Hopping anisotropies: A candidate for BCS-BEC crossover

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In a two-dimensional *t-J* model that includes anisotropy in the hopping frequency of the charge carriers, the crossover scenario from a BCS superconductor to a condensate of tightly bound bosonic pairs is studied. The important length scales, such as the mean pair radius and penetration depth, are obtained as a function of the anisotropy parameter that distinguishes hopping in one direction with respect to the other. The results indicate a smooth evolution from a picture of highly overlapping Cooper pairs to a condensate of short-range bosonic pairs with increasing anisotropy. The claim for the crossover phenomena is supported by calculating the renormalized chemical potential which slips below the band minimum in the extreme anisotropy limit, implying the onset of a Bose phase.

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I. INTRODUCTION

The crossover phenomenon from a BCS superconductor to a Bose superfluid¹⁻³ and the associated physics have generated enormous attention among researchers in recent times. It is instructive to look at Refs. 4 and 5 for a comprehensive review on the subject. The fact that a condensate consisting of weakly interacting fermionic degrees of freedom evolves smoothly into one which is characterized by strongly interacting bosons is worth a problem to investigate. A controlled tuning of strength of the attractive interaction between the carriers in the presence of a magnetic field for a system of ultracold fermionic atoms has facilitated the study of the crossover phenomenon in the cold atom problem in laboratories.^{6–9} The excitement is further intensified with the recent experiments on optical lattices and its associated practical applications.^{10,11} Interestingly, the subject relates to both atomic physicists and the condensed matter community.

The unusual features of the normal state observed in the context of high- T_c superconductors have put a special focus on the physics governing the crossover. To be more specific, the appearance of a pseudogap in the form of a depletion of single-particle spectral weight around the fermi level below a certain critical temperature T^* in the underdoped regime of cuprates^{12–18} demonstrates the most comprehensive deviation from the mean-field (BCS) scenario for superconductors. The BCS picture may be viewed as a very special case where the pair formation and the condensation occur simultaneously; i.e., at the same temperature while at moderate values of the interaction strength, the pairs form and condense at different temperatures, as energetics favor pair formation within the normal phase. Finally, the system comprising of such bosonic degrees of freedom condenses at a different temperature, say, T_c (below T^*). The two temperature scales (T_c and T^*) signal the presence of two different gap parameters, one of them being the superconducting gap (related to T_c) and the other corresponding to the excitations of the normal state or pseudogap at temperature $T > T_c$. To summarize, the bosonic excitations in the pseudogap phase smoothly evolve into fermionic ones in the BCS regime, thereby proving the inextricable connection between the crossover phenomenon and the pseudogap.

Due to the somewhat controversial nature of the experimental data available on the subject, the origin of the pseudogap is not clearly understood. However, a large community^{19–21} believes that a crossover scenario is best suited to explain the origin of the pseudogap.

The crossover analysis has mostly concentrated on studies to explore how the gap in the energy spectrum and the chemical potential evolve as a function of the interaction strength between the fermions.^{1,2,22} It can be shown that the chemical potential changing sign can be regarded as the signature of crossover, at least at low densities. Physically, this remarkably simple result demarcates the two regions in the following way. At very weak interaction strengths (or large particle density), the binding energy of a pair is extremely small, thus the chemical potential is decided by the Fermi energy alone and hence corresponds to a regime comprising of overlapping Cooper pairs. In the other limit of strong interparticle interaction (or low density), the binding energy of the pair dominates and sets the scale for the chemical potential. In this way, the system consists of Bose-Einstein (BE) condensate of bosons and the gap in the quasiparticle spectrum is different than that of BCS theory.^{12,23}

In this paper, we study a simple model that incorporates anisotropy in the hopping frequencies of the charge carriers. In a two-dimensional t-J-U model, this means that the kinetic energies are different in the x and y directions (i.e., t_x $\neq t_{y}$; however, the charges are allowed to interact via an isotropic exchange J. The following may be noted about the on-site Hubbard term U. The limit $U \rightarrow \infty$ projects out the doubly occupied sites and reduces the model to a more familiar t-J model.²⁴ Such a model has previously been considered as a minimal model for stripelike anisotropies, where it was solved for the binding energy of a two-electron problem (zero density).²⁵ The calculations were extended later to finite densities to obtain the superconducting energy gap and transition temperature at low but finite electron densities.²⁶ The results obtained were remarkable. In the extreme anisotropy limit [i.e., $t_x \ge t_y$ (say)], a two-particle pairing is possible in the presence of an infinitesimal J (and infinite U), and at finite densities, fingerprints of a more robust superconducting condensate (the transition temperature; T_c being much higher) is found. Here, with a mixed symmetry ansatz for the gap amplitudes, we solve the BCS gap equation at

