BCS to BEC Quantum Phase Transition in Spin Polarized Fermionic Gases

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We discuss the possibility of a quantum phase transition in ultracold spin polarized fermionic gases which exhibit a p-wave Feshbach resonance. We show that when fermionic atoms form a condensate that can be externally tuned between the BCS and BEC limits, the zero temperature compressibility and the spin susceptibility of the fermionic gas are non-analytic functions of the two-body bound state energy. This non-analyticity is due to a massive rearrangement of the momentum distribution in the ground state of the system. Furthermore, we show that the low temperature superfluid density is also non-analytic, and exhibits a dramatic change in behavior when the critical value of the bound state energy is crossed.

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Introduction: Recent experiments in cold fermionic gases have shown that s-wave magnetic field induced Feshbach resonances can be used to form diatomic molecules of $^{39}$K [8] and $^6$Li [5, 6], which undergo Bose-Einstein condensation (BEC) on the higher magnetic field side of the resonance. On the lower magnetic field side of the resonance, it has also been established that Cooper pairing takes place and a BCS condensate is formed. These studies in cold fermionic gases led to the first experimental realization of the theoretically proposed BCS-to-BEC crossover in three dimensional continuum s-wave superfluids [2, 3]. Three early theoretical works that considered the possibility of s-wave superfluidity in the context of (what is known today as) the BCS-to-BEC crossover should be highlighted. The first is by Eagles [7], where the possibility of pairing without condensation is described in a continuum model in the context of superconductors with low carrier concentration. The second is Leggett’s seminal work [8], in which the $T = 0$ s and p-wave BCS-to-BEC evolution are discussed as a crossover phenomenon in the context of a variational ground state wavefunction. And the third is the work of Nozieres-Schmitt-Rink [9], where the s-wave BCS-to-BEC crossover in a lattice is described. Furthermore, much of the theoretical [10, 11] and experimental [12, 13] efforts that followed described only the BCS-to-BEC crossover in s-wave systems.

In this manuscript, we present a functional integral analysis of the BCS-to-BEC evolution in p-wave fully spin-polarized Fermi gases, where p-wave Feshbach resonances have already been observed [12, 13]. We show that a quantum phase transition takes place when the chemical potential crosses a critical value, instead of the usual smooth BCS-to-BEC crossover that occurs in s-wave superfluids [10]. The atomic compressibility and the spin-susceptibility of the Fermi gas are computed and are shown to be non-analytic in the p-wave case, as a consequence of a major rearrangement in the momentum distribution as the critical point is approached. This non-analytic behavior suggests the occurrence of a quantum phase transition, which is further confirmed by a discontinuous change in the temperature dependence of the superfluid density of the gas at the transition point, which goes from power-law on the BCS side of the resonance to exponential on the BEC side of the resonance.

We study the case of two-dimensional systems, which can be prepared experimentally through the formation of a one-dimensional optical lattice, where tunnelling between lattice sites is suppressed by a large trapping potential. The form of the trapping potential can be chosen to be $V_{\text{trap}} = -I_0 \exp[-2(x^2 + y^2)/w^2] \cos^2(k_z z)$, where $2\pi/k_z$ is the wavelength of the light used in the laser beam. We assume that the width $w$ is such that $w \gg \lambda_F$, where $\lambda_F = 2\pi/k_F$ is proportional to the interparticle spacing of a Fermi gas with Fermi wavevector $k_F$, such that the problem is essentially two-dimensional.

