Quasi two-dimensional superfluid Fermi gases

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We study a quasi two-dimensional superfluid Fermi gas where the confinement in the third direction is due to a strong harmonic trapping. We investigate the behavior of such a system when the chemical potential is varied and find strong modifications of the superfluid properties due to the discrete harmonic oscillator states. We show that such quasi two-dimensional behavior can be created and observed with current experimental capabilities.

Finite size effects often lead to pronounced quantum mechanical changes in the system behavior. Among other things, these effects are crucial in the physics of quantum dots\textsuperscript{1}, in studying how spontaneous emission is modified in cavities\textsuperscript{2,3,4}, and in understanding the properties of thin superconducting films\textsuperscript{5}. In addition, dimensional cross-over effects have been actively studied experimentally using ultracold bosons in combined magnetic and optical potentials\textsuperscript{6} as well as in optical lattices\textsuperscript{7,8,9}.

The possibility of fermionic superfluidity in ultracold atomic gases\textsuperscript{10} motivated a substantial experimental effort into controlling and manipulating cold fermionic atoms. Very recently, these efforts were rewarded with a spectacular success. A series of experiments demonstrated Bose-Einstein condensation of molecules composed of two fermions\textsuperscript{11,12,13,14}. Experiments\textsuperscript{15,16,17,18} employing the Feshbach resonance to vary the atomic interaction strength observed strong indications of fermion pairing. This was soon followed by the direct observation of the energy gap\textsuperscript{19}. This set of experiments has established fermionic pairing in atomic gases as an experimental fact, and provided a strong case for superfluidity, proven recently by the observation of vortices\textsuperscript{20}.

The dramatic progress with ultracold fermions, combined with the fact that there is no fundamental problem in changing the dimensionality of the system by using for example optical lattices\textsuperscript{21}, raises important questions about the role of dimensionality and finite size effects in cold fermionic gases. The purpose of this Letter is to elucidate how quantum size effects are manifested in a dilute quasi-two-dimensional Fermi gas. Such system can be created by confining atoms tightly along one direction by a harmonic trapping potential. Note that we do not assume a purely Gaussian density profile in the $z$-direction, an assumption often made in studies of quasi two-dimensional quantum degenerate gases. Our extension beyond the ground state Gaussian profile reveals discrete features in observable quantities, and is expected to be useful in studying how a true long range order at non-zero temperature is established as one crosses over from a purely two-dimensional into a three-dimensional system.

We assume a cloud of fermionic atoms confined by a potential $V(z) = \hbar \omega_z^2 z^2/2$ and an atomic density $n(z)$ which only depends on the $z$-coordinate. The cloud consists of equal amount of fermions on two different internal states denoted by $\uparrow$ and $\downarrow$. Let us first, for orientation, consider the behavior of a non-interacting system at zero temperature: The first atom inserted into the system will fill the lowest energy state which corresponds to a stationary atom in the $xy$-plane and whose axial wave function is the lowest harmonic oscillator state $\phi_0(z)$ of the axial potential. This atom then has the energy $\hbar \omega_z/2$. As we add more atoms, they fill the continuum of plane-wave states in the $xy$-plane with an axial wave function $\phi_0(z)$. However, once the two-dimensional density of atoms is such that the next available plane-wave state has an energy $\hbar \omega_z$, the density of states changes abruptly and an extra atom has two choices. Either, it can occupy this high energy plane-wave state or it can occupy the zero plane-wave momentum state in the first excited harmonic oscillator state $\phi_1(z)$. Similar doubling of choices occurs also with respect to higher harmonic oscillator states, when the continuum Fermi-energy matches the oscillator level energy. More quantitatively, the two-dimensional density (of both components combined) $n_{2D} = \int dz n(z)$ is related to the Fermi-momentum through $k_F^z = 2\pi n_{2D}$. If the Fermi-energy $E_F = \hbar^2 k_F^z/2m$ is equated with the level spacing $\hbar \omega_z$ we find a maximum density before atoms start to occupy the first excited state of the harmonic oscillator, $n_c = 1/(\pi l_z^2)$. (If not indicated otherwise, we use $\hbar \omega_z$ as a unit of energy and $l_z = \sqrt{\hbar/m \omega_z}$ as a unit of length.) As the density exceeds this threshold, extra atoms have available a new state with the same total energy as the plane-wave states, but with a different axial state. This indicates that the growth rate of $n_{2D}$ with $E_F$ is suddenly doubled from its earlier value of $\partial n_{2D}/\partial E_F = m/(\pi \hbar^2)$. Therefore, $\partial n_{2D}/\partial E_F$ for ideal fermions, at zero temperature, is a staircase with steps at $E_F = \hbar \omega_z (n + 1/2)$ with the height $m/(\pi \hbar^2)$.

