Strong Pairing in two dimensions: Pseudogap and other phenomena

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We analyze the Berezinskii-Kosterlitz-Thouless transition temperature $T_{\text{BKT}}$ as a function of attractive coupling strength $g$, in 2D superconductors, following earlier work on atomic Bose gases. As a calibration, we successfully address the continuum case associated with experiments on atomic Fermi gases. Our focus is on metallic superconductors with tight binding bandstructure, as might be relevant to new materials such as twisted bi-layer graphene. Importantly our calculations reproduce the known constraints on $T_{\text{BKT}}$ at both weak and strong couplings. Here we provide physical insight into our surprising observation that $T_{\text{BKT}}$ decreases with $g$ in the physically relevant, intermediate coupling regime. Given the measured size of $T_{\text{BKT}}$, our calculations establish the magnitude of related quantities such as the excitation (pseudo)gap and coherence length.

Introduction—Recently there has been a resurgence of interest in superconductivity in (quasi-)2D materials. This has been driven by exciting discoveries of novel superconductors such as twisted magic-angle bilayer graphene [1], FeSe monolayers [2,3] and transition metal dichalcogenides [4,5]. For the former, one of the most striking features of this superconductivity is its correlation with the appearance of flat bands, where the kinetic energy of the electrons becomes small compared to the interaction energy [6]. Indeed, within a BCS mean-field formulation, flat bands have been argued to lead to very high transition temperatures which scale as a power-law in the attractive pairing interaction strength [7]. At the same time, the Uemura plot [8] suggests that BCS theory has a restricted applicability and that many interesting superconductors [1,9–11] appear to belong to the more strongly correlated class which are intermediate between BCS and Bose Einstein condensation (BEC). Adding to this complication, is the complexity of treating strongly correlated superconductivity in two dimensions where the long-range superconducting instability is replaced by a Berezinskii-Kosterlitz-Thouless (BKT) transition [12,13].

These two observations form the basis of this paper which deals with BKT superconductivity in the presence of strong pairing correlations. It is well known from Monte Carlo calculations [14,15] and other calculations [16] that plots of $T_{\text{BKT}}$ vs coupling $g$ ($>0$) yield a superconducting “dome” shape. It is generally believed [14] that the downturn in $T_{\text{BKT}}$ within the dome at larger $g$ arises from the BEC asymptotics; we show here that there are rather two important features: a dome and a separate BEC regime at even larger $g$, where the superconducting transition temperature is suppressed by the reduced pair hopping associated with the added expense of unbinding paired fermions [17].

The approach in this paper follows the spirit of earlier work on atomic Bose gases [18]. There the criterion for the BKT instability is based on the bosonic phase-space density:

$$D_B(T) \equiv \frac{n_B(T)}{\Omega_B(T)} \frac{2\pi}{T},$$

where $n_B(T)$ represents the areal number of bosons and $M_B(T)$, their effective mass. (In this notation $k_B = 1$ and $\hbar = 1$). The BKT transition temperature $T_{\text{BKT}}$ occurs when $D_B(T)$ reaches a critical value determined from previous Monte Carlo calculations [19]. It is important to calibrate these results. To this end we first address the continuum case associated with experiments on atomic Fermi gases [20–22] and show reasonably good agreement with experiment.

Our goal here is to focus on the lattice case and to provide analytical insights which serve to explain not only the general magnitude of $T_{\text{BKT}}$ but yield estimates of other correlated variables such as the excitation gap, $\Delta$ and the coherence length. We build on an analytical approach to BCS–BEC crossover which was developed to address superconductivity (and related pseudogap effects) in the cuprates [23–25]. Important is a very definite signature of this stronger-than-BCS-pairing which yields a crucial falsifiability criterion, i.e., the normal state above $T_{\text{BKT}}$ must have a pseudogap in the electronic spectrum due to formation of quasi-bound Cooper pair states. Such effects are enhanced in 2D systems and have been clearly observed in 2D atomic Fermi gases [26].