Hamiltonian: We study a two-dimensional continuum model of spin polarized (all atoms in the same hyperfine state) fermionic atoms of mass $m$ and density $n = k_F^2/\pi \hbar^2$. In the presence of an external magnetic field $\hbar$, the system is described by the Hamiltonian ($\hbar = k_B = 1$)

$$\mathcal{H} = \sum_k \xi_k \hat{\psi}_k \hat{\psi}_k^\dagger + \frac{1}{2} \sum_{k,k',q} V_{kk'} b_{k q}^\dagger b_{k' q}, \quad (1)$$

where $b_{k q} = \hat{\psi}_{-k+q} \hat{\psi}_{k+q}$ and $\xi_k = \epsilon_k - \mu$, with $\epsilon_k = k^2/2m$, and $\zeta_k = \epsilon_k - \tilde{\mu}$, with $\mu = \hbar \zeta \tilde{\mu}^* B_B \hbar_z$. The direction of the magnetic field $\hbar$, which was chosen to define the spin quantization axis $\zeta$, need not to coincide with the spatial direction $\hbar_z$ of propagation of the laser beam.

The interaction potential is approximated by the following separable function in $k$-space,

$$V_{kk'} = -\lambda \Gamma(k) \Gamma(k'), \quad (2)$$

where $\lambda$ is the interaction strength and $\Gamma(k) = h(k) \cos(\varphi)$, where the function $h(k) = (k/k_1)/[1 + k/k_0]^{3/2}$ controls the range of the interaction, $\varphi$ is the momentum angle in polar coordinates, and $R_0 \sim k_0^{-1}$ plays the role of the interaction range. The functional form of $\Gamma(k)$ can be shown to produce the correct asymptotic behavior at small and large momenta [13], and its angular dependence reflects equal contributions from the angular momentum channels $\ell = \pm 1$. In the limit

[...]

By studying the low temperature superfluid density, we can extract the non-analytic behavior of the BCS-to-BEC crossover, which is further confirmed by a discontinuous change in the temperature dependence of the superfluid density of the gas at the transition point, which goes from power-law on the BCS side of the resonance to exponential on the BEC side of the resonance.
of small momenta, this approach is identical to the T-matrix formalism \cite{3}, but has the added advantage of making unnecessary to introduce the scattering length as a relevant parameter, which is quite problematic in two-dimensions \cite{15}. The BCS-BEC evolution can be safely analyzed provided that the system is dilute enough \((k_F^2 \ll k_0^2)\), i.e., the square of the interparticle spacing \((\sim k_F^{-1})\) is much larger than the square of the interaction range \((\sim k_0^{-1})\). Throughout the manuscript, we choose to scale all energies with respect to the Fermi energy \(\epsilon_F = k_F^2/2m\) and all momenta with respect to \(k_F\).

**Effective Action:** The partition function \(Z\) at a temperature \(T = \beta^{-1}\) is written as an imaginary-time functional integral with action \(S = \int_0^\beta d\tau \sum_{k} \psi_k^\dagger(\tau)\partial_\tau \psi_k(\tau) + \mathcal{H}\). Introducing the usual Hubbard-Stratonovich field \(\phi_q(\tau)\), which couples to \(\psi^\dagger \psi^\dagger\), and integrating out the fermionic degrees of freedom, we obtain

\[
Z = \int \mathcal{D}\phi \mathcal{D}\phi^* \exp(-S_{\text{eff}}[\phi, \phi^*]),
\]

with the effective action given by

\[
S_{\text{eff}} = \int_0^\beta d\tau \left[ U(\tau) + \sum_{k,k'} \left( \frac{\xi_k}{2} \delta_{k,k'} - \text{Tr} \ln \frac{1}{2} G_{k,k'}^{-1}(\tau) \right) \right],
\]

where \(U(\tau) = \sum_k |\phi_k(\tau)|^2/(2\lambda)\) and \(G_{k,k'}^{-1}(\tau)\) is the (inverse) Nambu matrix,

\[
G_{k,k'}^{-1}(\tau) = \begin{pmatrix} -\partial_\tau + \xi_k & \Lambda_{k,k'}(\tau) \\ \bar{\Lambda}_{k',k}(\tau) & -\partial_\tau - \xi_{k'} \end{pmatrix},
\]

with \(\Lambda_{k,k'}(\tau) = \phi_{k-k'}(\tau) \Gamma((k+k')/2).

