Anomalous dispersion of the collective modes of an ultracold $^6$Li–$^{40}$K mixture in a square optical lattice

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We report numerical calculations of the collective excitation spectrum and the speed of sound of the superfluid phase of an atomic Fermi-Fermi mixture of population-imbalanced Lithium-6 and Potassium-40 atoms in a square lattice. It is predicted that in the exotic states of matter, known as the Fulde-Ferrell phase, an anomalous dispersion of the collective modes may be realized at some values of polarization, interacting strength and temperature, i.e., the collective-mode dispersion initially bends upward before bending over as the quasimomentum increases.

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I. INTRODUCTION

The anomalous dispersion of the collective modes in a superfluid phase is a phenomenon which describes the upward deviation of the collective-mode spectrum from linearity. In this case, the conservation laws of energy and momentum allow processes which do not conserve the number of excitations, such as the three-particle process in which one particle decays into two with lower energy, or two interacting particles combining into one. The energy conservation condition requires that the dispersion relation first bends up as quasimomentum increases, before bending over. From an experimental point of view, the existence of anomalous dispersion can be confirmed by neutron scattering, which allows the direct determination of the collective-mode dispersion. However, neutron measurements are difficult to be conducted because rather small scattering angles must be employed. The anomalous dispersion is well established in superfluid $^4$He for pressures $\leq 20$ bar. In this region, one long-wavelength excitation (referred to as a superfluid phonon) can decay into another one by absorbing a second phonon (the Landau damping), or one long-wavelength phonon can decay into two others (the Beliaev damping).

The subject of anomalous dispersion of the collective modes in a Bose gas in a periodic optical lattice potential at low temperatures has been explored in Refs. [1,2]. It was found that the spectrum of the collective modes of the Bose-Hubbard model exhibits an anomalous phonon dispersion under some critical on-site inter-atom interaction. This may cause Landau damping of collective modes in Bose condensates in a one-, two-, and three-dimensional periodic optical lattice potential.

The question naturally arises as to whether it is possible for the collective-mode dispersion of the Fermi-Hubbard model in the long-wavelength limit to convex concave up and thus exhibit an anomalous dispersion. Turning our attention to the theoretical description of the single-particle and collective-mode excitations of superfluid alkali atom Fermi gases in optical lattice potentials, we find that there have been impressive theoretical achievements [2,4]. Despite the fact that the anomalous dispersion of the collective modes in Fermi condensates has not been predicted to exist in these papers, it was found that when the anomalous dispersion of interacting Fermi atoms is represented by the relation $\omega(Q) = cQ(1 + \gamma Q^2 - \delta Q^4)$, where $c$ is the speed of sound, and $\gamma, \delta > 0$, then the scattering amplitude is formally equivalent to the corresponding expression obtained in the case of three-phonon damping in superfluid $^4$He [4].

In what follows, we use the generalized random phase approximation (GRPA) to calculate the long-wavelength limit of the collective excitation spectrum, and the corresponding speed of sound, of an interacting Fermi mixture of Lithium-6 and Potassium-40 atoms in a two-dimensional optical lattice at finite temperatures with the Fulde-Ferrell (FF) order parameter. Our numerical calculations show that at some values of polarization, interacting strength and temperature the collective-mode dispersion $\omega(Q)$ initially bends upward before bending over as the quasimomentum $Q$ increases.