finite temperature and hence evaluate the two important length scales that characterize the condensate, namely, mean pair radius ξ_{pair} and the penetration depth λ for the anisotropic system. As the hopping frequency in x and y directions are made progressively different, the mean pair radius decreases and, finally, in the limit of strongest anisotropy, becomes as small as a few lattice spacings, while the penetration depth diverges in a direction in which the hopping is suppressed. If the coherence length is loosely taken as the radius of the Cooper pair (the difference will be discussed in Sec. II), the rapid suppression of ξ_{pair} in the limit of large anisotropy is indicative of a phase consisting of nonoverlapping, albeit tightly bound pairs, a feature that distinguishes a Bose condensate from a BCS superconductor. In addition, the divergence of the penetration depth as a function of the strength of anisotropy implies a small superfluid density, again pointing toward a Bose-Einstein condensate (BEC) phase. Thus the claim of a crossover phenomenon occurring in the presence of strong hopping anisotropies receives support from the data of ξ_{pair} and λ .

We organize our paper as follows. Section II deals with the calculation of ξ_{pair} and λ for the anisotropic model. Section III analyzes the results obtained in Sec. II and, based on those results, discusses the emergence of a crossover from a BCS superconductor to a Bose superfluid in the presence of large anisotropies. The crossover scenario is supported by the chemical potential crossing the band minimum as seen via solving BCS equations self-consistently. A brief conclusion is presented in Sec. IV.

II. MEAN PAIR RADIUS AND PENETRATION DEPTH

To understand the nature of the superconducting condensate, it is intuitive to look at the two characteristic lengths, namely, the coherence length and the penetration depth. There is another length scale having values very similar to that of the coherence length for a BCS superconductor, i.e., the average size or radius of the Cooper pairs. The similarity has often led these quantities to be considered indistinguishable.¹² However, they are different quantities and the difference is very conspicuous in the BEC regime. As for a BCS superconductor, the two length scales are very similar and have values much larger than the interparticle spacing and close to $\frac{\hbar v_F}{\pi \Delta}$, the well-known Pippard result.²⁷ In the opposite limit of extremely low density, the mean pair radius is much smaller than the coherence length;²³ the latter being comparable to interparticle spacing. It was emphasized that the single-particle excitation spectrum (broken Cooper pairs) with an exponentially small gap is related to the pair radius, while the energy coherence range is defined by the coherence length, both being the same in the large density limit.

The other important quantity, namely, the penetration depth, signifies the distance over which an applied magnetic field is exponentially screened from the interior of a superconductor. The linear response of the current density to the magnetic field defines the penetration depth and hence the superfluid density; the latter having an inverse square dependence on the penetration depth. In this paper, we calculate the mean radius of the Cooper pairs and the penetration depth that describe the nature of the condensate in the presence of hopping anisotropies.

The mean pair radius is defined by the following relation:²⁹

$$\xi_{pair}^{2} = \frac{\int |f(r)|^{2} r^{2} d^{3} r}{\int |f(r)|^{2} d^{3} r},$$
(1)

where f(r) is the wave function for a Cooper pair in real space. Fourier transforming the above equation, one gets

$$\xi_{pair}^2 = \frac{\sum_k |\nabla_k g_k|^2}{\sum_k |g_k|^2},\tag{2}$$

where g_k is the amplitude of the pair wave function. In BCS theory, g_k at finite temperatures is given by

$$g_k = \frac{\Delta_k}{2E_k} [1 - 2f(E_k)], \qquad (3)$$

with $E_k = \sqrt{(\epsilon_k - \mu)^2 + |\Delta_k|^2}$, $f(E_k)$ being the Fermi distribution function, and $\epsilon_k = -2t(\cos k_x + r \cos k_y)$, where $r(=\frac{t_y}{t_x} = \frac{t_y}{t})$ is the anisotropy parameter that distinguishes the carrier's ability to move from one direction to another. The gap functions in *k* space Δ_k (vanishing of which determines T_c) and the chemical potential μ are obtained by solving BCS gap equations (including the number equation) self-consistently, with an isotropic exchange for the pair potential at finite temperature,^{26,30}

$$\Delta_{k} = -\sum_{k'} \frac{V_{kk'} \Delta_{k'} [1 - 2f(E_{k'})]}{2E_{k'}},$$

$$n = 1 - \sum_{k} \frac{(\epsilon_{k} - \mu)[1 - 2f(E_{k})]}{E_{k}}.$$
(4)