We emphasize that analytical approaches to the BKT transition temperature in fermionic superfluids must accommodate the fact that it depends fundamentally on bosonic variables. Thus to estimate $T_{\text{BKT}}$, commonly, one converts to the fermionic sector by introducing the fermionic mass ($m$) and 2D density ($n$) via $n_B = n/2$ and $M_B = 2m$ [27]. This, however, does not capture the known physics [14,17] on a lattice as a function of the coupling strength $g$. In the attractive Hubbard model one expects a very small $T_{\text{BKT}} \propto t^2/g$ in the large $g$ limit. (Here $t$ is the nearest neighbor hopping.) One also expects that in the small $g$ limit the BKT transition temperature should become arbitrarily small whether the 2D system has a gas or lattice dispersion. And this appears somewhat problematic if one makes the factor of 4 adjustment in $D_B$. The one situation where this transcription works is in a 2D gas, and at large $g$, or more precisely, in the BEC regime.

In our approach, the fermions enter $T_{\text{BKT}}$ because the fundamental bosonic variables $n_B$ and $M_B$ depend on the fermionic excitation gap $\Delta(T)$ (which is non-zero at $T_{\text{BKT}}$ as expected for a pseudogap). With an understanding of the limiting very weak and very strong coupling cases, we are able
then to address the intermediate coupling regime and deduce that the non-monotonic structure of the BKT transition temperature for both the gas and lattice dispersions depend on an interesting competition between $n_B(T)$, which increases, and $1/M_B(T)$, which decreases with increasing $g$. Importantly, this non-monotonicity appears well before the system enters the asymptotic high $g$ regime.

**Background Theory** — Our treatment of the BCS–BEC crossover follows an approach to BCS theory proposed by Kadanoff and Martin [23, 28]. BCS theory is associated with a propagator for (virtual) non-condensed pairs (called $t_{pg}$) given by

$$t_{pg}^{-1}(i\Omega_n, q) = -\frac{1}{g} + \sum_{\nu, \mu} G(i\omega_n, \nu, \mu) G(-i\omega_n + i\Omega_n, -\nu - \mu + q)$$

(1)

Here the dressed electronic Green’s function, $G$, assumes the BCS form with the Bogoliubov quasiparticle dispersion $E_k = \sqrt{\epsilon_k^2 + \Delta^2}$, and usual coherence factors $\{\nu^2_k, \nu_k\}$. Here $\epsilon_k = \epsilon_k - \mu$.

Analytically continuing Eq. (1) (for 4-vector $\Omega \equiv (q, \Omega) \neq 0$) leads to

$$t_{pg}^{-1}(Q) = -\frac{1}{g} + \sum_k \left[ 1 - f(E_k) - \frac{f(\epsilon_k - q) - \epsilon_k - \mu - i\gamma}{\epsilon_k - \mu - i\gamma} \right]$$

(2)

It is important to recognize that the statement $t_{pg}^{-1}(0) = 0$ is equivalent to the BEC condition that pairs have zero chemical potential $\mu_{pair} = 0$ for all $T \leq T_c$. In this way Eq. (2) yields the well-known temperature dependent BCS gap equation.

For the most part our interest will be on the long-wavelength and small-frequency limit, where the propagator can be approximated to be:

$$t_{pg}(Q) \approx \frac{a_0^{-1}}{\frac{q^2}{2M_B} + \mu_{pair} + i\gamma}.$$

(3)

Here $a_0^{-1}$ is the pair fluctuation strength, $\gamma$ is the decay rate due to the two-electron continuum. In the presence of a quasiparticle excitation gap, the pair decay rate at small frequencies vanishes. From now on we omit $i\gamma$ in the pair propagator.

