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DOI
10.1103/PhysRevLett.105.215302
Publication date
2010
Document Version
Final published version
Published in
Physical Review Letters

Link to publication

Citation for published version (APA):
Pikovski, A., Klawunn, M., Shlyapnikov, G. V., & Santos, L. (2010). Interlayer superfluidity in bilayer systems of fermionic polar molecules. *Physical Review Letters*, *105*(21), 215302. https://doi.org/10.1103/PhysRevLett.105.215302

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Interlayer Superfluidity in Bilayer Systems of Fermionic Polar Molecules

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(Received 24 August 2010; revised manuscript received 12 October 2010; published 17 November 2010)

We consider fermionic polar molecules in a bilayer geometry where they are oriented perpendicularly to the layers, which permits both low inelastic losses and superfluid pairing. The dipole-dipole interaction between molecules of different layers leads to the emergence of interlayer superfluids. The superfluid regimes range from BCS-like fermionic superfluidity with a high T_c to Bose-Einstein (quasi-) condensation of interlayer dimers, thus exhibiting a peculiar BCS–Bose-Einstein condensation crossover. We show that one can cover the entire crossover regime under current experimental conditions.

DOI: 10.1103/PhysRevLett.105.215302 PACS numbers: 67.85.−d, 03.75.Ss, 74.78.−w

Ultracold gases of dipolar particles attract great interest because the dipole-dipole interaction drastically changes the nature of quantum degenerate regimes compared to ordinary short-range interacting gases [1,2]. This has been demonstrated in experiments with a Bose-Einstein condensation (BEC) of chromium atoms which have a magnetic moment of $6\mu_B$ equivalent to an electric dipole moment of 0.05 D [3–5]. The recent experiments on creating polar molecules in the ground ro-vibrational state [6,7] and cooling them towards quantum degeneracy [6] have made a breakthrough in the field. For such molecules polarized by an electric field the dipole-dipole interaction is several orders of magnitude larger than for atomic magnetic dipoles. This opens fascinating prospects for the observation of new quantum phases [1,2,8–12]. The main obstacle is the decay of the system due to ultracold chemical reactions, such as $\mathrm{KRb} + \mathrm{KRb} \Rightarrow \mathrm{K}_2 + \mathrm{Rb}_2$ found in recent experiments [13]. These reactions are expected to be suppressed by the intermolecular repulsion in 2D geometries where the molecules are oriented perpendicularly to the plane of their translational motion [14].

In this Letter we consider fermionic polar molecules in a bilayer geometry where the dipoles are oriented perpendicularly to the layers [Fig. 1], which leads to low inelastic losses and allows for the possibility of superfluid pairing. The interaction between dipoles of different layers may lead to the emergence of an interlayer superfluid, that is a superfluid 2D gas where Cooper pairs are formed by fermionic molecules of different layers. We show that the interlayer dipole-dipole interaction provides a higher superfluid transition temperature than that for 2D spin-1/2 fermions with attractive short-range interaction.

Interestingly, an increase in the interlayer dipole-dipole coupling leads to a novel BCS-BEC crossover resembling that studied for atomic fermions near a Feshbach resonance [15,16]. The reason is that two dipoles belonging to different layers can always form a bound state [17]. As long as the binding energy ϵ_b is much smaller than the Fermi energy E_F, or equivalently the size of the interlayer two-body bound state greatly exceeds the intermolecular spacing in the $\{x, y\}$ plane, the ground state of the system is the BCS-paired interlayer superfluid. Once a reduction of the interlayer spacing λ or an increase of the molecular dipole moment d by an electric field make $\epsilon_b \gg E_F$, dipolar fermions of different layers form true bound states in real space and the ground state is a Bose-condensed system of these composite bosons. We describe this peculiar BCS-BEC crossover and show that interlayer superfluids may be observed for typical parameters of ongoing experiments. Strictly speaking, at a finite temperature T in the thermodynamic limit this is a crossover from a BCS-paired algebraic superfluid to an algebraic bosonic superfluid (quasi-BEC) of dimers. However, we keep the term BCS-BEC crossover for brevity .