Subsequently, Eq. (2) is solved for ξ_{pair}^x and ξ_{pair}^y . The results are presented in Fig. 1 as a function of the anisotropy parameter *r*. It may be noted that the parameters chosen are, J/t = 1/3 (physical value for cuprates), n=0.15 (low density), where our starting point, i.e., BCS gap equations, are most appropriate, and the on-site term *U* is set to infinity. $\xi_{pair}^{x,y}$ decreases from a few thousands of lattice spacing (expected for a BCS superconductor²⁸) with an increase in anisotropy and becomes very small (order of one lattice spacing) as $r \rightarrow 0$.

Physically, the shrinking of the pair size occurs due to the constrained hopping of the charge carriers along one direction as compared to the other. Quantitatively, the pair wavefunction in k space is noted to be enhanced, thereby implying a decrease in the pair radius in real space with anisotropy. Thus the system smoothly evolves from a large number of overlapping Cooper pairs to a condensate of much fewer but tightly bound pairs carrying the signature of a BCS-BEC crossover.



FIG. 1. The mean pair radii, ξ_{pair}^x and ξ_{pair}^y , are plotted as a function of anisotropy *r*. The electron density and the interaction parameters are chosen as n=0.15, J/t=1/3, and $U/t=\infty$, respectively. The temperature *T* is very small and chosen to be $0.1T_c$, T_c being the superconducting transition temperature. Both ξ_x and ξ_y show similar variation with *r* and shrinks to a value of the order of lattice spacing as $r \rightarrow 0$.

The other length scale, namely, the penetration depth, is defined through long-wavelength limit $(q \rightarrow 0)$ of static ($\omega = 0$) response kernel in the following manner:²⁸

$$\mathbf{J}_{\delta}(\mathbf{q}) = -\frac{1}{4\pi} K_{\delta}(\mathbf{q} \to 0) \mathbf{A}_{\delta}(\mathbf{q}), \quad \delta = x, y, \tag{5}$$

where

$$K_{\delta} = \frac{1}{\sqrt{\lambda_{\delta}}}.$$
 (6)

J and **A** are the current density and the vector potential, respectively. **J** includes both the paramagnetic and diamagnetic contributions (which tend to cancel each other) and hence the corresponding response kernels K^P and K^D are defined by³¹

$$K_{\delta}^{P} = \frac{32\pi e^{2}}{\hbar^{2}} \frac{1}{N} \sum_{k} \sin^{2} k_{\delta} \frac{\partial f(E_{k})}{\partial E_{k}},$$
$$K_{\delta}^{D} = \frac{8\pi e^{2}}{\hbar^{2}} \frac{1}{N} \sum_{k} \cos k_{\delta} \left(1 - \frac{\epsilon_{k} - \mu}{E_{k}} [1 - 2f(E_{k})]\right).$$
(7)

The total kernel is the sum of these two, which may be substituted in Eq. (6) to obtain λ . λ_x and λ_y , the penetration depths in the *x* and *y* directions, respectively, are plotted as a function of the anisotropy parameter *r*. While λ_x remains almost constant in the entire interval, λ_y diverges as $r \rightarrow 0$. Thus there is an efficient screening (Meissner effect) in the *x* direction where the carriers move unhindered, while, due to a severely restricted motion along *y*, the field penetrates to the interior of the sample. Since the penetration depth is inversely proportional to the square of the superfluid density, the scenario signals a condensate characterized by a smaller number of superconducting electrons and hence fewer pairs in the presence of large anisotropies.2



FIG. 2. The penetration depth along x and y axis are plotted vs r. The parameters chosen are the same as those of Fig. 1. λ_y shows a divergence in the limit $r \rightarrow 0$, while λ_x remains constant.

In the spirit of the discussion presented at the beginning of Sec. II, we loosely consider the mean pair radius as a characteristic length, indistinguishable from the coherence length (which is strictly true in the BCS limit), and calculate the Ginzburg-Landau characteristic parameters $\kappa_{x,y}$ $(=\lambda_{x,y}/\xi_{pair}^{x,y})$ along the *x* and *y* directions. Both κ_x and κ_y increase by three and six orders of magnitude, respectively, in the limit $r \rightarrow 0$ from a very small value corresponding to the isotropic case (where κ_x and κ_y are indistinguishable), implying the evolution of a very different phase.

