The Lifshitz Transition in d-wave Superconductors

S. S. Botelho and C. A. R. Sá de Melo
School of Physics, Georgia Institute of Technology, Atlanta Georgia 30332
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I. INTRODUCTION

The evolution from BCS to Bose-Einstein condensation (BEC) superconductivity/superfluidity has attracted considerable amount of interest in the condensed matter and atomic physics communities. In the atomic physics community, this interest resulted from the possibility of studying condensation phenomena in fermionic atomic gases, where the scattering length (and, thus, the effective interaction strength) can be tuned via Feshbach resonances for a given density. In the condensed matter physics community, the interest in the BCS to BEC evolution arose in the context of high-$T_c$ superconductivity, where the nature of the superconducting and normal states changes as function of carrier concentration. Furthermore, experimentalists seem to start having some control over the carrier concentration using electronic doping via ferroelectric oxides. The fundamental issue that needs to be addressed is whether there is a quantum phase transition in the evolution from a BCS to BEC ground state, as particle density or scattering length (interaction strength) are varied. In this paper we show that for a two-dimensional d-wave superconductor there is a Lifshitz transition between the BCS and BEC ground states. The transition is second order according to Ehrenfest’s classification of phase transitions, but it occurs without change in symmetry as Landau’s classification would demand. To illustrate the nature of the transition, we compute the compressibility and the superfluid density as functions of particle density.

in Section V an analogy with the Lifshitz transition in metals is discussed. The superfluid density is analyzed in Section VI and, finally, our concluding remarks are summarized in Section VII.

II. HAMILTONIAN AND INTERACTION POTENTIAL

We study a two-dimensional continuum model of fermions of mass $m$ described by the Hamiltonian ($\hbar = k_B = 1$)

$$\mathcal{H} = \sum_{k,\sigma} \epsilon_k \psi_{k\sigma}^\dagger \psi_{k\sigma} + \sum_{k,k',q} V_{kk'} b_{kq}^\dagger b_{k'q},$$

where $b_{kq} = \psi_{-k+q/2\uparrow}^\dagger \psi_{k+q/2\uparrow}$ and $\epsilon_k = k^2/2m$. We consider the following separable potential in k-space,

$$V_{kk'} = -\lambda_0 \Gamma(k)\Gamma(k'),$$

which includes only the dominant angular momentum channel, assumed to be d-wave. The interaction term can be written as $\Gamma(k) = \hbar(k)g(k)$, where $\hbar(k) = (k/k_1)^2/[1 + k/k_0]^{5/2}$ controls the range of the interaction, $g(k) = \cos(2\varphi)$ sets its angular dependence, and $\varphi$ is the momentum angle in polar coordinates. In this case, $k_0 \sim R_0^{-1}$, where $R_0$ plays the role of the interaction range, and both $k_0$ and $k_1$ set the momentum scales in the short and long wavelength limits. We work under the assumption that the system is dilute enough, i.e., $k_F^2 \ll k_0^2$. When computing physical properties throughout the manuscript, we scale momenta by $k_F^*=\epsilon_F^*=\hbar k_F^*/2m$, energies by $\epsilon_F^*=k_F^*/2m$, velocities by $v_F^*=k_F^*/m$, and particle density $n$ by $n_{\text{max}}/2\pi$, where $n_{\text{max}}^*=k_F^*/2\pi$. If we choose, for instance, $k_0 = \sqrt{10} \text{Å}^{-1}$ ($R_0 \approx 0.32 \text{Å}$) and define $k_F^* = k_0/10$, then $n_{\text{max}}^* \approx 1.59 \times 10^{14} \text{cm}^{-2}$. We next discuss the effective action and analyze the effects of Gaussian fluctuations about the saddle point solution.