II. LONG-WAVELENGTH DISPERSION OF THE COLLECTIVE MODES OF AN ULTRACOLD $^6$Li–$^{40}$K MIXTURE

From a theoretical point of view, the simplest approach to the fermions in optical lattices is the tight-binding approximation, which requires a sufficiently deep lattice potential. In the tight-binding limit, two alkali atoms of opposite pseudospins on the same site have an interaction energy $U$, while the probability to tunnel to a neighboring site is given by the hopping parameters. The hopping parameters as well as the interaction energy depend on the depth of the lattice potential and can be tuned by varying the intensity of the laser beams. We assume that the interacting fermions are in a sufficiently deep periodic lattice potential described by the Hubbard Hamiltonian. We restrict the discussion to the case of atoms confined to the lowest-energy band (single-band Hubbard model), with two possible states described by pseudospins $\sigma$. We consider different amounts of $^6$Li and $^{40}$K atoms in each state ($\sigma = \uparrow = Li, \sigma = \downarrow = K$) achieved by considering different chemical potentials $\mu_\uparrow$ and $\mu_\downarrow$. 
There are $M = M_{t} + M_{i}$ atoms distributed along $N$ sites, and the corresponding filling factors $f_{t,i} = M_{t,i}/N$ are smaller than unity. The Hubbard Hamiltonian is defined as follows:

$$H = - \sum_{\sigma} J_{\sigma} \psi_{i,\sigma}^{\dagger} \psi_{j,\sigma} - U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} - \sum_{i,\sigma} \mu_{\sigma} n_{i,\sigma},$$

(1)

where $J_{\sigma}$ is the single electron hopping integral, and $n_{i,\sigma} = \psi_{i,\sigma}^{\dagger} \psi_{i,\sigma}$ is the density operator on site $i$. The Fermi operator $\psi_{i,\sigma}^{\dagger}$ ($\psi_{i,\sigma}$) creates (destroys) a fermion on the lattice site $i$ with pseudospin projection $\sigma$. The symbol $\sum_{<ij>}$ means sum over nearest-neighbor sites of the two-dimensional lattice. The first term in (1) is the usual kinetic energy term in a tight-binding approximation. All numerical calculations will be performed assuming that the hopping (tunneling) ratio $J_{L_{i}}/J_{K} \approx 0.15$. In our notation the strength of the on-site interaction $U > 0$ is positive, but the negative sign in front of the interaction corresponds to the Hubbard model with an attractive interaction. In the presence of an (effective) attractive interaction between the fermions, no matter how weak it is, the alkali atoms form bound pairs, also called the Cooper pairs. As a result, the system becomes unstable against the formation of a new many-body superfluid ground state. The superfluid ground state comes from the U(1) symmetry breaking, characterized by a nonzero order parameter, which in the population-balanced case is assumed to be a constant in space $\Delta_{0}$. Physically, it describes a superfluid state of Cooper pairs with zero momentum. A superfluid state of Cooper pairs with nonzero momentum occurs in the population-imbalanced case between a fermion with momentum $k + q$ and spin $\uparrow$ and a fermion with momentum $-k + q$, and spin $\downarrow$. As a result, the pair momentum is $2q$. A finite pairing momentum implies a position-dependent phase of the order parameter, which in the FF case varies as a single plane wave $\Delta(k) = \Delta_{0} \exp(2\pi q_{x} a)$, where $\Delta_{0}$ is a real quantity. The order parameter can also be a combination of two plane waves as in the case of the Larkin-Ovchinnikov (LO) superfluid states. In both cases, we are dealing with spontaneous translational symmetry breaking and an inhomogeneous superfluid state. When continuous and global symmetries are spontaneously broken the collective modes, known as the Nambu-Goldstone modes, appear.

