Stable Topological Superfluid Phase of Ultracold Polar Fermionic Molecules

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We show that single-component fermionic polar molecules confined to a 2D geometry and dressed by a microwave field may acquire an attractive $1/r^3$ dipole-dipole interaction leading to superfluid p-wave pairing at sufficiently low temperatures even in the BCS regime. The emerging state is the topological $p_x + ip_y$ phase promising for topologically protected quantum information processing. The main decay channel is via collisional transitions to dressed states with lower energies and is rather slow, setting a lifetime of the order of seconds at 2D densities $\sim 10^8$ cm^{-2}.

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Remarkable progress in the studies of ultracold atomic Fermi gases [1,2] has opened up prospects for creating novel phases of fermionic atoms. Of particular interest is the topological superfluid $p_x + ip_y$ phase for identical fermions in two dimensions (2D) [3], discussed in the contexts of superfluid ^{3}He and the fractional quantum Hall effect [4,5]. The intense interest arises from the exotic topological properties of the phase at positive chemical potential $\mu > 0$ (i.e., in the BCS regime). In the presence of vortices, the ground state becomes highly degenerate, spanned by zero-energy Majorana modes on the vortex cores [5,6]. The highly nonlocal character of these states is expected to suppress decoherence processes and allow this degenerate subspace to be used for topologically protected quantum information processing [7].

The $p_x + ip_y$ topological phase has been predicted to be the ground state of ultracold fermionic atoms interacting via a p-wave Feshbach resonance [3]. However, the realization of the $p_x + ip_y$ phase in this way encounters serious difficulties. Away from a Feshbach resonance, the superfluid transition temperature is vanishingly low. While it may be increased on approach to the resonance, in this case the system becomes collisionally unstable. Fermions form long-lived diatomic quasibound states and their collisions with the atoms cause relaxation into deep molecular states, leading to a rapid decay of the gas [8,9].

In this Letter, we show that a stable topological $p_x + ip_y$ phase can be created with fermionic polar molecules with large dipole moment. Ultracold clouds of polar molecules in the ground rovibrational state have been obtained in recent successful experiments [10,11]. Fermionic ^{40}K^{87}Rb molecules [10] have a permanent dipole moment $d \simeq 0.6$ D, and the dipole moment of ^{6}Li^{133}Cs fermionic molecules should be close to 6 D, the same as for the created bosonic molecules ^{7}Li^{133}Cs [11]. Being electrically polarized, such molecules interact via long-range anisotropic dipole-dipole forces, which has crucial consequences for the nature of quantum degenerate regimes. In particular, this provides the possibility of superfluid pairing at sufficiently low temperatures in a single-component Fermi gas. In 3D, the ground state of a gas of fermions with dipole moments aligned in the z direction has a pairing function which vanishes for $p_z = 0$ [12]. The 2D Fermi gas of canted dipoles has a ground state with a pairing symmetry of a similar form [13]. In both cases, the presence of nodes in the order parameter makes these phases distinct from the $p_x + ip_y$ topological phase. Our route to a stable $p_x + ip_y$ phase is somewhat simpler than other approaches [14].

Our idea is to use polar molecules confined to a 2D geometry and dressed by a microwave (MW) field which is nearly resonant with the transition between the lowest and the first excited rotational molecular levels. As we describe below, the dressed polar molecules acquire an attractive $1/r^3$ dipole-dipole interaction, which leads to superfluid pairing of $p_x + ip_y$ symmetry. Staying in the BCS limit, the superfluid transition temperature can be made sufficiently large and decay processes sufficiently slow to allow realization of this phase in experiment. The effects of MW dressing of polar molecules have been considered as a way to tune the intermolecular potential [15] and to form a repulsive shield for suppressing inelastic losses [16]. The possibility of attractive interactions, which we consider here, has very important consequences for the nature of the phases that can arise and for the stability.

We consider a gas of fermionic polar molecules that are tightly confined in one (z) direction and assume that the confinement length l_z still greatly exceeds the size of a molecule. Then the translational motion of the molecules is 2D, but rotational eigenstates $|J, M_J\rangle$ are those of the 3D molecule. The operator of the dipole moment $\hat{\boldsymbol{d}}$ can have nonzero matrix elements only between states with different rotational quantum numbers J. The transition dipole moment for $J = 0 \rightarrow J = 1$ is $d_t = |\langle 0, 0|\hat{\boldsymbol{d}}|1, M_J\rangle| = d/\sqrt{3}$, with $M_J = 0, \pm 1$ and d the permanent dipole moment of the molecule.