Let us now consider an attractive binary contact interaction with a coupling strength $g$ between atoms in different internal states and allow for a non-zero temperature. Interaction between atoms is assumed to be sufficiently weak so that the Bardeen-Cooper-Schrieffer
(BCS) theory provides a reliable framework to study this many-body system also at finite temperature. If the Hamiltonian is expanded around the order parameter $\Delta(z) = g(\psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r}))$, one finds the usual quadratic mean field Hamiltonian

$$H = \int d\mathbf{r} \sum_\sigma \frac{\hbar^2}{2m} \nabla^2 - \mu + V(z) \hat{\psi}_\sigma(\mathbf{r}) + \Delta(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}) \hat{\psi}_\downarrow(\mathbf{r}) + \Delta^*(\mathbf{r}) \hat{\psi}_\downarrow(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}).$$

(1)

This Hamiltonian is diagonalized using a Bogoliubov transformation $\hat{\psi}_\sigma(\mathbf{r}) = \sum_\zeta u_\zeta(\mathbf{r}) \hat{b}_\zeta,\uparrow + v_\zeta(\mathbf{r}) \hat{b}_\zeta,\downarrow$ and $\hat{\psi}_\dagger(\mathbf{r}) = \sum_\zeta -v_\zeta(\mathbf{r}) \hat{b}_\zeta,\uparrow + u_\zeta(\mathbf{r}) \hat{b}_\zeta,\downarrow$, where the quasiparticle amplitudes $u_\zeta(\mathbf{r})$ and $v_\zeta(\mathbf{r})$ are solutions to the Bogoliubov-de-Gennes (BdG) equations

$$\begin{pmatrix} H_0 & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -H_0 \end{pmatrix} \begin{pmatrix} u_\zeta(\mathbf{r}) \\ v_\zeta(\mathbf{r}) \end{pmatrix} = E_\zeta \begin{pmatrix} u_\zeta(\mathbf{r}) \\ v_\zeta(\mathbf{r}) \end{pmatrix},$$

where $H_0 = -\hbar^2\nabla^2/2m - \mu + V(z)$. Furthermore, the amplitudes are normalized $\int |u_\zeta(\mathbf{r})|^2 + |v_\zeta(\mathbf{r})|^2 = 1$. Self-consistency then imposes the well known gap equation

$$\Delta(z) = -g \sum_\zeta |u_\zeta(\mathbf{r})| v_\zeta^*(\mathbf{r}) [1 - 2n_F(E_\zeta)],$$

(2)

where $n_F(E) = 1/(\exp(\beta E) + 1)$ is the Fermi distribution. Finally, the chemical potential is related to the atom density through the number equation $n(\mathbf{r}) = \sum_\zeta |u_\zeta(\mathbf{r})|^2 n_F(E_\zeta) + |v_\zeta(\mathbf{r})|^2 (1 - n_F(E_\zeta))$.

In the quasi-two-dimensional system considered here, it is natural to expand the Bogoliubov quasiparticle amplitudes in terms of the harmonic oscillator states $\phi_n(\mathbf{z})$ and radial plane waves $\sim \exp(i \mathbf{k} \cdot \mathbf{r}_\perp)$. This amounts to

$$u_\zeta(\mathbf{r}) = \sum_n \sum_k \frac{1}{\sqrt{A}} \phi_n(\mathbf{z}) e^{i \mathbf{k} \cdot \mathbf{r}_\perp} u_{n,k}^\zeta$$

(3)

and the same expression for $v_\zeta(\mathbf{r})$, where $A$ is the quantization area in the $xy$-plane. We include only the three lowest lying harmonic oscillator states and the solution to the BdG equations for the amplitudes $u_{n,k}^\zeta$ and $v_{n,k}^\zeta$ amounts to a diagonalization of the matrix

$$M = \begin{pmatrix} \xi_{0,0,k} & \Delta_0 & 0 & 0 & 0 & \Delta_{02} \\ \Delta_0 & -\xi_{0,0,k} & 0 & 0 & \Delta_{02} & 0 \\ 0 & 0 & \Delta_1 & 0 & 0 & \xi_{0,1,k} \\ 0 & 0 & 0 & \Delta_2 & 0 & \xi_{0,2,k} \\ \Delta_{02} & 0 & 0 & 0 & \Delta_2 & -\xi_{0,2,k} \end{pmatrix},$$

where $\xi_{0,n,k} = \hbar \omega_z (n + 1/2) + \hbar^2 k^2/2m - \mu$, $\Delta_n = \int dz \Delta(z)|\phi_n(z)|^2$, and $\Delta_{02} = \int dz \Delta(z) \phi_0^*(z) \phi_0(z)$. This matrix is almost block-diagonal with respect to different harmonic oscillator states. However, since $\phi_0(z)$ and $\phi_2(z)$ are both symmetric, $\Delta_{02}$ is non-zero and the simple block diagonality is broken. This coupling between $n = 0$ and $n = 2$ channels is evident as an avoided crossing between two of the three (positive) dispersion branches.