The BCS to BEC evolution has been recently the focus of studies in superconductors and cold atomic gases. For a d-wave system, we show that a Lifshitz transition occurs at a critical particle density which separates two topologically distinct phases according to their quasiparticle excitation energies: a BCS-like gapless superconductor in the higher density limit and a BEC-like fully gapped superconductor in the lower density limit. This transition is second order according to Ehrenfest’s classification, but it occurs without a change in the symmetry of the order parameter, and thus can not be classified under Landau’s scheme. To illustrate the nature of the transition, we compute the compressibility and the superfluid density as functions of particle density.
III. EFFECTIVE ACTION AND GAUSSIAN FLUCTUATIONS

The partition function $Z$ at a temperature $T = \beta^{-1}$ is written as an imaginary-time functional integral with action $S = \int_0^\beta \! d\tau \sum_{k,k'} \! \langle \psi k \psi k' \rangle (\partial_\tau - \mu) \psi k \psi k', + \mathcal{H}$. Introducing the usual Hubbard-Stratonovich field $\phi_k(\tau)$, which couples to $\bar{\psi} \psi$, and integrating out the fermionic degrees of freedom, we obtain $Z = \int \! D\phi D\dot{\phi} \exp(-S_{\text{eff}}[\phi, \dot{\phi}],)$, with the effective action given by

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

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

$$G_{k,k'}^{-1}(\tau) = \begin{pmatrix} - (\partial_\tau + \xi_k) \delta_{kk'} & \Lambda_{k,k'}(\tau) \\ \Lambda_{k',k}(\tau) & - (\partial_\tau - \xi_k) \delta_{kk'} \end{pmatrix},$$

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

To study the BCS to BEC evolution it is necessary to go beyond the standard saddle point approximation, and include at least Gaussian fluctuations. Assuming $\phi_k(\tau) \approx \Delta_0 \delta_{\eta(0)}(\tau)$, and performing an expansion in $S_{\text{eff}}$ to quadratic order in $\eta$, one obtains

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

where $S_0$ is the saddle point action, $\eta^\dagger = [\eta^\dagger(q), \eta(q-\eta)]$, and $q \equiv (q, i\gamma_m)$ with $i\gamma_m \equiv 2m\pi/\beta$. The inverse fluctuation propagator $M$ is a $2 \times 2$ matrix to be defined later.

The Saddle Point Equation: Starting with the stationarity condition $[\delta S_{\text{eff}} / \delta \eta^\dagger(q)(\tau')]|_{\Delta_0} = 0$, Fourier transforming from imaginary time to Matsubara frequency, $ik_\alpha = i(2n + 1)\pi/\beta$, and performing the frequency sum, the saddle point condition can be written as

$$1/\lambda_d = \sum_k \frac{\Gamma^2(k)}{2E_k} \tanh \left( \frac{\beta E_k}{2} \right),$$

where $E_k = \sqrt{\xi_k^2 + \Delta_0^2 \Gamma^2(k)}$ is the quasiparticle excitation energy, with $\xi_k = \epsilon_k - \mu$. Fig. 1 shows a plot of $\pm E(k, \mu)$ as a function of $k$ for three different values of the chemical potential $\mu$. Notice that the Dirac cones collapse at $\mu = 0$.

The Number Equation: Using the thermodynamic relation $N = -\partial \Omega / \partial \mu$, and taking $\Omega = \Omega_{\text{Gauss}} + \Omega_{\text{fluct}}$, where $\Omega_0 = S_0[\Delta_0] / \beta$ and $\Omega_{\text{fluct}} = \beta^{-1} \sum_q \ln \det[M(q)]$, one can write the number equation as

$$N_{\text{Gauss}} = N_0 + N_{\text{fluct}},$$

where $N_0 = -\partial \Omega_0 / \partial \mu = 2 \sum_k n_k$, with $n_k = 1/2 [1 - \xi_k \tanh(\beta E_k/2)/E_k]$ being the momentum distribution, and

$$N_{\text{fluct}} = -\frac{\partial \Omega_{\text{fluct}}}{\partial \mu} = T \sum_q \sum_{\eta_n} \left[ -\partial (\det M) / \partial \mu \right] \left[ \det M(q, i\eta_n) \right]$$

