BCS–BEC crossover in a quasi-two-dimensional Fermi superfluid

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Abstract
We study the crossover from the Bardeen–Cooper–Shrieffer regime to the Bose–Einstein-condensation regime in an anisotropic trapped quantum gas of ultracold fermionic atoms. Using an effective two-dimensional Hamiltonian with renormalized interactions between atoms and dressed molecules, we extend the Gaussian pair fluctuation theory to quasi-two-dimensional systems. The equation of state, pair size and sound velocity as well as the convexity parameters of the Goldstone mode are investigated to show how Fermi superfluidity is affected by reduced dimensionality and Gaussian fluctuations at zero temperature in a wide range of crossover. We compare our results with the recent experiment of $^6$Li atomic gases and find good agreements.

1. Introduction

The effect of reduced dimensionality on pairing states of fermions is an intriguing yet open question, especially in the context of superfluids and superconductors. Owing to the restriction of motional degrees of freedom and the existence of strong fluctuations in low dimensions, exotic pairing phases may be stabilized, such as the Fulde–Ferrell–Larkin–Ovchinnikov state with a finite pairing momentum [1] and the Berezinskii–Kosterlitz–Thouless phase with vortex-antivortex pairs [2–4]. Of particular interest are two-dimensional (2D) Fermi systems, which not only give the highest critical temperature superconductors at ambient pressure [5] and high temperature superfluidity with large gap [6, 7], but also feature quantum anomaly in their collective excitations [8–11].

Recently, rapid experimental progresses have greatly promoted the research on 2D superconductivity and superfluidity. In condensed matter systems, precise control of carrier density, geometric strain and lattice structure significantly bring forward the study of multiband layered superconductors such as FeSe [12], FeSe$\_1-x$S$_x$ [13, 14], Li$_x$ZrNCl [15], and magic-angle twisted trilayer graphene [16]. In atomic systems, highly anisotropic traps or one-dimensional optical lattices have been implemented to realize quasi-two-dimensional (Q2D) Fermi gases with tunable inter-particle interaction via Feshbach resonances [17–26]. A very recent experiment in ultracold gases of $^6$Li atoms [25] has now provided benchmark results on Q2D superfluidity by evolving the system from a weakly interacting Bardeen–Cooper–Schrieffer (BCS) superfluid to a tightly-bound Bose–Einstein condensate (BEC). For 2D and 3D Fermi systems, Gaussian pair fluctuation (GPF) theory have been applied in a wide variety of theoretical studies [27–38], which demonstrate the significant role of Gaussian fluctuations and on the understanding of system properties both qualitatively and quantitatively. However, for Q2D systems, a framework of GPF which incorporates both the interaction and reduced dimensionality effects is still lack.
In this paper, we theoretically investigate the BCS–BEC crossover of a Fermi gas subjected to a tight harmonic confinement along one spatial dimension (the z direction), under conditions compatible with the recent experiment of 6Li atoms [25]. In the BCS regime, the confinement provides the dominant energy scale and the system approaches the 2D limit. In the BEC regime, the binding energy \( E_B \) of the two-body bound state exceeds the confinement such that the excited harmonic oscillator states along the z-direction are significantly populated [39], and the 2D regime may become difficult to reach [40]. To account for such a Q2D configuration, we adopt an effective two-channel model [36–38, 41, 42] with a phenomenological bosonic particle of dressed molecule [43–46], and extend the GPF approach to study the pairing properties at zero temperature. Compared with the results (with or without Gaussian fluctuations) for purely 2D systems and Q2D systems with different trapping frequencies, our Q2D GPF theory shows the best agreement with the 6Li experiment [25] in superfluid gap, chemical potential, and pair size. These results reveal the remarkable effect of reduced dimensionality and the GPF correction on equation of state and pair size, which can also be drawn from the sound velocity and convexity parameters of the Goldstone mode.

2. GPF theory for Q2D Fermi systems

2.1. Effective Hamiltonian

We consider an ultracold gas of fermionic atoms confined in an axially symmetric anisotropic harmonic trap with trapping frequency along the axial direction (\( \omega_z \)) much stronger than that in the radial plane. When the reduced chemical potential \( \bar{\mu} = \mu + E_B/2 \) and the thermal energy scale \( k_B T \) are both much smaller than the trapping energy scale \( h\omega_z \), the low-energy/long-range physics of the system is effectively 2D. Meanwhile, by tuning the inter-atomic interaction into the BEC regime, the excited harmonic oscillator states of the tightly confined direction are inevitably populated [44]. Therefore, the high-energy/short-range details must be renormalized by either an energy dependent scattering length [11, 40] or a phenomenological degree of freedom of dressed molecule [43–46]. In the following, we adopt the latter approach and write the effective 2D Hamiltonian in the form of a two-channel model (with natural units \( \hbar = 1 \)),

\[
H_{\text{eff}} = \sum_{k\sigma} \xi_k a_{k\sigma}^\dagger a_{k\sigma} + \sum_q (\xi_q + \delta_q)d_q^\dagger d_q + \alpha_b \sum_{kq} (d_q^\dagger a_{-k+q/2,\uparrow} a_{k+q/2,\uparrow} + \text{h.c.}) + V_b \sum_{kk'q} a_{k+q/2,\uparrow}^\dagger a_{-k+q/2,\downarrow}^\dagger a_{k'+q/2,\downarrow} a_{k'+q/2,\uparrow}.
\]