We consider the bilayer system of Fig. 1, assuming no interlayer hopping. The interaction potential between two dipoles belonging to different layers has the form

$$V(r) = d^2 \frac{r^2 - 2\lambda^2}{(r^2 + \lambda^2)^{5/2}}, \tag{1}$$

where r is the in-plane separation between these dipoles. The potential $V(r)$ is attractive for $r < \sqrt{2}\lambda$, and repulsive at larger distances r. It satisfies the relation

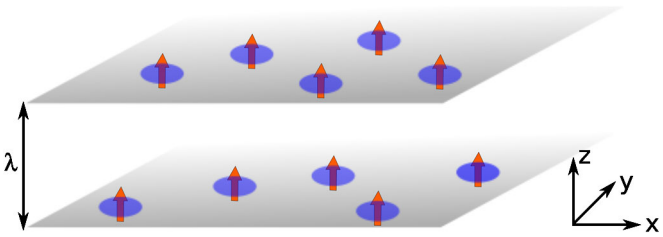

FIG. 1 (color online). Bilayer dipolar system under consideration.

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$$\int V(r)d^2r = 0, \tag{2}$$

which precludes the ordinary method of finding a bound state in 2D potentials finite at the origin [18]. However, it has been proven that $V(r)$ always has a bound state [17], at any dimensionless strength $\beta = r_*/\lambda$, with $r_* = md^2/\hbar^2$ being the dipole-dipole length. For $\beta \ll 1$ the binding energy is exponentially small [19],

$$\epsilon_b \simeq E_0 \exp[-8(1-\beta)/\beta^2 - (5 + 2\gamma - 2\ln 2)], \tag{3}$$

where $E_0 = \hbar^2/m\lambda^2$, and $\gamma = 0.5772$ is the Euler constant. One finds numerically that Eq. (3) is valid up to $\beta \simeq 1$. Note that the unusual dependence on the interaction, $\epsilon_b \sim \exp(-8/\beta^2)$, is a consequence of Eq. (2).

Dipoles of different layers undergo the 2D s-wave scattering from each other in the interlayer potential $V(r)$. We define the off-shell scattering amplitude as

$$f(\mathbf{k}, \mathbf{k}') = (m/\hbar^2) \int \exp(-i\mathbf{k}'\mathbf{r}) V(r) \psi_{\mathbf{k}}(\mathbf{r}) d^2r, \tag{4}$$

where $\psi_{\mathbf{k}}(\mathbf{r})$ is the true wave function of the relative motion with momentum $\mathbf{k}$. The potential $V(r)$ shows a slow power law decay $\sim 1/r^3$ at large distances r. Therefore, at low relative momenta $k \ll r_*^{-1}$, λ^{-1} and $k' \ll r_*^{-1}$, λ^{-1} one has two contributions to the scattering amplitude: the contribution from short distances and the so-called anomalous contribution from distances $r \sim 1/k$ [18] obtained using a perturbative approach in $V(r)$. The leading short-range and anomalous contributions yield the following s-wave part of $f(\mathbf{k}, \mathbf{k}')$:

$$f(k, k') = \frac{2\pi}{\ln(\kappa/k) + i\pi/2} - 2\pi k r_* F_1\left(\frac{k'}{k}\right), \tag{5}$$

omitting higher order terms. The short-range (logarithmic) contribution is obtained by putting $k' = 0$ and proceeding along the lines of the 2D scattering theory [18]. The k dependence of the s-wave part of $\psi_{\mathbf{k}}$ at distances in the interval r_*, $\lambda \ll r \ll k^{-1}$ is given by a factor $[\ln(\kappa/k) + i\pi/2]^{-1}$, where κ depends on the behavior of $V(r)$ at small r and in the presence of the weakly bound state we have $\kappa = \sqrt{m\epsilon_b}/\hbar$ [18]. The anomalous term comes from distances where the motion is almost free. We then have $F_1(x) = (x^2/2)F(1/2, 1/2, 2, x^2) + F(1/2, -1/2, 1, x^2)$, where F is the hypegeometrical function, so $F_1(1) = 4/\pi$. This is valid for $k' < k$; for $k' > k$ one should interchange k' and k. A detailed derivation of $f(k, k')$, including k^2 terms, will be given elsewhere.