being the fluctuation contribution to $N_{\text{Gauss}}$. At $T = 0$, we will consider a well defined Goldstone modes for all couplings, provided that $|q|$ is sufficiently small. This collective mode appears as a pole in the two-particle excitation spectrum determined by $\det[M(k, z)] = 0$, with $i\eta_n \to z$. This pole has the form $z = c|q| - id|q|^2$, where $c > 0$ is the speed of sound and $d \geq 0$ is the damping coefficient. For $\mu < 0$, $d$ vanishes and the contribution from the collective mode pole $z = c|q|$ dominates at sufficiently low temperatures, since the two-particle excitations are gapped. For $\mu > 0$, $d$ becomes positive, and the spectrum of two-particle excitations is gapless due to the presence of the Dirac points. Thus, unlike the $s$-wave case, Landau damping occurs even at $T = 0$. However, for small $|q|$, the Goldstone mode is underdamped, i.e., the real part of the pole dominates. Therefore, for either $\mu > 0$ or $\mu < 0$, these fluctuation effects lead to

$$\frac{N_{\text{fluct}}}{N_{\text{max}}} \approx \frac{3}{2} \frac{1}{\lambda_d} \frac{1}{\beta},$$

which vanishes in the limit of $T \to 0$. Thus, we recover the $d$-wave equivalent of Leggett’s variational result. At $T = 0$ for the saddle point and number equations in the context of $^3$He.

Denoting $\xi_k$ and $E_k$ by $\xi$ and $E$, and $\xi_{k+q}$ and $E_{k+q}$ by $\xi'$ and $E'$, the matrix elements of $M$ become

$$M_{11}(q) = \frac{1}{\xi_d} + \sum_k \left( \frac{E' + \xi' \xi}{2EE'} \right) \left( \frac{E + \xi \xi' / 2}{(\xi + \xi') / 2} \right),$$

$$M_{12}(q) = -\sum_k \left( \frac{\xi'}{2EE'} \right) \left( \frac{\xi' \xi / 2}{(\xi + \xi') / 2} \right),$$

where the element $M_{11}(q) = M_{11}^0(q) + M_{11}^1(q)$ was split into an even ($E$) and an odd ($O$) part in $i\eta_n$, and $M_{12}(q) = M_{12}(q)$ and $M_{22}(q) = M_{22}(q)$ is subtracted. Performing the analytic continuation $i\eta_n \to \omega + i0^+$ and defining $\eta(q) = |\eta(q)| \exp(i\phi(q)) = (\lambda + i\theta(q)) / \sqrt{2}$, the correction to the effective action assumes the form

$$\left( \lambda^{\ast} \theta \right) \left( \frac{M_{11}^0 + M_{12}}{M_{11}^0 - M_{12}} \right) \left( \frac{\lambda}{\theta} \right),$$

where $\lambda(q)$ and $\theta(q)$ are real functions that may be identified with amplitude and phase fluctuations, respectively. Since the excitation spectrum is gapped for $\mu < 0$, one can make a direct small $q$ and $\omega$ expansion, resulting in $M_{11}^0 + M_{12} = A - Bq^2 + Qq^4 + \ldots$, $M_{11}^1 = Cq^2 + \ldots$, and $M_{11}^1 - M_{12} = -Dq^2 + Fq^4 + \ldots$, where the coefficients are given by $A = \sum_k \Gamma^2(k) \Delta_0^2 / 2E^3$, $B = \sum_k 2\xi \Gamma^2(k)/16E^3$, $C = \sum_k \xi \Gamma^2(k)/4E^3$, $D = \sum_k 2\xi^2 \Gamma^2(k)/16E^3$, etc.
IV. ELECTRONIC COMPRESSIBILITY AND PHASE DIAGRAM