Now consider non-condensed pairs in the normal state [23, 24] where there is no condensate. We assume, throughout, that the pairing gap $\Delta$ is the pseudogap so that $\Delta \equiv \Delta_{pg}$. This excitation gap is to be distinguished from the order parameter. The self consistency condition can be written $t_{pg}^{-1}(0) = a_0 \mu_{pair}$, where $\mu_{pair}$ smoothly vanishes at the transition into the ordered phase. This same analysis applies to two dimensions where $\mu_{pair}(T)$ will be shown to assume small values, but never reach zero, except at $T = 0$.

We note that the self energy associated with these non-condensed pairs in the dressed Green’s function is more completely given by

$$\Sigma(i\omega_n, \nu, \mu) = T \sum_{\nu, \mu} t_{pg}(i\Omega_n, \nu)G(-i\omega_n + i\Omega_n, -\nu - \mu + q)$$

$$\approx -\Delta^2 G(-i\omega_n, -\nu - \mu + q),$$

(4)

where in this last step we have assumed that the system is near an instability where $t_{pg}(Q)$ is strongly peaked at $Q = 0$. Eq. (4) is a standard approximation in the cuprate literature for the pseudogap-related self-energy [25, 29].

We stress that the second line in Eq. (4) is the only approximation used here, aside from the overarching assumption implicit in Eq. (1) that we are dealing with a BCS-like gap equation and ground state, albeit extended to BCS–BEC crossover. Note that this approximation effectively ignores Hartree as well as incoherent contributions to the fermionic self-energy, which may, as well, introduce particle-hole asymmetry effects. There is an additional complication near half filling and this is associated with competing charge density wave order in the particle-hole channel [13], which we are ignoring here. It is, however, convenient to make such a simplifying assumption in the vicinity of small $\mu_{pair}$ (which is appropriate near $T_{BKT}$) for analytical tractability.

Combined with the parametrization in Eq. (3), we derive the following self-consistent equations for a fixed-density system:

$$a_0 \mu_{pair} = -\frac{1}{g} + \sum_k \left[ \frac{1 - 2f(E_k)}{2E_k} \right],$$

(5)

$$a_0 \Delta^2 = n_B = \sum_q b \left( \frac{q^2}{2M_B} - \mu_{pair} \right),$$

(6)

$$n = \sum_k \left[ 1 - \frac{\epsilon_k}{E_k} \left( 1 - 2f(E_k) \right) \right],$$

(7)

where $b(x)$ is the Bose-Einstein distribution function.

At finite temperatures, Eq. (6) can be inverted exactly to give the pair chemical potential: $\mu_{pair} = T \ln \left( 1 - e^{-\frac{n_{BKT}}{T}} \right)$.

The size of $|\mu_{pair}|$, which measures how close the normal fluid is to a long range-ordered superfluid phase, reflects the bosonic phase-space density: $D_B(T) \equiv \frac{\mu_{pair}^2}{2\pi M_B}$, $\frac{\mu_{pair}}{n_B(T)} \lambda_B^2$, where $\lambda_B$ is the thermal wavelength for the pairs.

This (dimensionless) phase space density is of fundamental importance in studies of 2D Bose superfluids [18, 30]. In the literature on 2D superfluid Bose gases, one establishes the BKT transition temperature by knowing the critical value which $D_B(T)$ assumes at $T = T_{BKT}$.

By contrast the literature on 2D fermionic superfluids focuses on the Nelson-Kosterlitz (NK) criterion [31] which considers only the superfluid contribution to the phase space density, called $D_{B}(T)$. This NK criterion states that the superfluid component $D_{B}(T) = \frac{n_{BKT}^2}{M_B}$ is $4$ at $T_{BKT}$. Note that this does not determine the value of the total phase space density ($D_B$) at the transition. Rather it introduces [18] the constraint $D_{B}(T_{BKT}) > 4$.