(1)

Here, \( a_{k\sigma} \) and \( d_q \) are the annihilation operators for fermionic atoms and dressed molecules with mass \( m \) and \( 2m \), respectively, and \( \xi_k \equiv \epsilon_k - \mu = k^2/2m - \mu \) and \( \xi_q = \epsilon_q/2 - 2\mu \) are the corresponding dispersions shifted by chemical potentials \( \mu \) and \( 2\mu \) with 2D momenta \( \mathbf{k} \) and \( \mathbf{q} \). The bare detuning \( \delta_q \), bare coupling constant between atom and dressed molecule \( \alpha_b \), and bare background interaction in the open channel \( V_b \) should be renormalized to their corresponding physical parameters \( \delta_p, \alpha_p \) and \( V_p \), via a standard procedure to eliminate divergence and to recover the two-body physics at low energy [44]

\[
\frac{1}{V_{\text{eff}}}^p = \frac{1}{V_{\text{eff}}}^0 - \sum_k \frac{1}{2\epsilon_k + \omega_z}.
\]

(2)

where \( V_{\text{eff}}^p = V_b + \alpha_p^2/(2\mu - \delta_p) \) is the bare renormalized effective interaction between atoms and \( V_{\text{eff}}^0 = V_p + \alpha_p^2/(2\mu - \delta_p) \) is the physical correspondence.

The 2D physical parameters \( \delta_p, \alpha_p \) and \( V_p \) can be determined by matching the solution of two-body bound state in an axially symmetric Q2D trap [44], with the background interaction between atoms \( U_p = 4\pi a_{bg}/m \), the coupling between atom and Feshbach molecule \( g_{bg}^p = \mu_{co}\omega U_p \), and the detuning between the open and closed channels \( \delta_p = \mu_{co}(B_B) \). Here, \( a_{bg} \) is background scattering length, \( \mu_{co} \) is the difference in magnetic moments between the open and close channels, \( W \) is the resonance width, and \( B_B \) is the resonance position. To compare with the experiment of Q2D 6Li atomic gases [25], we consider an effective 2D density per spin state of \( n = 0.8 \text{ atoms/\mu m}^2 \) and an axial trapping frequency \( \omega_z = 2\pi \times 9.2 \text{ kHz} \), and use the parameters \( a_{bg} = -1405a_0, W = 300 \text{ G}, \) and \( \mu_{co} = 2\mu_B \) for the wide Feshbach resonance near 834 G, where \( a_0 \) and \( \mu_B \) are respectively the Bohr radius and Bohr magneton.

The first matching condition is for the two-body bound state energy \( E_B \), which is determined by the solution of the eigen-equation

\[
\frac{1}{U_{\text{eff}}^0(E_B)} = S_p(E_B),
\]

(3)
where $U_{\text{eff}}^{p}(E) = U_{p} + g_{p}^{2}/(E - \nu_{p})$, and

$$S_{p}(E) = -\frac{1}{2\sqrt{2\pi}} \int_{0}^{\infty} dx \left[ \frac{\Gamma(x - E/2)}{\Gamma(x + 1/2 - E/2)} - \frac{1}{\sqrt{x}} \right].$$

(4)

In the off-resonance deep BCS limit, this condition leads to

$$V_{p}^{-1} = \sqrt{2\pi}(U_{p}^{-1} - C_{p}),$$

(5)

where $C_{p} = \lim_{\nu_{p} \to \infty} \left[ S_{p}(E_{b}) - \sigma_{p}(E_{b}) \right]$ and

$$\sigma_{p}(E) = \frac{\ln|E|}{2\sqrt{2\pi}x^{1/2}}.$$

(6)

The second matching condition is for the atomic population in the ground harmonic oscillator state of the $z$ confinement. Together with the bound state energy condition, one obtains the parameters of the effective 2D Hamiltonian equation (1) [44]

$$\delta_{p} = E_{b} - \frac{\sigma_{p}(E_{b})}{\partial_{E} \left[ 1/U_{\text{eff}}^{p}(E) - (S_{p}(E) - \sigma_{p}(E)) \right]} \left[ 1 - \frac{\sigma_{p}(E_{b})}{U_{p}^{-1} - C_{p}} \right],$$