We now discuss the behavior of the electronic compressibility and phase diagram of the system as the \( \mu = 0 \) point is crossed. A simple analysis of \( E_k \) indicates that, for \( \mu > 0 \), \( E_k \) is gapless, while for \( \mu < 0 \), \( E_k \) is gapped. Simultaneously, there is a massive rearrangement of the momentum distribution \( n_k \) as \( \mu \) passes through \( \mu_c = 0 \), leading to the vanishing of the first derivative of \( \mu \) with respect to the density \( n = N/L^2 \) at \( n = n_c \). An important thermodynamic quantity that depends directly on both \( n_k \) and \( E_k \) is the isothermal electronic compressibility \( \kappa \), defined by \( n^2\kappa = \left[ -\partial^2\Omega/\partial \mu^2 \right]/L^2 \). This quantity can be written as

\[
n^2\kappa = \alpha_0 + \alpha_{\text{fluct}}, \quad (10)
\]

where \( \alpha_0 = \partial n_0/\partial \mu \) and \( \alpha_{\text{fluct}} = \partial n_{\text{fluct}}/\partial \mu \). The term \( \alpha_0 \) at \( T = 0 \) can be explicitly rewritten as \( \alpha_0 = (4/L^2) \sum_k n_k (1 - n_k)/E_k \), while the term \( \alpha_{\text{fluct}} \propto T^3 \) vanishes as \( T \to 0 \). In the vicinity of \( \mu = \mu_c = 0 \), \( \kappa \) diverges logarithmically at \( T = 0 \) as

\[
\kappa \approx [-c_1 \ln |1 - n/n_c| + c_2] \quad (11)
\]

in the d-wave case, suggesting the existence of a quantum phase transition (QPT). This singular behavior of the compressibility is shown in Fig. 2 and the corresponding phase diagram is shown in Fig. 3 together with a plot of \( \mu \) as function of \( n \) (inset). The critical line \( \mu = \mu_c = 0 \) in the \( \lambda_d \times n \) space separates a BCS-like region, where Dirac points exist and there are gapless excitations \( (\mu > \mu_c) \), from a BEC-like region which is fully gapped \( (\mu < \mu_c) \). One critical line ends at the two-body bound state threshold \( \lambda^*_{2} = 8 \) (see Fig. 3) when \( n \to 0 \). Thus, the QPT between the BEC and BCS regimes requires that \( \lambda_d > \lambda^*_{2} \). In the s-wave case there is no QPT, since \( \kappa \) is continuous and changes in \( n_k \) are always smooth. Notice that the contribution of the collective modes to \( n \) and to \( \kappa \) at \( T = 0 \) vanishes identically. Thus, Gaussian fluctuation effects of the superconducting order parameter are not important for the \( T = 0 \) electronic compressibility. This divergence in the second derivative of \( \Omega \) at \( T = 0 \) signals a second order quantum phase transition, according to Ehrenfest’s classification. However, the symmetry of the order parameter does not change, and a Landau symmetry classification of the phase transition is not possible. So, if the symmetry is not changing at the transition point, what is?