From the fermionic and bosonic swells we are left with two choices on how to proceed. One can either compute the
bosonic superfluid density $n^s_B/M_B$ and use the constraint that $D_B = 4$ at the transition or alternatively one must appeal to other calculations to provide the critical value for the total phase space density precisely at the transition. The complication with the first approach is that it is not straightforward to deduce the “phase stiffness” or helicity which appears in $n^s_B$ and depends in a complicated way [32] on the fermionic quasi-particles, and long wavelength phase fluctuations. BCS-like approximations [16] to the superfluid density, which seem most natural, do not assure that $n^s_B$ strictly vanishes above $T_{BKT}$, nor that the resulting transition temperature vanishes at weak $g$.

Our approach belongs to the bosonic school and is based on Monte Carlo work [19] and on prior analysis of atomic Fermi gases [20][21]. Here one estimates $D_B/T_{BKT} = 4.9$ [21]. Note this is near but somewhat larger than the minimum value of 4. As a consequence $T_{BKT}$ in the present formalism is derived from the condition

$$\frac{2\pi}{4.9} \frac{n_B(T)}{M_B(T)} = T$$

at $T = T_{BKT}$.

Important here is that $n_B$ and $M_B$ in the above equation should be thought of as $\Delta(T)$ dependent rather than fixed in temperature. They vary in a way which reflects the fermionic degrees of freedom.

**Numerical results**– The detailed numerical results in this section are based on Eqs. [3][7]. We begin with the atomic Fermi gases where we calibrate our theoretical framework directly by comparison with experiment [20][21] on trapped superfluids (although, in contrast to Ref. [22] trap effects have not been included). Here in place of the attractive coupling constant $g$, we introduce the 2D scattering length $a_{2D}$ via $g^{-1} = \sum_{k} \frac{1}{2\epsilon_k + \epsilon_B}$, where $\epsilon_k = k^2/2m$ and $\epsilon_B = 1/ma_{2D}^2$.

Figure 1 presents a plot of $T_{BKT}$ in units of $E_F$ versus $-\ln(k_F a_{2D})$, with $E_F$ being the non-interacting Fermi energy and $k_F$ the Fermi wave-vector. From left to right on the horizontal axis represents the transition from BCS-like to BEC. Indicated are the asymptotic values for $n_B = n/2$ and $M_B = 2m$. Note that $T_{BKT}$ has a dome shape for $a_{2D} > k_F^{-1}$, and saturates to a constant at strong coupling. Notable is the transition point or “kink” in the plot where the fermionic chemical potential $\mu = 0$. Beyond this point, $T_{BKT} \approx \frac{1}{2} E_F$. (That the asymptotic value is slightly different from $\frac{1}{2}$ is due to the fact that the critical value for $D_B(T)$ is slightly larger than 4.)

We now focus exclusively on the lattice case. Figure 2 provides a summary of our results at two representative electron densities. Panels (a-c) are characteristic of low electron density $n = 0.3$. As shown from (a), at weak to intermediate couplings, $T_{BKT}$ has a dome shape followed by a long slow tail. In (b), we see that this is driven by a competition between an increase in the density of Cooper pairs $n_B$ (which saturates to $n/2$ above $g_c$) and an even stronger increase in the mass $M_B$. Here the critical coupling $g_c$ is associated with the point where $\mu$ changes sign, as depicted in panel (c). For strong coupling $g > g_c$, the normal state purely consists of bosonic pairs without any unbound electrons, and the pair mass scales linearly with $g$. This gives rise to the expected asymptotic tail in $T_{BKT} \propto t^2/g$. We emphasize here that the dome at intermediate couplings is not determined by the $t^2/g$ asymptotics seen in strong coupling. For completeness, in Fig 2(a) we also present the temperature $T^*$ where the pseudogap sets in. Over most of the BKT dome, the magnitude of the gap $\Delta(T_{BKT})$ at the transition temperature is essentially unchanged from its zero-temperature value.