The mean-field treatment of the FF and LO phases in a variety of systems shows that the FF and LO states compete with a number of other states, such as the Sarma ($q = 0$) states, and the superfluid-normal separation phase (also known as the phase separation phase). It turns out that in some regions of momentum space the FF (or LO) phase provides the minimum of the mean-field expression of the Helmholtz free energy. Phase diagrams for a $^{6}\text{Li} - ^{40}\text{K}$ mixture at zero temperature were obtained in Ref. [11], but the calculations were limited to the emergence of insulating phases during the evolution of superfluidity from the BCS to the BEC regime, and the competition between the FF and Sarma phases was ignored. The polarization versus temperature diagrams in Fig. 1 show that there are three phases in the mass-imbalanced case: the Sarma phase, the FF phase, and the normal phase in which the Helmholtz free energy is minimized for gapless phase. The zero polarization line is the conventional Bardeen-Cooper-Schrieffer state. Contrary to the phase diagram of population-imbalanced $^{6}\text{Li}$ Fermi gas, where the phase separation appears for low polarizations, the existence of a polarization window for the FF phase was found. This means that as soon as the system is polarized it goes into the FF phase if the temperature is low enough. This polarization window is larger for a majority of $^{40}\text{K}$ atoms compared to the majority of $^{6}\text{Li}$ atoms. Since the GRPA is a good approximation in a weak-coupling regime, we have chosen the on-site interaction to be $U/J_{Li} = 2$. The mean-field number-, gap- and q-equations [22] were solved at a temperature $T/J_{Li} = 0.01$ for three polarizations: $P = (f_{K} - f_{Li})/(f_{K} + f_{Li}) = 0.1, 0.3$, and $P = 0.4$, where the total filling factor is $f = f_{K} + f_{Li} = 0.5$. The corresponding mean-field results for the Fulde-Ferrell wave vector $q = (\tilde{q}\pi/a, 0)$ ($a$ is the lattice constant), the two chemical potentials $\tilde{\mu}_{Li,K} = \mu_{Li,K}/J_{Li}$, and the gap $\Delta = \Delta/J_{Li}$ are as follows:

$$P = 0.1, \tilde{q} = 0.049, \tilde{\mu}_{Li} = 2.091, \tilde{\mu}_{K} = 0.551, \tilde{\Delta} = 0.367,$$

$$P = 0.3, \tilde{q} = 0.122, \tilde{\mu}_{Li} = 1.894, \tilde{\mu}_{K} = 0.479, \tilde{\Delta} = 0.170,$$

$$P = 0.4, \tilde{q} = 0.153, \tilde{\mu}_{Li} = 1.683, \tilde{\mu}_{K} = 0.493, \tilde{\Delta} = 0.108.$$  

(2)

Generally speaking, the collective excitations of the Hamiltonian [11] manifest themselves as poles of the two-particle Green’s function (or equivalently, as poles of the density and spin response functions). Since the fermion self-energy does depend on the two-particle Green’s func-

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**FIG. 1:** The phase diagrams of a $^{6}\text{Li} - ^{40}\text{K}$ mixture in a square lattice [12]. The interaction strength is $U = 2J_{Li}$. The polarization is defined as $P = (f_{K} - f_{Li})/f$, where the total filling is $f = 0.5$ atoms/lattice site. Colors: Sarma states = blue (black), FF = red (dark grey), and normal gas = white.
the long-wavelength limit and the corresponding speed of sound.

The mean-field system parameters are given in the text. The anomalous dispersion appears for polarization $P=0.4$.

![Image](image.png)

**FIG. 2:** The collective-mode dispersion $\omega(Q_x)$ in positive $Q_x$-direction calculated by the Bethe-Salpeter formalism for a 2D system with $U = 2J_{Li}$ and $T = 0.01J_{Li}$ and three different polarizations: $P = 0.1$ - diamonds (blue), $P = 0.3$ - circles (red), and $P=0.4$ - triangles (black). The red, blue and black straight lines define the slope of the curves in the long-wavelength limit and the corresponding speed of sound. The mean-field system parameters are given in the text. The anomalous dispersion appears for polarization $P=0.4$.

![Image](image.png)

**FIG. 3:** The collective-mode dispersion $\omega(Q_x)$ in negative $Q_x$-direction calculated by the Bethe-Salpeter formalism for a 2D system with $U = 2J_{Li}$ and $T = 0.01J_{Li}$ and three different polarizations: $P = 0.1$ - diamonds (blue), $P = 0.3$ - circles (red), and $P=0.4$ - triangles (black). The red, blue and black straight lines define the slope of the curves in the long-wavelength limit and the corresponding speed of sound. The mean-field system parameters are given in the text. The anomalous dispersion appears for polarization $P=0.4$.