For a weakly interacting system the restriction to just three harmonic oscillator states is expected to be sufficient, if the chemical potential is below the energy $7\hbar \omega_z/2$ of the third excited state and if the temperature is small compared to $\hbar \omega_z$. In our examples both these conditions are well satisfied. The coupling between $n = 0$ and $n = 2$ states influences, depending on $\mu$, $\Delta(z) = 0$ by about 10%. As a validity test, we included the $n = 3$ channel in the numerics and found a quantitative change of a few percent, while the qualitative behavior was unchanged.

The eigenvectors $\mathbf{w}_{\zeta,k} = (u_{0,k}^\zeta, v_{0,k}^\zeta, u_{1,k}^\zeta, v_{1,k}^\zeta, u_{2,k}^\zeta, v_{2,k}^\zeta)$ with eigenvalues $E_{\zeta,k}$ can then be inserted into Eq. (3) to find a self consistent solution for $\Delta(z)$. Since the Bogoliubov quasiparticle amplitudes are polynomials multiplied by the same exponential (in trap units) $\exp(-z^2/2)$, it is convenient to expand the symmetric order parameter as $\Delta(z) = \sum_{n=0}^2 a_{2n} z^{2n} \exp(-z^2)$. When the above expansion is used in Eq. (2) in conjunction with eigenvectors $\mathbf{w}_{\zeta,k}$, we find, by comparing terms with different powers of $z$, a set of three coupled self-consistency equations

$$a_0 = -\frac{g}{\sqrt{\pi}} \sum_\zeta \sum_k \left[ u_{0,k}^\zeta v_{0,k}^\zeta + \frac{1}{2} u_{2,k}^\zeta v_{2,k}^\zeta \right]$$

$$- \frac{1}{\sqrt{2}} \left[ u_{0,k}^\zeta v_{2,k}^\zeta + u_{2,k}^\zeta v_{0,k}^\zeta \right] \left[ 1 - 2n_F(E_{\zeta,k}) \right],$$

$$a_2 = -\frac{g}{\sqrt{\pi}} \sum_\zeta \sum_k \left[ 2 u_{1,k}^\zeta v_{1,k}^\zeta - 2 a_{2,k}^\zeta \right]$$

$$+ \sqrt{2} \left[ u_{0,k}^\zeta v_{2,k}^\zeta + u_{2,k}^\zeta v_{0,k}^\zeta \right] \left[ 1 - 2n_F(E_{\zeta,k}) \right],$$

$$a_4 = -\frac{g}{\sqrt{\pi}} \sum_\zeta \sum_k \left[ 2 a_{2,k}^\zeta v_{2,k}^\zeta \right] \left[ 1 - 2n_F(E_{\zeta,k}) \right].$$

We solve this set of equations numerically.

Replacing the sums over $k$ with two-dimensional integrals gives rise to equations which are formally divergent. The ultraviolet divergence has its origin in approximating the interaction between atoms with a contact interaction. Most elegantly this divergence is removed by renormalizing $g$ to two-body scattering matrix, which amounts to subtracting the divergent part away from the integral. However, for computational reasons, we remove the divergence using a simple Gaussian energy cut-off. The cut-off energy is high enough so that our results are not sensitive to the cut-off procedure.

The integrals are also infrared divergent and this divergence is due to the bound state appearing in the two-dimensional problem. This bound state has an energy $\epsilon_0/\hbar \omega_z \sim \exp(-\sqrt{2\pi l_z/a})$, where $a$ is the three dimensional scattering length $[22]$. This weakly bound state
causes a logarithmic energy dependence for the coupling strength \( g \sim \ln^{-1}(\epsilon_0/\epsilon) \) which in turn results in non-separable gap equations. In our case this makes the computations exceedingly complicated. Furthermore, the bound-state energy also depends on the axial wave function. This implies that the relevant bound state energy would also depend on the harmonic oscillator quantum number \( n \) and consequently one would have to deal with several different coupling strengths. However, in the BCS theory, the most interesting effects originate in the neighborhood of the Fermi surface. System behavior is therefore largely insensitive to the details of the low energy behavior of the coupling strength. In fact, we found that the use of a sharp low energy cut-off is sufficient for the examples presented here. As long as the low energy cut-off was \( \ll 1 \), we could change it by an order of magnitude without affecting the results seriously.