(7a)

$$\alpha_{p}^{2} = \frac{1}{\sqrt{2\pi}} \frac{1}{\partial_{E} \left[ 1/U_{\text{eff}}^{p}(E) - (S_{p}(E) - \sigma_{p}(E)) \right]} \left[ 1 - \frac{\sigma_{p}(E_{b})}{U_{p}^{-1} - C_{p}} \right]^{2}.$$

(7b)

2.2. GPF theory

Adopting the functional path-integral formalism over imaginary time $\tau$ and applying the Hubbard–Stratonovich transformation in real space [47], we decouple the interaction term by introducing an auxiliary bosonic field $\Delta(x) = \epsilon_{0}\phi(x) + \Delta(x)$ with $\phi(x) = \langle d(x) \rangle$, $\Delta(x) = V_{p}(a_{x}a_{x}^{\dagger}(x))$, and $x = (x, \tau)$ the short-hand notation. The effective action is then given in term of the fermionic Nambu spinor $A(x) = [a_{\tau}(x), a_{\tau}^{\dagger}(x)]^{T}$ as

$$S = \beta \sum_{k} \xi_{k} + \int dx dx' A(x)^{\dagger} \left[ -\mathcal{G}_{a}^{-1}(x,x') \right] A(x') - \frac{|\Delta(x)|^{2}}{V_{k}} + \overline{d}(x) \left( \partial_{\tau} + \omega_{q} \right) d(x) + \overline{\phi}(x)\Delta(x) + \text{h.c.}.$$

(8)

Here, $\beta = 1/k_{B}T$ is the inverse temperature, $\mathcal{G}_{a}(x,x')$ is the Green’s function (GF) of atoms, $\overline{d}(\Delta)$ is the complex conjugate of $d(\Delta)$, and $\omega_{q} = q^{2}/4m - 2\mu + \delta_{b}$ is the pair dispersion shifted by chemical potential. Under the mean-field approximation $\Delta(x) = \Delta$ and $\phi(x) = \phi$, the inverse GF is given by

$$\mathcal{G}_{a}^{-1}(x,x') = \begin{pmatrix} -\partial_{\tau} - H_{0}^{b} & -\Delta \\ -\Delta & -\partial_{\tau} - H_{0}^{b} \end{pmatrix} \delta(x - x') \delta(\tau - \tau'),$$

(9)

where $H_{0}^{b} = -\nabla^{2}/2m - \mu$ is the kinetic energy of atoms. By minimizing the mean-field effective action with respect to $\phi$, we obtain the zero-temperature thermodynamic potential ($\Omega_{\text{MF}} = \lim_{T \to 0} k_{B}T\Omega_{\text{MF}}$)

$$\Omega_{\text{MF}} = \sum_{k} \left( \xi_{k} - E_{k} + \frac{\Delta^{2}}{2\epsilon_{k} + \omega_{2}} \right) - \frac{\Delta^{2}}{V_{\text{eff}}^{p}},$$

(10)

where $E_{k} = \sqrt{\xi_{k}^{2} + \Delta^{2}}$ is the quasiparticle dispersion. Note that the bare parameters have been replaced by the physical ones by the renormalization relation equation (2). The saddle point conditions of $\Omega_{\text{MF}}$ lead to the gap and number equations in the mean-field level

$$\frac{1}{V_{\text{eff}}^{p}} = -\sum_{k} \left( \frac{1}{2E_{k}} - \frac{1}{2\epsilon_{k} + \omega_{2}} \right),$$

(11a)

$$n_{\text{MF}} = -\frac{\partial \Omega_{\text{MF}}}{\partial \mu} = 2\phi^{2} + \sum_{k} \left( 1 - \frac{\xi_{k}}{E_{k}} \right),$$

(11b)

where $\phi^{2} = \Delta^{2}/[\alpha_{p} + V_{p}(2\mu - \delta_{p})/\alpha_{p}]^{2}$ is the population of dressed molecules.

We then introduce the fluctuation of the pairing order parameters $\Delta(x) = \Delta + \delta\psi(x)$ and $\phi(x) = \phi + \delta\phi(x)$, and calculate the contribution to the effective action up to the second order. This leads to the following Gaussian term at zero temperature.
\[ S_{\text{GPF}} = \frac{1}{2} \sum_q \overline{\Psi}_m(q) D_0^{-1}(q) \Phi_m(q) - \frac{1}{2} \overline{\Psi}(q) \Gamma_0^{-1}(q) \Psi(q) + \frac{\alpha_p}{2V_b} \left[ \overline{\Psi}_m(q) \Psi(q) + \text{h.c.} \right], \]