**Saddle Point Equation:** After Fourier transforming from imaginary time to Matsubara frequency \(i\epsilon_n = (2n+1)\pi/\beta\) and performing the frequency sum, the saddle point condition \(\delta S_{\text{eff}}/\delta \phi_q(\tau)|_{\Delta_0 = 0}\) can be cast in the form of the familiar order parameter equation,

\[
\frac{1}{\lambda} = \sum_k \frac{\Gamma^2(k)}{2E_k} \tanh \left( \frac{\beta E_k}{2} \right),
\]

where \(E_k = \sqrt{\xi_k^2 + \Delta_0^2}\) is the quasiparticle excitation energy, and \(\Delta_0 = \Delta_0(\Gamma(k))\) plays the role of the order parameter function. We eliminate the interaction strength \(\lambda\) in favor of the two-body bound state energy \(E_b(h_z)\) in vacuum (and in the presence of a magnetic field) by using the relation \(1/\lambda = \sum_k \Gamma^2(k)/(2E_k - E_b)\), where \(E_b = E_b(h_z) + 2g_{zz}\mu_B h_z\). The renormalized gap equation in terms of \(E_b\) then takes the form

\[
\sum_k \Gamma^2(k) \left[ \frac{1}{2E_k - E_b} - \frac{\tanh(\beta E_k/2)}{2E_k} \right] = 0.
\]

**Number Equation:** Using the relation \(N = -\partial \Omega/\partial \mu\) and the saddle point approximation for the thermodynamic potential, \(\Omega_0 = S_{\text{eff}}|\Delta_0|/\beta\), one can write the number equation as \(N_0 = \sum_k n_k\), where the momentum distribution \(n_k\) is given by

\[
n_k = \frac{1}{2} \left[ 1 - \frac{\xi_k}{E_k} \tanh \left( \frac{\beta E_k}{2} \right) \right].
\]

Thus, at \(T = 0\), the saddle point and number equations reduce to \(\sum_k \Gamma^2(k)(2E_k - E_b)^{-1} - (2E_k^{-1}) = 0\) and \(N_0 = \sum_k (1 - \xi_k/E_b)/2\), respectively. The solutions for \(\Delta_0\) and \(\mu\) at \(T = 0\) as functions of the binding energy \(E_b\) in the case of p-wave pairing symmetry are plotted in Fig. 1 for \(k_0 = k_1 = 10k_F\). The point \(\mu = 0\) is achieved for \(E_b = -0.87\epsilon_F\) and corresponds to \(\Delta_0 = 19.063\epsilon_F\).

**Gaussian Fluctuations:** We now investigate the effect of Gaussian fluctuations in the pairing field \(\phi_q(\tau)\) about the static saddle point value \(\Delta_0\). Assuming \(\phi_q(\tau) = \Delta_0\delta_{q,0} + \eta_q(\tau)\) and performing an expansion in \(S_{\text{eff}}\) to quadratic order in \(\eta\), one obtains

\[
S_{\text{Gauss}} = S_0[\Delta_0] + \frac{1}{2} \sum_q \eta_q^\dagger M(q) \eta(q),
\]

where \(S_0\) is the saddle point action, the vector \(\eta(q)\) is such that \(\eta_q(q) = [\eta^\dagger(q), \eta(q)]\), and \(q \equiv (q, \eta_m)\), where \(\eta_m = i2m\pi/\beta\) is a bosonic Matsubara frequency. The \(2 \times 2\) matrix \(M(q)\) is the inverse fluctuation propagator.