The anomalous term in Eq. (5) corresponds to attraction and so does the logarithmic term if $\kappa \ll k$, i.e., if the collision energy is much larger than ϵ_b. Thus, both the short-range and anomalous contribution may lead to superfluid interlayer pairing. Note that for short-range potentials, like all interatomic potentials decaying as $1/r^6$, only the logarithmic term is present in Eq. (5). We will show that the anomalous scattering drastically influences the superfluid pairing. The inlayer dipole-dipole interaction is repulsive and it simply renormalizes the chemical potential. This is valid as long as the inlayer repulsion is sufficiently weak to exclude crystallization [10,11].

Treating molecules of the first and second layers as spin-up and spin-down fermions, our problem is mapped onto spin-1/2 fermions with a peculiar interaction potential. For a weak interlayer attractive interaction we use the BCS approach and obtain the standard gap equation for the momentum-space order parameter,

$$\Delta(\mathbf{k}) = -\int \frac{dk'^2}{(2\pi)^2} \frac{V(\mathbf{k} - \mathbf{k}')\Delta(\mathbf{k}')}{2\epsilon_{k'}} \tanh\left(\frac{\epsilon_{k'}}{2T}\right), \tag{6}$$

where $\epsilon_k = \sqrt{(E_k - \mu)^2 + |\Delta(k)|^2}$ is the gapped dispersion relation, μ is the chemical potential, and $E_k = \hbar^2k^2/2m$. We rewrite Eq. (6) expressing the Fourier component of the interaction potential, $V(\mathbf{k} - \mathbf{k}')$, through the off-shell scattering amplitude [20]. Assuming that the s-wave interaction is the leading channel of superfluid pairing the renormalized gap equation reads

$$\Delta(k) = -\frac{\hbar^2}{2m} \int \frac{d^2k'}{(2\pi)^2} f(k, k')\Delta(k') \times \left\{\frac{\tanh(\epsilon_{k'}/2T)}{\epsilon_{k'}} - \frac{1}{E_{k'} - E_k - i0}\right\}. \tag{7}$$

As long as the interaction is really weak and $\mu \simeq E_F$ [21], Eq. (7) may be employed for calculating $\Delta(k)$ and the superfluid transition temperature. As known, in 2D the transition from the normal to superfluid state is of the Kosterlitz-Thouless type. However, in the BCS limit the Kosterlitz-Thouless transition temperature is very close to the critical temperature T_c given by the BCS gap equation [22]. Using Eq. (7) we obtain the relation between T_c and the order parameter on the Fermi surface at $T = 0$, $\Delta_0(k_F)$, which is the same as in 3D [23]

$$T_c = (e^\gamma/\pi)\Delta_0(k_F). \tag{8}$$

When the short-range logarithmic contribution to Eq. (5) dominates, the anomalous term can be omitted. This is, in particular, the case for β approaching unity and sufficiently small values of $k_F\lambda$. Then, using Eq. (7) we recover the well-known results [22,24]:

$$\Delta_0(k_F) = \sqrt{2E_F\epsilon_b}; \qquad T_c = (e^\gamma/\pi)\sqrt{2E_F\epsilon_b}. \tag{9}$$

Note that we do not include here the second order Gor'kov–Melik-Barkhudarov corrections. They decrease both $\Delta_0(k_F)$ and T_c by a factor of e [25], but Eq. (8) remains valid. A detailed analysis of the BCS limit up to the second order will be given elsewhere.

For $\beta < 1$ the anomalous scattering dominates, at least for not very low k_F. Then the logarithmic term in Eq. (5) reduces to $-\pi\beta^2/2$, and it is necessary to include quadratic terms in k. In this case the scattering amplitude can be calculated using the second order Born approximation.

The expression for the off-shell amplitude is cumbersome. The on-shell amplitude is $f(k, k) = f'/(1 + if'/4)$, where $f'(k)$ is real and given by

$$f' = -8kr_* + \frac{4\pi(kr_*)^2}{\beta} - \frac{\pi\beta^2}{2} + 3\pi(kr_*)^2 \times \ln\left[\frac{k\lambda}{2} e^{\gamma+(23/12)}\right], \quad (10)$$

where the first term is dominant and it follows from the second term in Eq. (5) at $k' = k$.