(12)

where the bosonic Nambu spinors are defined as \( \Phi_m(q) = [\delta \phi(q), \delta \bar{\phi}(-q)]^T \) and \( \overline{\Psi}(q) = [\delta \psi(q), \delta \bar{\psi}(-q)]^T \), with \( q = (q, \nu_n) \) denoting both the 2D pairing momentum \( q \) and the bosonic Matsubara frequency \( \nu_n \). The inverse of the bosonic GF of dressed molecule reads

\[ D_0^{-1}(q) = \begin{pmatrix} i\nu_n - \omega_q + \frac{\alpha_p^2}{V_b} & 0 \\ 0 & -i\nu_n - \omega_q + \frac{\alpha_p^2}{V_b} \end{pmatrix}. \]

(13)

The elements of the \( 2 \times 2 \) inverse vertex function \( \Gamma_0^{-1} \) are

\[
\Gamma_{0,11}^{-1}(q) = \Gamma_{0,22}^{-1}(-q) = -\sum_k G_{11}(k) G_{22}(k - q) + \frac{1}{V_b},
\]

\[
\Gamma_{0,12}^{-1}(q) = \Gamma_{0,21}^{-1}(q) = -\sum_k G_{12}(k) G_{12}(k - q),
\]

(14)

where \( G \) is the saddle-point GF with the notation \( k = (k, \omega_m) \),

\[ G(k) = \frac{1}{(i\omega_m)^2 - E_k^2} \begin{pmatrix} i\omega_m + \xi_k & -\Delta \\ -\Delta & i\omega_m - \xi_k \end{pmatrix}. \]

(15)

By integrating over the two bosonic Nambu spinors \([47]\), we find that the thermodynamic potential \( \Omega_{\text{GPF}} = k_B T S_{\text{GPF}} \) contributed by quantum pair fluctuations is given by

\[ \Omega_{\text{GPF}} = \frac{1}{2} \sum_q \ln [M_{11}(q) M_{22}(q) - M_{12}(q) M_{21}(q)] e^{i\omega_0^+}, \]

(16)

where an extra factor \( e^{i\omega_0^+} \) is added to ensure the convergence of the summation over \( q \). The expressions of \( M_{ij}(q)(i, j = 1, 2) \) can be worked out explicitly and at zero temperature lead to

\[
M_{11}(q) = \sum_k \left( \frac{\nu_k^2 + \nu_{k}^2}{i\nu_n - E_{k+} + E_{k-}} - \frac{\nu_{k+}^2 \nu_{k-}^2}{i\nu_n - E_{k+} + E_{k-}} + \frac{1}{2\epsilon_k + \omega_m} \right) - \frac{1}{V_{\text{eff}}(q)},
\]

(17)

\[
M_{12}(q) = \sum_k \left( \frac{\nu_{k+} \nu_{k-}}{i\nu_n + E_{k+} + E_{k-}} - \frac{\nu_{k+} \nu_{k-}}{i\nu_n - E_{k+} + E_{k-}} \right),
\]

where

\[ V_{\text{eff}}(q) = V_p + \frac{\alpha_p^2}{i\nu_n - (q^2/4m - 2\mu + \delta_p)}. \]

(18)

In the expressions above, we define \( k_{\pm} = q/2 \pm k \), and BCS superfluid parameters \( \nu_k^2 = (1 + \xi_{k\pm}/E_{k\pm})/2 \) and \( \nu^2_{k\pm} = (1 - \xi_{k\pm}/E_{k\pm})/2 \) to simplify notation, where \( \xi_{k\pm} = k_{\pm}/2m - 2\mu \) and \( E_{k\pm} = \sqrt{k_{\pm}^2 + \Delta^2}. \) With that, the number equation including the Gaussian fluctuation effect reads

\[ n = -\frac{\partial \Omega_{\text{MF}}}{\partial \mu} - \frac{\partial \Omega_{\text{GPF}}}{\partial \mu}, \]

(19)

which is solved self-consistently with the mean-field gap equation equation (11a) numerically to determine the chemical potential \( \mu \) and order parameter \( \Delta \).

**3. BCS–BEC crossover and numerical results**

In this section, we present our numerical results of superfluid gap, chemical potential, pair size and sound velocity as well as convexity parameters of the Goldstone mode across the BCS–BEC crossover for Q2D Fermi gases.
Figure 1. (a) Superfluid gap and (b) chemical potential versus the dimensionless 2D interaction strength $\ln(k_F a_{2D})$. (c) Superfluid gap versus chemical potential. Results obtained via GPF approach are shown for a strictly 2D (gray dotted line) gas of $^6$Li atoms and Q2D gases with trapping frequency $\omega_z = \omega_0$ (red solid line) and $\omega_z = 5\omega_0$ (blue dashed-dotted line), which are compared with results via MF approach for Q2D gases with $\omega_z = \omega_0$ (green dashed line). Experimental data are extracted from the recent work of Q2D $^6$Li atomic gases [25] (red triangles) and the 2D QMC calculations [48] (red dots) with the correction of Q2D binding energy $E_B$.