Panels (d-f) are representative results for high electron densities (here we use $n = 0.7$ for illustrative purposes). Just as in the previous case with $n = 0.3$, there is also a superconducting dome in the range of $g/E_F \leq 8$. In addition, the maximal transition temperature $T_{BKT} \sim 0.1 E_F$ in both cases. However, a notable difference is that we do not find the long tail as it is not possible to achieve a purely bosonic regime where all electrons bind into Cooper pairs. This is reflected in the fact that the fermionic chemical potential (panel (f)) never changes sign before $T_{BKT}$ reaches zero. This occurs concurrently with the vanishing of $\frac{1}{\epsilon_B}$, corresponding to Cooper pair localization [33].

The fact that the fermionic regime is so robust at high densities is intimately connected to the (near-) particle-hole symmetry of the underlying lattice Hamiltonian. In a bipartite lattice at exactly at half-filling, the fermionic chemical potential is pinned at $\mu = 0$ regardless of the interaction strength, and as a result a purely bosonic regime can never be achieved.

Interestingly, within our approach, we observe re-entrant superconductivity in a narrow range of intermediate electron densities around $n = 0.55$. Here in addition to the dome for $g < g_c$, there is a strong coupling tail with $t^2/g$ asymptotic behavior that sets in at a slightly larger $g$ [34].

We can compare to earlier Quantum Monte Carlo data on...
the attractive Hubbard model at \( n = 0.7 \) [15]. There it was found that the BKT transition temperature reaches a maximum of about 0.15\( T_c \) which occurs at \( g = 5t \), as compared with the maximum we find of 0.3\( T_c \) which occurs at \( g \approx 7t \). The Monte Carlo data do not extend beyond \( g = 8t \). It is likely that the self-energy based approximation [25, 29] we make as shown in Eq. [4] leads to an over estimate of particle-hole symmetry and may be in part responsible for the differences from Monte Carlo data. Also important may be short-ranged charge density wave fluctuations which are neglected in the present study.

**Conclusions-** We turn finally to Table I for a more quantitative understanding of the various energy and length scales in the intermediate coupling regime, where for a given ratio of \( T_{\text{BKT}}/T_c \), there are two possible values of the coupling strength \( g/E_F \). For concreteness we choose the ratio to be 0.06, motivated by estimates made for twisted bilayer graphene (TBG) [1]. However, it should be acknowledged that our calculation was performed for an attractive 2D Hubbard model, and not directly applicable to TBG. Nonetheless, as in more conventional BCS theory, once one knows the transition temperature a number of additional properties can be quantified regardless of the underlying microscopic details.

Of particular interest are the size of the pseudogap \( \Delta \) at the transition in comparison to \( T_{\text{BKT}} \), the size of the Cooper pairs [35], and the bare coherence length \( \xi_0 = 1/\sqrt{2}M_F T_{\text{BKT}} \) for each case [36]. The lower of the two \( g \) values appears most reasonable physically when compared to estimates in TBG [37]. In both cases the amplitude of \( \Delta \) is relatively the same at \( T_{\text{BKT}} \) and \( T = 0 \); notably, for the smaller \( g \), the chemical potential is close to \( E_F \), so that the system is far from BEC.

A central message of this paper is that when the BKT transition temperature is large, say of the order of 0.06\( E_F \), we have shown that this corresponds to a strongly correlated superconductor and is always accompanied by substantial pseudogap effects.

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**TABLE I.** Estimates of dimensionless physical quantities near the value \( T_c/E_F \approx 0.06 \) based on our calculations for \( n = 0.3 \). Here the two length scales are in units of the lattice constant.

| \( g/E_F \) | \( \Delta(T_{\text{BKT}})/T_{\text{BKT}} \) | pair size | \( \xi_0 \) |
|------------|---------------------------------|----------|--------|
| 1.62       | 2.21                            | 2.14     | 12.44  |
| 5.03       | 26.51                           | 0.22     | 1.85   |

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