We now use Eq. (7) to calculate T_c. For $T \to T_c$, we set $\Delta(k') = 0$ in the dispersion relation which becomes $\epsilon_{k'} = |E_{k'} - E_F|$. The main contribution to the integral over dk' comes from the region near the Fermi surface, where we put $k' = k_F$ in the arguments of Δ and f, and taking $k = k_F$ use $f(k_F, k_F)$ from Eq. (10). For the rest of the integration it is sufficient to use $f(k_F, k')$ given by the second term of Eq. (5) and employ the relation $\Delta(k) \simeq \Delta(k_F) f(k, k_F)/f(k_F, k_F)$ following from Eq. (7). After a straightforward algebra we then find

$$T_c = 0.1E_F \left(\frac{E_0}{E_F}\right)^{0.46} \exp\left\{-\frac{\pi}{4k_F r_*} G(k_F\lambda, \beta)\right\}, \quad (11)$$

where $G(x, y) = (1 - \pi x/2 + \pi y/16x)^{-1}$. The validity of Eq. (11) requires $1 \gg k_F\lambda \gg \pi\beta/16$. One easily checks that Eq. (11) gives a significantly higher T_c than that given by Eq. (9). The numerical solution of Eq. (7) also confirms this conclusion for $k_F\lambda$ approaching unity. Figure 2 shows that T_c strongly departs from Eq. (9) for small β, an anomalous behavior stemming from the long-range character of the interlayer interaction.

For sufficiently strong interactions μ deviates from E_F, and Eq. (7) should be complemented by the number equation [26,27] for the 2D density n in one layer

$$n = \frac{1}{2}\int \frac{d^2k}{(2\pi)^2}\left\{1 - \frac{E_k - \mu}{\epsilon_k} \tanh\left(\frac{\epsilon_k}{2T}\right)\right\}. \quad (12)$$

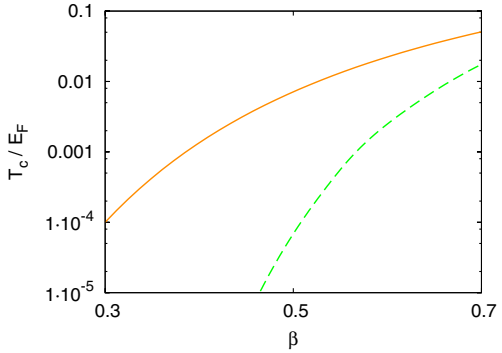

FIG. 2 (color online). Critical temperature T_c as a function of the dipole-dipole strength β for $k_F\lambda = 0.5$. The numerical solution (solid) is higher by at least an order of magnitude than the result of Eq. (9) (dashed).

We found numerically μ and $\Delta(k)$ from the self-consistent solution of Eqs. (7) and (12). Alternatively, we used Eq. (6) together with (12), which is adequate since the potential $V(r)$ is finite and strongly bounded at small r.

This approach provides a qualitative description of the strongly interacting regime [26,27]. An increase of ϵ_b by, e.g., increasing β leads to bound interlayer dimers when ϵ_b becomes much larger than E_F and the chemical potential for the fermionic molecules is $\mu \simeq -\epsilon_b/2$, in contrast to $\mu \simeq E_F$ in the BCS regime. These composite bosons condense and we thus have a BCS-BEC crossover. An approximate crossover line is marked by the condition $\mu = 0$ [27] [Fig. 3]. At sufficiently low T, well above this line a dimer (quasi)-BEC occurs, whereas well below the line the system is a Fermi gas which is superfluid or normal, depending on T and density [Fig. 3].

For strong interactions, T_c calculated from Eqs. (7) and (12) cannot be interpreted as the critical temperature for the onset of superfluidity. Instead, it corresponds to the temperature of pair dissociation [28]. The temperature of the Kosterlitz-Thouless transition, T_{KT}, below which the system is superfluid, satisfies the equation [29]