3.1. Superfluid gap and chemical potential

Based on the coupled equations (11a) and (19), we determine the superfluid gap $\Delta$ and the chemical potential $\mu$ self-consistently in a wide range of crossover, where the interaction strength can be parameterized by the effective 2D dimensionless interaction parameter $\ln(k_F a_{2D})$ with a 2D scattering length $a_{2D} = 2e^{-\gamma E}/\sqrt{mE}$ and the Euler constant $\gamma_E \approx 0.577$. We compare the superfluid gap and chemical potential obtained from the GPF theory for Q2D systems with experimental data [25] of ultracold atoms gases in Q2D traps with the axial trapping frequency $\omega_z = \omega_0 \equiv 2\pi \times 9.2$ kHz, as functions of $\ln(k_F a_{2D})$ in figures 1(a) and (b), respectively. For comparison, results for strictly 2D systems and the MF predictions for Q2D systems are also presented. The Fermi energy $E_F$ and Fermi momentum $k_F$ are used as the energy and momentum units, respectively. Among them, the Q2D GPF results with trapping frequency $\omega_z = \omega_0$ not only qualitatively but also quantitatively show the best agreement with the experiment data. The pronounced discrepancy between Q2D GPF results with different trapping configurations ($\omega_z = \omega_0$ and $\omega_z = 5\omega_0$) and 2D GPF results in figures 1(a) and (b) indicates the important effect of the axial confinement along $z$-axis. Notably, the Q2D MF predictions with $\omega_z = \omega_0$ always lie above the corresponding GPF results, showing the strong suppression of the superfluid gap and chemical potential attributed to the Gaussian fluctuations. In the experiment [25], the BCS–BEC crossover is tuned by changing the interaction strength via a Feshbach resonance, and the chemical potential is extracted with assistance of the auxiliary field quantum Monte Carlo (QMC) calculations [48], together with the modified binding energy $E_B$ for a Q2D geometry, which is given by $[39]$

$$a_z \equiv \sqrt{1/m\omega_z}$$

$$a_s = \int_0^{+\infty} \frac{du}{\sqrt{4\pi u^3}} \left[ 1 - \frac{e^{-\frac{E_B}{\omega_z}u}}{\sqrt{(1-e^{-\frac{E_B}{\omega_z}})/(2u)}} \right]$$

with $a_s \equiv 1/\sqrt{m\omega_z}$ the characteristic length of the axial trap. This result of $E_B$ is equivalent to the one obtained in our effective 2D Hamiltonian equation (1) since it is a matching condition to determine the Hamiltonian parameters. As shown in figure 1(b), a self-consistent GPF calculation of the chemical potential for a Q2D system is in excellent agreement with the 2D QMC results when the binding energy $E_B$ is corrected by the Q2D results. This indicates that the correction plays an essential role in the connection between Q2D and purely 2D systems. We stress that while the QMC study is conducted in a strictly 2D system and the
Figure 2. The pair size $\xi/\xi_\infty$ as a function of the effective interaction $V_{p}\text{eff}/\omega_z$ for Q2D systems with trapping frequency $\omega_z = \omega_0$ (red solid line), $\omega_z = 3\omega_0$ (yellow dashed line) and $\omega_z = 5\omega_0$ (blue dashed-dotted line).

many-body fluctuations are only considered within the 2D plane, the Q2D theory presented here also allows fluctuation of the dressed molecule, hence can describe many-body effects along the confined direction.

Also, the relation between the superfluid gap and the chemical potential in all these cases are plotted in figure 1(c), where the chemical potential is taken as a measure of the interaction strength. Obviously, the MF results overestimate the superfluid gap as expected in the whole range of crossover. In the weakly interacting regime $\mu/E_F \rightarrow 1$, theoretical calculations with Gaussian fluctuations for all cases nearly fall into a single curve as one would expect for a BCS superconductor. However, with increasing interaction ($\mu \rightarrow -\infty$), the superfluid gaps in different geometric configurations exhibit a certain degree of disagreement, owing to the difference of density of states. Furthermore, when plotted against the reduced chemical potential $\tilde{\mu} = \mu + E_F/2$, the superfluid gap obtained from GPF theory for Q2D systems increases monotonically with increasing trapping frequency, and is eventually upper-bounded by that for strictly 2D systems, as shown in the inset of figure 1(c). This qualitative behavior is consistent with the physical picture that a stronger confinement can facilitate pairing owing to the enhancement of density of states. Our GPF result of superfluid gap for Q2D systems agree well with the experimental data obtained for the same configuration in both the BCS and BEC regimes, while the deviation is more drastic around unitarity $|\mu| \sim 0$ where quantum fluctuations are most significant and Gaussian fluctuation has been already known to be not enough [49]. Besides, the two-channel model we used is valid when the reduced chemical potential $\tilde{\mu}$ is much smaller than the trapping frequency and Fermi energy. Around unitarity, strong fluctuations can break this condition and compromise the validity of the two-channel model. Another fact that may bring discrepancy is finite temperature effect. The pairing state will be affected by the presence and damping of collective excitations at a finite temperature.