The Gaussian fluctuation term in the effective action leads to a correction to the thermodynamic potential, which can be rewritten as \(\Omega_{\text{Gauss}} = \Omega_0 + \Omega_{\text{fluct}}\), with \(\Omega_{\text{fluct}} = \beta^{-1} \sum_q \text{ln det}[M(q)]\). Therefore, using the relation \(N = -\partial \Omega/\partial \mu\), one can write the corrected number equation as \(N_{\text{Gauss}} = N_0 + N_{\text{fluct}}\), where \(N_0\) is the saddle-point level number of particles given above, and

\[
N_{\text{fluct}} = -\frac{\partial \Omega_{\text{fluct}}}{\partial \mu} = T \sum_q \sum_{\eta_m} \left[ -\frac{\partial \text{det}M(q)}{\partial \mu} \frac{\text{det}M(q, \eta_m)}{\text{det}M(q, \eta_m)} \right].
\]
At low $T$, the Goldstone mode $\omega = c|\mathbf{q}|$ dominates the contribution to $N_{\text{fluct}}$, leading to

$$N_{\text{fluct}} \sim -\frac{L^2}{2\pi} \zeta(3) \frac{1}{c^3} \frac{\partial c}{\partial \mu} T^3,$$

which vanishes in the limit of $T \to 0$. Therefore, analogously to the three-dimensional $s$-wave case [6], Eq. (7) provides a very accurate description of the number equation near and at $T = 0$, thus confirming Leggett’s suggestion [16]. However, it is well known that the same is not true near $T_c$, where the effects of temporal fluctuations are essential to describe the BEC regime [5]. The discussion of this interesting limit will be postponed to a future manuscript, and we will focus here on the low temperature properties, to be discussed next.

**Momentum distribution:** The momentum distribution $n_k$ given by Eq. (7), which at zero temperature reduces to $n_k = (1 - \xi_k/E_k)/2$, is plotted in Fig. 2 for the case of $p$-wave pairing symmetry as a function of $\mathbf{k} = (k_x, k_y)$, together with the contour plots. Notice that $n_k$ becomes discontinuous when the chemical potential crosses zero, which coincides with the collapse of the two Dirac points to a single point $\mathbf{k} = 0$ and the appearance of a full gap in the quasiparticle excitation spectrum. This major rearrangement of the momentum distribution has a dramatic effect in the atomic compressibility, which is discussed next.

**Atomic Compressibility:** The first derivative of the chemical potential with respect to the density $n = N/L^2$ becomes non-analytic at the critical value of the binding energy in the $p$-wave case. As a consequence, the isothermal atomic compressibility $\kappa$, defined by

$$\kappa = -\frac{L^2}{N^2} \frac{\partial^2 \Omega}{\partial \mu^2} = \frac{1}{n^2} \frac{\partial n}{\partial \mu},$$

will develop a cusp when expressed in terms of $\tilde{E}_b$, its first derivative with respect to $\tilde{E}_b$ diverging at the critical point, as shown in Fig. 3. In the $s$-wave case, however, $\kappa$ is smooth for all values of $\tilde{E}_b$ [14]. This non-analytic behavior of the $p$-wave atomic compressibility, combined with the appearance of a full gap in the excitation spectrum, suggests the existence of a quantum critical point at $\tilde{\mu} = 0$.

**Spin Susceptibility:** The phase transition discussed in the previous section also manifests itself in the spin susceptibility. The application of a small probe magnetic field $H_z$ along the same direction ($\tilde{z}$) of $\mathbf{h}$ generates the spin susceptibility response $\chi_{zz} = (-1/L^2)(\partial^2 \Omega / \partial H_z^2)$, which can be rewritten in the case of spin polarized atoms as

$$\chi_{zz} = \frac{1}{L^2 \rho_s \mu_B^2} \frac{\partial^2 \Omega}{\partial \mu^2} = g_s^2 \rho_s \frac{\partial n}{\partial \mu}.$$  

Thus, the graph in Fig. 3 also represents a universal plot of $\chi_{zz}/g_s^2 \mu_B^2$ as a function of $\tilde{E}_b$.