$$T_{\mathrm{KT}} = \pi\hbar^2\rho_s(T_{\mathrm{KT}})/2M^2, \quad (13)$$

where $M = 2m$ is the dimer (Cooper-pair) mass, and ρ_s is the superfluid mass density just below T_{KT}, which may be determined from our mean-field equations using the known expression for the normal density [23]. In Fig. 4 we depict T_{KT} and T_c versus β for $k_F\lambda = 0.5$. In the BCS regime we retrieve $T_{\mathrm{KT}} \approx T_c$ and see that the ratio T_c/E_F can reach 0.04. For strong interactions where $\Delta(k_F)$ is a sizable fraction of E_F we obtain $T_{\mathrm{KT}} = 0.125E_F$ (cf. [30]). In the intermediate regime T_{KT} interpolates smoothly between these limits [see Fig. 4]. On the BEC side of the crossover we take into account a noticeable normal fraction, which makes T_{KT} lower. We obtain that $T_{\mathrm{KT}} \simeq 0.1E_F$ for $\beta \simeq 2.2$ and very slowly decreases with increasing β (decreasing the interaction), in agreement with the result for bosons [31].

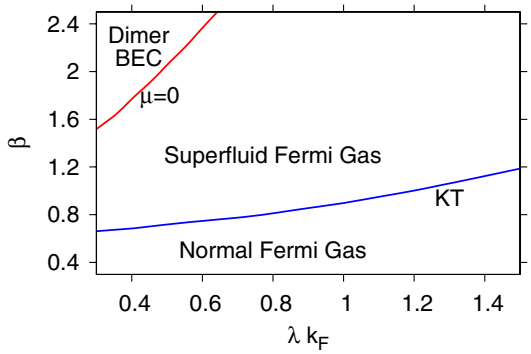

FIG. 3 (color online). Phase diagram for $T = 0.05E_F$, obtained from Eqs. (7) and (12). The curves indicate the Kosterlitz-Thouless (KT) transition and the $\mu = 0$ line.

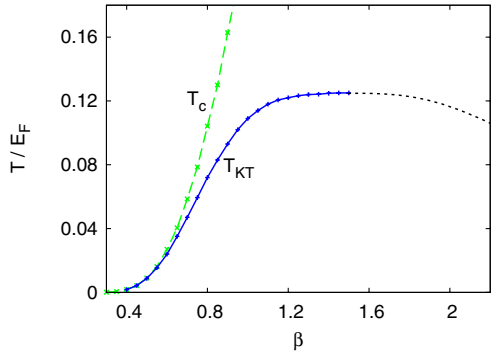

FIG. 4 (color online). Kosterlitz-Thouless transition temperature T_{KT} and the critical BCS temperature T_c versus the dipole-dipole strength β for $k_F\lambda = 0.5$.

In conclusion, we have shown that bilayer systems of fermionic polar molecules which are expected to have low inelastic losses, at the same time may allow the observation of interesting regimes of interlayer superfluidity. These regimes range from fermionic BCS-like superfluidity with a relatively high T_c and Cooper pairs formed by molecules of different layers, to quasi-BEC of interlayer dimers, thus exhibiting a peculiar BCS-BEC crossover. For example, by making the interlayer spacing $\lambda \simeq 250$ nm one achieves $k_F\lambda \simeq 2$ for KRb and LiCs molecules at densities $n \simeq 5 \times 10^8$ cm^{-2} corresponding to $E_F \simeq 110$ nK. Then, varying the LiCs dipole moment d from 0.35 to 1.3 D by increasing the electric field to about 1 kV/cm, one obtains β ranging from 1 to 14 and covers the entire crossover regime, with T_{KT} of a few nanokelvin. For KRb molecules the strongly interacting regime can be reached for the presently achieved $d \simeq 0.2$ D [14] by putting a shallow in-plane optical lattice and getting $\beta > 1$ due to an increase in the effective mass of molecules.

Our results open exciting perspectives for future studies. Imbalanced Fermi mixtures may be studied by preparing layers with different chemical potentials (effective magnetic field) or with different densities. An increase in the dipole-dipole interaction may lead to in-plane Wigner-like dimer crystallization, and perhaps opens routes towards a supersolid dimer gas.

We are grateful to T. Vekua and D. Jin for helpful discussions. A. P. was supported by the DFG (QUEST Cluster). We acknowledge support from the ESF (EuroQuasar and EuroQuam programs). G. S. acknowledges support from the IFRAF Institute, from ANR (Grant No. 08-BLAN0165), and from the Dutch Foundation FOM.

Note added.—After the completion of this work, we learned of a recent related work of Potter *et al.* [32], where interlayer dimerization and superfluidity in multistacks of polar Fermi molecules have been considered.

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