3.2. Pair size

Pair size is another fundamental physical quantity to characterize the BCS–BEC crossover, which is defined in a form independent of dimensionality

$$\xi^2 \equiv -\frac{\sum_k \langle \varphi_k | \nabla^2_k | \varphi_k \rangle}{\sum_k \langle \varphi_k | \varphi_k \rangle},$$

where $|\varphi_k\rangle = \Delta/2E_k$ is the zero temperature pair wave function. For 2D systems, the pair size can be obtained analytically [50],

$$\xi^2 = \frac{1}{4m\Delta} \left[ \frac{\mu}{\Delta} + \frac{\mu^2 + 2\Delta^2}{\mu^2 + \Delta^2} \left( \frac{\pi}{2} + \arctan \frac{\mu}{\Delta} \right)^{-1} \right].$$

In figure 2, we show the pair size $\xi$ as a function of the dimensionless 2D effective interaction strength $V_{p}\text{eff}/\omega_z$ for different choice of confining frequency. By scaling with the asymptotic value $\xi_\infty \equiv \xi(|V_{p}\text{eff}| \rightarrow \infty)$
Figure 3. Dimensionless pair size $k_F\xi$ as a function of (a) dimensionless chemical potential $\mu/E_F$, (b) dimensionless pairing order parameter $\Delta/E_F$, and (c) dimensionless interaction parameter $ln(k_Fa_{2D})$ for Q2D and 2D Fermi superfluids. Results from GPF theory for a strictly 2D (gray dotted line) gas and Q2D gases with trapping frequency $\omega_z = \omega_0$ (red solid line) and $\omega_z = 5\omega_0$ (blue dashed-dotted line), together with results within MF approximation for Q2D gases with $\omega_z = \omega_0$ (green dashed line) are shown for comparison. The gray dots represent the experimental raw data obtained from the onset momentum $k_o$ of the pair breaking continuum for Q2D gases of $^6$Li atoms [25]. The red diamonds are modified Q2D pair sizes calculated via equation (22) using the superfluid gap and the chemical potential obtained from reference [25]. The black dotted line in panel (b) presents the coherence length $\xi_p = k_F/\pi m\Delta$.

at infinitely large $|V_{\text{eff}}|$, the results for different trapping configurations show universal behavior, as also found in previous studies [51].

Further, we plot in figure 3(a) the pair size $k_F\xi$ as a function of the dimensionless chemical potential $\mu/E_F$ for Q2D and 2D systems via GPF or MF approach and compared with the experimental data. The GPF results for Q2D systems with $\omega_z = \omega_0$ show quantitative consistency with the experiment data. The results via GPF theory for Q2D systems with different trapping frequencies and 2D systems do not show obvious difference. Furthermore, the superfluid gap against pair size is plotted in figure 3(b), where the curves of Q2D and 2D systems almost collapse onto a same straight line in the BCS regime, and start showing deviation with increasing interaction. This observation is consistent with the results shown in figure 1(c). In the weak coupling regime, all systems have a same universal 2D equation of state as expected for a BCS superconductor, and the physical properties are solely determined by the density of states at the Fermi energy. With increasing interaction, when the superfluid order parameter is comparable to the Fermi energy and the pair size reaches the order of $1/k_F$, the specific shape of dispersion will play a key role in correcting the gap. In this case, a 2D system or a Q2D system in a tight trap is more favorable for pairing as compared with a Q2D system in a loose trap, as demonstrated both in figures 1(c) and 3(b).

The universal behavior of superfluid gap (figure 1(c)) and pair size (figure 3(a)) plotted as functions of chemical potential suggests that the BCS–BEC crossover of Q2D Fermi gases can be characterized by these physical quantities, regardless of the specific shape of confining potential. A previous mean field study of 3D superconductors suggests that the boundaries between BCS, crossover, and BEC regimes can be determined by universal values of $\Delta/E_F$ and $k_F\xi$ [52]. Our results indicate that this qualitative conclusion still holds for Q2D Fermi gases, while the quantitative values are quite different owing to the effects of Gaussian fluctuation and reduced dimensionality.