Equation. The kernel of the BS equation in the GRPA is obtained by summing ladder and bubble diagrams. The mean-field decoupling of the single-particle and two-particle Green’s functions leads to expressions for the Green’s functions that cannot be evaluated exactly because the interaction part of the Hamiltonian is quartic in the fermion fields. The simplest way to solve this problem is to transform the quartic term into quadratic form by making the Hubbard-Stratonovich transformation for the fermion operators. In contrast to the previous approaches, such that after performing the Hubbard-Stratonovich transformation the fermion degrees of freedom are integrated out; we decouple the quartic problem by introducing a model system which consists of a multi-component boson field interacting with fermion fields.

The mean-field single-particle Green’s function, used in our numerical calculations, is a $4 \times 4$ matrix, which takes into account all possible thermodynamic averages. The poles of the two-particle Green’s function (the solutions of the Bethe-Salpeter equation) are defined by the zeros of the corresponding $8 \times 8$ secular determinant. It is worth mentioning, that it is possible to reduce the single-particle Green’s function to the $2 \times 2$ one by neglecting some of the thermodynamic averages. As a result, the corresponding secular determinant reduces to a $4 \times 4$ determinant.

We have calculated the collective-mode dispersion in $Q_x$-direction using the $4 \times 4$ and the $8 \times 8$ secular determinants at three different polarizations. The corresponding mean-field system parameters are listed in (2). It turns out that the two secular determinants provide almost the same collective-mode dispersion (the difference is about 2% - 7% in the interval $-0.1\pi/a < Q_x < 0.1\pi/a$, and less than 1% out of this interval). The speed of sound, $c_{\pm}$, to the positive and negative directions of the $Q_x$ axis is defined by $d\omega(Q_x)/dQ_x$ at $Q_x \rightarrow 0$.

In Fig. 2 and Fig. 3, we have presented the three collective-mode dispersions $\omega(Q_x)$ numerically calculated by using the $8 \times 8$ secular determinant. The straight lines define the slope of the dispersion curves and the corresponding speeds of sound:

$$P = 0.1, \quad c_+ = 0.614J_{Li}a/h, \quad c_- = 0.534J_{Li}a/h$$

$$P = 0.3, \quad c_+ = 0.910J_{Li}a/h, \quad c_- = 0.793J_{Li}a/h$$

$$P = 0.4, \quad c_+ = 0.466J_{Li}a/h, \quad c_- = 0.500J_{Li}a/h.$$
dispersion curve has no quadratic term in $Q_x$, and the dependence $\omega(Q_z)$ is similar to the corresponding fit in the $^4$He case:

$$\omega(Q_z) = u Q_z \left[ 1 + \delta_1 (Q_z a)^2 - \delta_2 (Q_z a)^3 + \delta_3 (Q_z a)^4 + \ldots \right].$$

In positive $Q$-direction we have: $u = 0.478 J_z a / \hbar$, $\delta_1 = 9.78$, $\delta_2 = 24.37$, and $\delta_3 = 15.20$. In negative direction the parameters are: $u = 0.496 J_z a / \hbar$, $\delta_1 = 10.44$, $\delta_2 = 36.03$, and $\delta_3 = 30.6$. It is worth mentioning, that this fit represents better the curve compare with the relation $\omega(Q) = c Q (1 + \gamma Q^2 - \delta Q^4)$ assumed in Ref. [44].

In conclusion, we have shown that collective excitation spectrum of the Fulde-Ferrell superfluid phase of an atomic Fermi-Fermi mixture of population-imbalanced Lithium-6 and Potassium-40 atoms in a square lattice may exhibit anomalous dispersion at some values of polarization, interacting strength and temperature, and therefore, it is possible to have the damping of collective modes due to the three-particle process in which one particle decays into two with lower energy, or two interacting particles combine into one.

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