In Fig. 1 we show, for the \(^{6}\text{Li}\) atoms, an example of the order parameter in the center of the system \( \Delta(z = 0) \) as a function of temperature and chemical potential. The gap \( \Delta(0) \) increases with the chemical potential and shows a clear staircase structure especially around \( \mu = 3\hbar\omega_z/2 \). The behavior around \( \mu = 5\hbar\omega_z/2 \) is smoother. Also the critical temperature rises quite suddenly when the chemical potential is close to the harmonic oscillator levels. This increase reflects the abrupt increase of the density of states. While \( \Delta(0) = \alpha_0 \) increases monotonically with chemical potential, this is not generally true for other coefficients of \( \Delta(z) \). Having solved the gap equations, the derivative \( \partial n_{2D}/\partial \mu \) can be easily computed. The staircase structure one expects for an ideal Fermi gas is still present, but now the interactions have rounded the steps.

In a homogeneous superfluid, the energy gap for the single particle excitations coincides with the order parameter. In the inhomogeneous case, the order parameter becomes position dependent and Andreev bound states (in-gap states) appear. Note that in the RF-spectroscopy experiments so far, the final state was initially empty, i.e. there is no Pauli blocking for transfer of particles from the lowest momentum states, unlike in superconductor-normal metal tunneling experiments. In a strongly interacting Fermi gas, however, the order parameter can be as large as half of the Fermi energy and even the lowest momentum states are strongly affected by pairing. As a result, it turns out that the peak position is of the same order of magnitude as the order parameter. In contrast, in the BCS limit, pairing takes place near the Fermi level and the transfer of particles from the lowest momentum states leads to a very small shift of the peak position of the order \( \Delta^2/(2\mu) \). Such small shifts are difficult to observe. However, in the near future it will be possible to trap stable mixtures of Fermions in three internal states of one atom (or, say, in one state of \(^{40}\text{K}\) and two of \(^{6}\text{Li}\)). Then, selected transitions can be Pauli blocked by preparing the Fermi level of the final state at will. This provides a new degree of control in the spectroscopy of the gas and the resolution at the BCS limit could be dramatically increased. In this way, also the Andreev state energy could be via suppression of collective mode frequencies.

We calculated the RF-spectra for our system and from that determined the location of the spectral peak as a function of chemical potential. This peak position and the lowest Andreev state energy together with the order parameter at \( z = 0 \) are shown in Fig. 2. In the main figure, the peak position is calculated by assuming Pauli blocking of the final state, i.e. the final state chemical potential equals the initial state one. The spectral peak is closer to \( \Delta(0) \) than to the lowest Andreev state. This trend becomes more clear as the chemical potential increases, meaning that the experimental signal in RF-spectroscopy from the lowest Andreev state becomes negligible when several axial harmonic oscillator states are occupied. This might, however, be changed by the choice of the final state chemical potential. In the inset we show the peak position when the final state was initially empty. The spectral shift is now much smaller. However, both the main figure and the inset demonstrate that the steps in the order parameter are directly reflected in observable quantities. This behavior originates from the change in the density of states and demonstrates the many body nature of the pairing.

Probing experimentally the regime we are interested in here requires a sufficiently tight axial confinement. In practice, the interesting two-dimensional density scale is \( n_{2D} \sim 1/(\pi l_z^2) \) and when the axial profile of the cloud is that of the lowest harmonic oscillator state, this corresponds to a density scale \( n_{3D} \sim 1/(\pi l_z^2) \) at \( z = 0 \). If
inhomogeneity of energy scale come small if it is much smaller than the interaction energy.

\( \Delta(\omega) \) and the absence of long range order (when \( T \neq 0 \)) as required by the Coleman-Mermin-Wagner-Hohenberg theorem. Here we have ignored such fluctuations with the implicit assumption that the modulus \( |\Delta(z)| \) of the order parameter can be reliably calculated with the BCS theory. Understanding how the couplings between harmonic oscillator levels suppress phase fluctuations and establish true long range order would be an interesting future extension of the work.

In summary, we have shown how finite size effects appear and can be observed in a superfluid Fermi gas that is quasi two-dimensional via a tight harmonic confinement in one dimension. We introduced a theoretical approach which employs the first few oscillator states. Such an approach is sufficient to describe finite size effects, yet it is simple and transparent, which should be very useful in studies of phase coherence and fluctuations in dimensional crossovers, of strong interactions, as well as of superfluid fermion dynamics in this system.

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