III. BCS-BEC CROSSOVER

In the context of the two-electron problem, in the presence of hopping anisotropy, it was shown earlier that a twoparticle bound state is possible with an infinitesimal attractive interaction in the limit of extreme anisotropy.²⁵ Further, it was shown that the bound state is distinctly more favorable for the carriers to be moving across the chains than along the chains as $r \rightarrow 0$, and the bound state energy was found to increase considerably, implying a very stable pair in this limit. Thus we are provided with a scenario where a twodimensional plane of exchange-coupled chains facilitates bound-state formation in the zero-density limit. Extrapolation of the anisotropic model to finite densities has yielded a much higher superconducting transition temperature in the limit of large anisotropy.²⁶ In this paper, we further calculate two length scales associated with this model. The average pair radius shrinks remarkably from a few thousands of lattice spacings corresponding to the isotropic case to a few lattice spacings in the limit $r \rightarrow 0$. Thus a large number of overlapping Cooper pairs evolve smoothly to a system of tightly bound, much smaller pairs. Further, a large penetration depth implies an anomalously low superfluid density in the presence of large anisotropies, thus strengthening the possibility of breakdown of the standard BCS scenario and the onset of an unconventional phase bearing fingerprints of local, short-range pairing in the superconducting condensate.32

To support the claim for a crossover scenario, we consider the chemical potential μ [obtained by solving Eq. (4)], which

TABLE I. BCS-BEC crossover is investigated by computing μ as a function of anisotropy parameter r for a few values of density n and interaction strength J. The value of r at which μ falls below the lower band edge [=-2t(1+r)] and thus signals a crossover is denoted by r_c . The empty slots represent the absence of a CROSS-OVER for the corresponding parameter values.

n	r _c		
	J/t=1/3	J/t = 1	J/t=2
0.02	0.007	0.11	0.57
0.1		0.006	0.08
0.15			0.026
0.2			

when it slips below the band minimum as a function of anisotropy parameter r (the Leggett condition), the system evolves into a Bose superfluid. To gain insight on the dependence of crossover on the electronic density, we investigate the variation of μ as a function of r for different values of n corresponding to a few representative values of J, e.g., J/t=1/3, 1, and 2. The results obtained are presented in Table I. It may be noted that there is no crossover for larger values of *n* for any J. Physically, at higher densities, the pairs overlap, thereby resulting in an increase in correlation between the carriers. To compensate for this, the system organizes itself with a larger average pair size so as to minimize the total energy of the system. Thus, at higher densities, the system bears resemblance to a BCS condensate even for larger values of J. However, in general, at moderate values of density, the crossover phenomenon is more robust for stronger exchange coupling J.

The table clearly indicates the absence of a crossover for the isotropic case (r=1) for J to be as large as 2t. The hopping anisotropy thus plays a crucial role and drives the system from a BCS phase to a Bose regime at lower densities.

IV. CONCLUSIONS

In this paper, we have calculated two important length scales that characterize the superconducting condensate, namely, the mean radius of the Cooper pairs and the penetration depth, for a two-dimensional t-J model with hopping anisotropies. It is observed that a BCS superconductor evolves smoothly into a phase with much shorter and fewer (although tightly bound) pairs, characteristic of a BE phase with increasing anisotropy. This crossover picture is supported by calculating the chemical potential which falls below the band minimum in the extreme anisotropy limit at low densities.

The emergence of a Bose phase consisting of tightly bound local pairs from a condensate of overlapping Cooper pairs has been studied mostly as a function of the interaction strength between the pairs.^{33,34} The weak-coupling limit corresponds to a BCS superconductor, while the strong-coupling limit applies to the BE phase. Experimental signatures of such crossover with oxygen concentration were observed in YBa₂Cu₃O_{7- δ}.³⁵ Also, effects of structural disorder on the crossover phenomenon have been discussed.³⁶

Thus it leaves a number of relevant and unresolved questions associated with the crossover phenomena. Which are the other influencing parameters that drive a system consisting of fermionic excitations to smoothly evolve into one having bosonic degrees of freedom, and what is the influence of interaction and fluctuation effects on the driving parameters, to name a few. A detailed analysis is required to address these important issues.

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