**Superfluid Density:** We now turn our attention to the behavior of the low temperature superfluid density tensor $\rho_{ij}(T, \tilde{E}_b)$ as the critical value of the binding energy $\tilde{E}_b$ is crossed. This tensor is associated with phase twists of the superconductor order parameter [17], and can be obtained by taking $\phi_{\mathbf{q}} \to \phi_{\mathbf{q}} \exp(i \theta_{\mathbf{q}})$ and expanding the effective action $S_{\text{eff}}$ in powers of $\theta_{\mathbf{q}}$ about the saddle point with $\theta_{\mathbf{q}} = 0$. The resulting difference in the action, $\Delta S = S_{\text{eff}}(\theta_{\mathbf{q}}) - S_{\text{eff}}(\theta_{\mathbf{q}} = 0)$, becomes

$$\Delta S(T) = -(L^2/2) \sum_{\mathbf{q}} \theta_{\mathbf{q}} \theta_{-\mathbf{q}} q_i q_j \rho_{ij}(T),$$

with the super-


\[
\rho_{ij}(T) = \frac{1}{2L^2} \sum_k \left[2\eta_k \partial_i \xi_k - Y_k \partial_j \xi_k \partial_j \xi_k \right], \quad (13)
\]

where \(\eta_k\) is the momentum distribution, \(Y_k = (2T)^{-1} \text{sech}^2(E_k/2T)\) is the Yoshida distribution, and \(\partial_i\) denotes the partial derivative with respect to \(k_i\). Notice that \(\rho_{xx} = \rho_{yy} \equiv \rho\), while \(\rho_{xy} = \rho_{yx} = 0\). In addition, notice that at \(T = 0\), \(\rho_{ij}(0) = n/m\), such that \(\partial \rho_{ij}/\partial \mu = (1/m) \partial n/\partial \mu\) and \(\partial \rho_{ij}/\partial H_2 = (1/m) \partial n/\partial H_2\). Using our energy and momentum scales, we define the dimensionless quantity \(\Delta \rho(T) = m \rho(T)/n - 1\), which is shown in Fig. 4 as a function of temperature for different values of the binding energy. The linear behavior of \(\Delta \rho(T)/T^2\) for values of \(E_b\) that correspond to \(\tilde{\mu} > 0\) indicates a \(T^3\) dependence of the superfluid density on temperature on the BCS side of the transition. This behavior is in fact confirmed by our analytical calculation of \(\Delta \rho(T)\) at low temperatures and in the case of short range interactions \((k_0 \to \infty)\). In the BCS limit, we found \(\Delta \rho(T) \sim C T^3\), with the coefficient \(C\) weakly dependent on \(E_b\). This power-law behavior reflects the nodal (gapless) structure of the \(p\)-wave excitation spectrum. In the BEC limit, we obtained \(\Delta \rho(T) \sim \exp(-|\tilde{\mu}/T|)\), the exponential behavior reflecting the appearance of a full gap to the addition of quasiparticles for \(\tilde{\mu} < 0\). Fig. 4 also shows (inset) the zero temperature slope of \(\Delta \rho(T)/T^3\) as a function of the binding energy \(E_b\), which is clearly discontinuous at the critical point \(E_b = -1.087 \epsilon_F\). These results further confirm the existence of a quantum phase transition along the BCS-to-BEC evolution as a function of interaction strength (binding energy) in the case of \(p\)-wave spin polarized atoms.

**Summary:** We proposed the existence of a quantum phase transition in the BCS-to-BEC evolution of \(p\)-wave fully spin polarized Fermi gases as a function of the two-body bound state energy. We have shown that, at a critical value of this binding energy, the momentum distribution undergoes a major rearrangement in \(k\)-space, which leads to a non-analytic behavior of the atomic compressibility and spin susceptibility of the gas. Furthermore, the low temperature superfluid density of the system presents a dramatic change in behavior as the critical point is crossed, its temperature dependence going discontinuously from power-law on the BCS side of the transition to exponential on the BEC side of the transition.

We conclude by suggesting that this phase transition may be observable in traps of \(^6\text{Li}\) and \(^{40}\text{K}\) gases which exhibit \(p\)-wave Feshbach resonances \(^\text{[12,13]}\). The occurrence of this phase transition may be investigated through the direct measurement of the atomic compressibility, spin susceptibility or superfluid density as functions of binding energy or magnetic field.

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