We note that the pair size of Q2D $^6$Li atomic gases is not directly measured in experiment [25]. Instead, one determines the onset momentum $k_o$ of the pair breaking continuum from the interaction point of a bilinear fit of the dynamic structure at a transferred energy of $\omega = 2\Delta$, which is related to pair size via $k_o = \alpha/\xi$. The prefactor $\alpha$ is evaluated by comparing the experimental results of $1/k_o$ to theoretical predictions of the pair size of 2D Fermi gases. The raw data of pair size in Q2D $^6$Li Fermi gases [25] is shown
Three Q2D configurations with decreases from \(-1\) with for Q2D systems with different trapping frequencies and interactions of (a) \(1/k_{a_2} = -1\) and (b) \(1/k_{a_1} = 1\). Three Q2D configurations with \(\omega = 1\omega_0\) (red solid line), \(3\omega_0\) (yellow dashed line), and \(5\omega_0\) (blue dashed-dotted line) are shown for comparison. The shades with different colors represent the continuum of pair breaking excitations for corresponding trapping configurations.

3.3. Collective mode

In addition to the ground state properties discussed above, collective modes are also important since they may play a significant role in the response of system to external probes, and have been intensively studied for cold Fermi gases [53–55]. The low-energy collective mode spectrum \(\omega_q\) is well-known as the Goldstone mode arising from the broken of \(U(1)\) symmetry, which is determined by the pole of the inverse Gaussian fluctuation bosonic propagator \(M\), i.e. the solution of \(\det[M(q, \omega_q)] = 0\). The two-particle continuum begins at \(E_s(q) = \min_q(E_s + E_+ - \omega_0)\), corresponding to the single particle excitation from the pair breaking threshold.

In figure 4, we present the Goldstone mode by lines and pair breaking continuum by shades with different trapping frequencies on the BCS side with the interaction strength \(1/k_{a_2} = -1\) (figure 4(a)), and on the BEC side with interaction strength \(1/k_{a_1} = 1\) (figure 4(b)). The trapping frequencies are \(1\omega_0\) by red solid lines and red shades, \(3\omega_0\) by yellow dashed lines and yellow shades, and \(5\omega_0\) by blue dashed-dotted lines and blue shades. In the long-wavelength limit, the dispersions exhibit linear shape for all configurations, and the slope of which determines the sound velocity. We find that \(\omega_q\) is always below the two-particle continuum, indicating the existence of a two-body bound state in a Q2D system over a wide range of crossover.

As shown in figure 4(a), in the BCS regime, we observe a wide pair breaking continuum and the pairs are weakly bound. When the transferred energy is strong enough to break a Cooper pair, the atoms will be excited to the continuum state with a sharp energy threshold of \(2\Delta\). In particular, for large transferred momentum, the Goldstone mode touches the pair breaking continuum and bends down instead of keeping a linear slope. However, in the BEC regime where the atom pairs condense as tightly-bound molecules, the continuum is notably lifted until moves out of the spectra, as shown in figure 4(b).

3.4. Speed of sound and convexity of the Goldstone mode

In this subsection, we consider the first sound velocity \(C_s\), which represents the propagating speed of density waves in superfluid and is defined as the slope of the Goldstone mode in the long-wavelength limit. Specifically, we expand the elements of the Gaussian fluctuation matrix \(M(q, \omega)\) to quadratic order in both \(q\) and \(\omega\), and determine the speed of sound by requiring \(\det[M(q, \omega)] = 0\). For strictly 2D systems within the mean-field approximation, the sound velocity is (incorrectly) independent on the interaction strength and reads \(C_s = v_F/\sqrt{2}\) as shown in figure 5, where \(v_F\) is the Fermi velocity. For Q2D systems (taking the \(\omega_0 = 1\omega_0\) case for an example) within the mean-field approximation, however, \(C_s/v_F\) decreases from \(1/\sqrt{2}\) with
The sound velocity $C_s/v_F$ as a function of the interaction parameter $\ln(k_Fa^2_D)$. Results are obtained from GPF theory for strictly 2D systems (gray dotted line) and three Q2D configurations with $\omega_z = \omega_0$ (red solid line), $3\omega_0$ (yellow dashed line), and $5\omega_0$ (blue dashed-dotted line), and from mean-field approximation for Q2D systems with $\omega_z = \omega_0$ (green dashed line) and 2D systems (black solid line).

increasing interaction since the excitation of high energy modes in the confined direction suppress the propagation of density waves. Taking into account the contribution of pair fluctuations, $C_s$ shows an obvious down-shift compared with the mean-field result, which is naturally expected since fluctuations will reduce the superfluid order parameter and consequently the sound velocity. To further elaborate the effect of Q2D confinement, we also show in figure 5 the results of $C_s$ for different trapping frequencies. Note that $C_s$ increases monotonically with a stronger confinement, and is bounded from the top by the asymptotic value in 2D systems, where the axial fluctuations are completely frozen out.

