Pi_{mn}(\omega_\lambda) = (g_{bf})^2 N_b \sum_{ph}\left[\frac{\langle mh|p0\rangle\langle 0p|hn\rangle}{\hbar\omega_\lambda - \epsilon_p^{ho} + \epsilon_h^{ho}} - \frac{\langle mp|h0\rangle\langle 0h|pn\rangle}{\hbar\omega_\lambda - \epsilon_h^{ho} + \epsilon_p^{ho}}\right]. \tag{49}$$

The matrix elements in Eq. (49) are defined by

$$\langle mh|p0\rangle = \int dz\, \phi_m^{ho}\phi_h^{ho}\phi_p^{ho}\varphi_0, \tag{50}$$

where the single-particle wave functions in Eq. (50) have been replaced by the HO eigenfunctions ϕ_n^{ho}. It should be noted that the matrix element, Eq. (50), has a transition probability only in the spatial region where the condensate exists. It is important at this point to contrast the finite system to the homogeneous system in which the condensate is present all over the range.

We restrict the present discussion to the parameter region $\hbar\omega_r > \mu_f > \mu_b > \hbar\omega_a$. Under these conditions, we can take several approximations. Because $\mu_b > \hbar\omega_a$, the system is in the Thomas-Fermi (TF) regime, so that we can take the TF approximation for the order parameter:

$$\Phi = \sqrt{N_b}\varphi_0 \propto \sqrt{1 - \frac{z^2}{z_{TF}^2}}\,\theta(z_{TF} - |z|). \tag{51}$$

The z_{TF} in Eq. (51) is a cutoff length in the TF approximation:

$$z_{TF} = \sqrt{2}a_{ho}\left(\frac{3N_b\beta}{4\sqrt{2}}\right)^{1/3}, \tag{52}$$

where $\beta = mg_{bb}a_{ho}/\hbar^2$ with $a_{ho} = \sqrt{\hbar/m\omega_a}$ (the HO length in the axial direction).

As we have seen in Sec. III, the 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 "wave number" $k_n = \sqrt{2n}/a_{ho} \sim 2k_F$. 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 ϕ_n^{ho} in the middle of the trap $|z| < z_{TF} < L_n$ [32]:

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

For a bosonic eigenstate with higher nodal mode, the negative energy amplitude $v_n^\lambda = 0$ of Eq. (47) can be neglected.

Using these approximations, the matrix elements like $\langle 0p|hn\rangle$ become linear combinations of the form $J_1(z_{TF}K)/z_{TF}K$, where $J_1(x)$ is the first-order Bessel function and the K is a wave-number difference between the initial and 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 $|x| \leqslant \mathcal{O}(1)$ can contribute to the matrix elements. Under the restriction of wave numbers $k_h \leqslant k_F$ and $k_p > k_F$ with $k_n \sim 2k_F$ ($k_F = \sqrt{2N_f}/a_{ho}$), the main contributions of the matrix element are from the scattering processes $k_n \to k_p + k_h$ and $k_n + k_h \to k_p$. To make an estimate, we replace a product of Bessel functions as

$$\frac{J_1(x_1)}{x_1}\frac{J_1(x_2)}{x_2} \simeq \frac{1}{4}\theta(1 - |x_1|)\theta(1 - |x_1 - x_2|) \tag{54}$$

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

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

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

Contrary to the uniform system, the static polarization potential, the second term of the 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 $4\epsilon_F$:

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

where $v_B(0) = \sqrt{g_{bb}n_b(0)/m}$. This is the Peierls instability condition where a boson-fermion density wave may occur.

We roughly estimate the parameters according to experimental conditions. When $m_b/m_F \sim 1$, we can express the velocity ratio and the dimensionless coupling constant by

$$\frac{v_B^2}{v_F^2} = \frac{1}{4N_f}\left(3N_b\frac{\omega_r}{\omega_a}\frac{a_{bb}}{a_{ho}}\right)^{2/3}, \tag{57}$$

$$\zeta = \sqrt{\frac{2}{\pi^2 N_f}}\frac{\omega_r}{\omega_a}\frac{a_{bf}^2}{a_{bb}a_{ho}}. \tag{58}$$

As a possible candidate for the Peierls instability, we take the rubidium isotope system: ^{87}Rb-^{84}Rb mixtures. Taking the scattering lengths in [33], $a_{bb} = 5.3$ nm and $a_{bf} = 29.1$ nm, and the typical trapping frequencies $\omega_a = 2\pi \times 10$ Hz and ω_r

$=2\pi\times 15$ kHz, Eq. (56) gives $N_f=10^3$ and $N_b=2\times 10^4$ for realization of the Peierls instability.

VI. SUMMARY

In the present paper, we studied the occurrence of a Peierls instability in Q1D Bose-Fermi mixtures at zero temperature. We analyzed the bosonic collective-excitation spectra in the random phase approximation. It shows that the mixtures of a uniform BEC and a Fermi gas are unstable against spontaneous formation of a collective mode of wave number $2k_F$; this type of instability is known as the Peierls instability. This result suggests that the ground state of bosons is a periodic condensate with period π/k_F. In the variational method, the boson-fermion density wave state has 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 the Peierls instability condition.

It is well known that density waves in Q1D conductors lead to generations of Lee-Rice-Anderson [34] and phase soliton [26] modes. Thus, studies of the dynamical properties of boson-fermion density waves should be interesting problems in the future.

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