V. THE LIFSHITZ TRANSITION

To answer this question we make an immediate connection to the Lifshitz transition in the context of ordinary metals at \( T = 0 \) and high pressure. The Lifshitz transition should not be confused with the Lifshitz point, where a finite temperature phase transition occurs separating the high temperature disordered phase, the spatially uniform ordered phase, and the spatially modulated ordered phase. In the conventional Lifshitz transition, the Fermi surface \( \epsilon(k, P) = E_F \) changes its topology as the pressure \( P \) is changed. For an isotropic pressure \( P \), the deviation \( \Delta P = P - P_c \) from the critical pressure \( P_c \) is proportional to \( \Delta \mu = \mu - \mu_c \). A typical example of the Lifshitz transition is the disruption of a neck of the Fermi surface which leads to a non-analytic behavior of the number of states \( N(\mu) \) inside the Fermi surface. In this case, \( N(\mu) \) behaves as \( A(\mu_c) + B(\mu - \mu_c)^{3/2} \) for \( \mu < \mu_c \), and as \( A(\mu_c) \) for \( \mu > \mu_c \), in the vicinity of \( \mu_c \). Here, \( \kappa = (3/2)B(\mu - \mu_c)^{1/2}/n^2 \), where \( n_c = N_c/V \). Notice that \( \kappa \) is non-analytic, but it is not singular. The
quantity that signals a phase transition in this case is not \( \kappa \), but the thermopower \( Q \), which is proportional to \(-\partial \ln(n)/\partial \mu\), thus leading to \( Q \propto -|\Delta \mu|^{-1/2} \). In the conventional Lifshitz transition, the system lowers its energy by \( \Delta E \propto -|\mu - \mu_c|^2 \ln|\mu - \mu_c| \). This logarithmic contribution originates from the simultaneous collapse of the four Dirac points at \( k = 0 \), which produces a gap in the excitation spectrum \( E_k \) and a massive discontinuous rearrangement of the momentum distribution \( n_k \) in the ground state as \( \mu \rightarrow \mu_c = 0 \). A direct topological analogy with the standard Lifshitz transition can be made by noticing the collapse of the Dirac cones at \( \mu = \mu_c \) (and the disruption of a neck for \( \mu < \mu_c \)) in the excitation spectrum of the system, as shown in Fig. 4.

VI. SUPERFLUID DENSITY

Now we analyze the behavior of the superfluid density tensor \( \rho_{ij}(T, n) \) across the Lifshitz transition, given by

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

where \( n_k \) is the momentum distribution and \( Y_k = (2T)^{-1} \text{sech}^2(E_k/2T) \) is the Yoshida distribution. Notice that \( \rho_{xx} = \rho_{yy} \equiv \rho \), while \( \rho_{xy} = \rho_{yx} = 0 \). Due to Galilean invariance of our continuum model, \( \rho(T = 0) = n/2m \) is well-behaved as the critical point is crossed. However, \( \partial \rho(T = 0)/\partial \mu = n^2 \kappa/m \) diverges at \( n = n_c \). Using our energy and momentum scales, we define \( \Delta \rho \equiv (\rho(T) - n)/2\pi \). In Fig. 4, we show \( \Delta \rho \) for various concentrations (inset), and the zero temperature slope \((m/2\pi)[\partial \rho/\partial T]_{T=0}\) as a function of particle density. Notice the discontinuity in the zero temperature slope as the critical point \( n = n_c \) is approached.

We have also calculated \( \Delta \rho \) analytically at low temperatures in the case of very short range interactions \((k_0 \rightarrow \infty) \). In the BCS limit, \( \Delta \rho = -2\pi k^2 T \Delta_0(n) \), due to the nodal structure of the d-wave symmetry. At the critical point \( \mu = 0 \) \((n = n_c) \), \( \Delta \rho = -\ln(2) F(\eta)/T \), where \( F(\eta) = (1 + \eta^2)^{-1/2} \), with \( \eta = \Delta_0(n)/k^2 T \). In the BEC limit, \( \Delta \rho = -(8/\pi) \exp(-|\mu|/T) F(\eta) \). This exponential behavior reflects the appearance of a full gap in the excitation spectrum for \( n < n_c \).

For all values of \( \mu \), there is further reduction of \( \rho(T) \) at low \( T \) due to Goldstone modes leading to \( \Delta \rho_G = -AT^3 \), which obviously does not affect the \( T = 0 \) slope of \( \Delta \rho \) through \( n = n_c \).

VII. SUMMARY

We have proposed the existence of a Lifshitz transition at \( T = 0 \) in clean d-wave superconductors, where a topological change in momentum space is responsible for a non-analytic behavior of the electronic compressibility and of the zero temperature slope of the superfluid density. We conclude by suggesting that the search for this transition may now be possible using the so-called ferroelectric field effect transistor (FFET), where some control over the particle density in cuprate superconductors may be achieved without chemical doping. In addition, it may be possible to investigate the occurrence of this transition by measuring the superfluid density as a function of doping, or through a direct measurement of the electronic compressibility as a function of particle density, as was done in the study of metal-insulator transitions.
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