Another characteristic property of the Goldstone mode is the convexity of its dispersion relation, which is important to determine the damping mechanism [56–59]. The convexity parameters have been theoretically investigated in 3D [58] and 2D [35] Fermi systems and experimentally measured in a 3D ultracold gas of $^6$Li atoms [26]. By expanding the dispersion of low-energy collective excitation up to a fifth order polynomial of $q = |q|$ as

$$\omega_q = C_s q \left[ 1 + \frac{\gamma}{8} \left( \frac{q}{mC_s} \right)^2 + \frac{\eta}{16} \left( \frac{q}{mC_s} \right)^4 \right], \quad (23)$$

and substituting it back into the elements of the $M$ matrix, we can rewrite the condition $\det M(q, \omega_q) = 0$ to the sixth order of $q$ and determine the convexity parameters $\gamma$ and $\eta$ from the coefficients of terms $q^4$ and $q^6$, respectively. In figure 6, we compare the results in 2D and Q2D systems with different trapping frequencies from GPF or MF theory. In the BEC regime, the convexity is convex ($\gamma > 0$), indicating that the dominant damping mechanism of collective excitation is the Landau–Beliaev two-photon to one-photon process. In the strongly interacting limit, $\gamma$ approaches a universal value of $1/4$, which is determined by the dispersion of Bogoliubov excitations in a weakly interacting Bose gas with mass $2m$ and is valid in all dimensions and trapping geometries. When the interaction is reduced, the system crosses over to the BCS regime where the damping mechanism is dominated by the Landau–Khalatnikov two-photon to two-photon process, and the convexity turns to concave ($\gamma < 0$). The sign changing point of $\gamma$ moves towards the BCS side with decreasing axial trapping frequency, presenting the same trend as the first sound velocity shown in figure 5.

In the BCS limit where $\Delta$ and $E_F$ are the only relevant energy scales, $\omega_q/\Delta$ becomes a universal function of $C_s q / \Delta$. A dimensional analysis suggests that $\gamma |\Delta|^2 / m^2 C_s^4$ for all the 2D and Q2D cases should approach a same asymptotic value of $-1/3$, as shown in figure 6(c). For the other parameter $\eta$, we observe qualitatively the same behavior where $\eta$ approaches a universal value of $-1/128$ in the BEC limit (figure 6(b)), and $\eta |\Delta|^4 / m^4 C_s^8$ saturates to $-1/72$ for all 2D and Q2D systems (figure 6(d)). Besides, the MF results can recover the asymptotic behaviors of convexity parameters in both the BCS and BEC limits but fail in the crossover region. Our results of the convexity parameters can be tested in future experiments of Q2D Fermi systems.

Figure 5. The sound velocity $C_s/v_F$ as a function of the interaction parameter $\ln(k_Fa^2_D)$. Results are obtained from GPF theory for strictly 2D systems (gray dotted line) and three Q2D configurations with $\omega_z = 1\omega_0$ (red solid line), $3\omega_0$ (yellow dashed line), and $5\omega_0$ (blue dashed-dotted line), and from mean-field approximation for Q2D systems with $\omega_z = \omega_0$ (green dashed line) and 2D systems (black solid line).
Figure 6. Convexity parameters $\gamma$ and $\eta$ for the collective modes versus $\ln(k_Fa_2D)$ for 2D and Q2D systems with different trapping frequencies. Results for a purely 2D system (gray dotted line) and three Q2D configurations with $\omega_z = \omega_0$ (red solid line), $3\omega_0$ (yellow dashed line), and $5\omega_0$ (blue dashed-dotted line) within GPF theory and a Q2D system with $\omega_z = \omega_0$ within MF level (green dashed line) are shown for comparison. The black dashed lines correspond to the limiting values of (a) $\gamma_{\text{BEC}} = 1/4$, (b) $\eta_{\text{BEC}} = -1/128$, (c) $\gamma_{\text{BCS}}|\Delta|^2/m^2C_s^4 = -1/3$, and (d) $\eta_{\text{BCS}}|\Delta|^4/m^4C_s^8 = -1/72$.

4. Summary and conclusion

We study the BCS–BEC crossover in a Q2D quantum gas of ultracold fermionic atoms. By adopting an effective model of dressed molecule to take into account the excited degrees of freedom and extending the GPF theory, we characterize various pairing parameters at zero temperature in a wide range of crossover. We have found that the order parameter and pair size for 2D and Q2D systems with different trapping frequencies show universal relations with chemical potential in the BCS limit, but behave distinctively with increasing interaction. Within GPF theory, our results of superfluid gap, chemical potential and pair size for Q2D systems show quantitatively agreement with the recent experiment of $^6$Li atomic gases [25]. These results reveal the notable effect of reduced dimensionality and pair fluctuations, which can also be concluded from the speed of first sound and convexity of Goldstone modes. The prediction of convexity of the Goldstone modes in Q2D Fermi gases over the BCS–BEC crossover can be verified in future experiments.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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