We then apply a circularly polarized MW field that propagates in the z direction and has a frequency ω close

to the frequency ω_0 of the transition between the states $|0,0\rangle$ and $|1,1\rangle$. If the Rabi frequency $\Omega_R \equiv d_t E/\hbar$ and the detuning $\delta \equiv \omega - \omega_0$ satisfy the inequality $|\delta|,\ \Omega_R \ll \omega_0$, then the rotating wave approximation is valid and the MW electric field $\boldsymbol{E}(t)$ couples only the states $|0,0\rangle$ and $|1,1\rangle$. The resulting states may be represented in the dressed-molecule picture, with wave functions [17]

$$|+\rangle = a|0,0;N\rangle + be^{-i\omega t}|1,1;N-1\rangle, \quad (1)$$

$$|-\rangle = b|0,0;N\rangle - ae^{-i\omega t}|1,1;N-1\rangle, \quad (2)$$

where N labels the number of photons in the field, and $a = -A/\sqrt{A^2+\Omega_R^2}$, $b = \Omega_R/\sqrt{\Omega_R^2+A^2}$, and $A = (\delta + \sqrt{\delta^2+4\Omega_R^2})/2$. We will consider $\delta \gtrsim \Omega_R$ and choose $\delta > 0$ such that the energy of the state $|+\rangle$ lies *above* the energies of $|-\rangle$ and $|1,-1\rangle$. If the MW field is ramped on adiabatically, then the ground state $|0,0\rangle$ evolves into the state $|+\rangle$, and all molecules can be prepared in this state. As described below, relaxation to the lower energy states, $|-\rangle$ and $|1,-1\rangle$, can be very slow.

We derive the interaction potential between two molecules within the Born-Oppenheimer approximation, in which the molecules are assumed to be at fixed locations with a separation $\boldsymbol{r} = r(\cos\phi, \sin\phi)$. At large separations, the molecules are both in the state $|+\rangle$. Each molecule has an effective electric dipole moment $d_{\rm eff} = -\sqrt{2}abd_t$, which rotates in the plane of translational motion: $\langle+|\hat{\boldsymbol{d}}|+\rangle = d_{\rm eff}(\cos\omega t, \sin\omega t, 0)$. The interaction potential at large distances is then

$$V(r) = \frac{\boldsymbol{d}_1\boldsymbol{d}_2 - 3(\boldsymbol{d}_1\hat{r})(\boldsymbol{d}_2\hat{r})}{r^3} = \frac{d_{\rm eff}^2}{r^3}[1-3\cos^2(\omega t-\phi)]. \quad (3)$$

Thus, the *time-averaged* interaction is attractive,

$$V_0(r\to\infty) = -d_{\rm eff}^2/2r^3, \quad (4)$$

and characterized by the length scale $r^* \equiv Md_{\rm eff}^2/2\hbar^2$, where M is the mass of a molecule. The quantity r^* is defined analogously to the van der Waals length for atoms and is a measure of the radius of the centrifugal barrier experienced by the (fermionic) molecules.

At smaller separations, the dipolar interactions between the molecules cause them to depart from the state $|+\rangle$. This occurs when the characteristic interaction energy d_t^2/r^3 becomes larger than the detuning $\hbar|\delta|$, setting a new length scale $r_\delta \equiv [d_t^2/(\hbar|\delta|)]^{1/3}$. We have found the resulting Born-Oppenheimer surfaces using a full coupled channel calculation containing all of the levels $|J, M_J; N\rangle$. Similar calculations are described in Refs. [15,16]. We choose a positive detuning $\delta > 0$ and assume that the length scale of the potential, r_δ, is larger than the confinement length l_z so that the interaction is 2D. The potential energy curves of even parity are illustrated in Fig. 1, showing a potential $V_0(r)$ that has a repulsive core for $r \lesssim r_\delta$ and is attractive at $r \gtrsim r_\delta$ with a long-range $1/r^3$ tail. As discussed below, the repulsive core prevents low-energy particles from approaching each other at distances $r \lesssim r_\delta$ and suppresses inelastic collisions, including "ultracold chemical reactions" recently observed at JILA for KRb molecules.

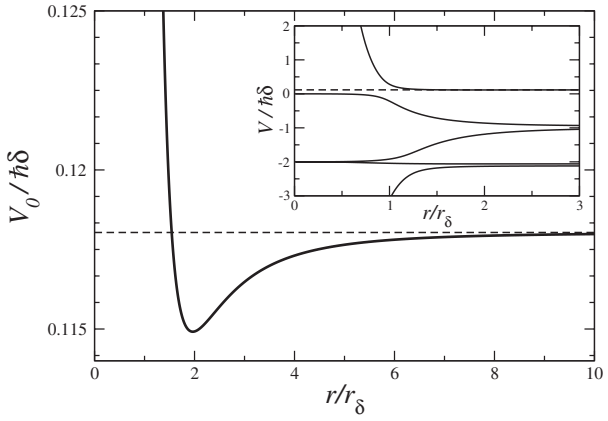

FIG. 1. Potential energy curve $V_0(r)$ for two $|+\rangle$ state molecules, computed for $\Omega_R = 0.25\delta$ (see text). Anticrossings with other field-dressed levels of even parity occur at distances $r \sim r_\delta$, as shown in the inset.

We now analyze the low-temperature phase of a 2D gas of identical fermions interacting via the potential $V_0(r)$, assuming that $r_\delta \ll r^*$. Because of the presence of an attractive $1/r^3$ tail given by Eq. (4), one expects that the Fermi gas is unstable to the formation of a superfluid state. In the ultracold dilute limit, where the momenta of colliding fermionic particles satisfy the inequality $kr^* \ll 1$, this tail provides a contribution $\propto(-kr^*)$ to the scattering amplitude. This is the so-called anomalous contribution coming from distances of the order of the de Broglie wavelength of the particles and obtained in the Born approximation [18]. It greatly exceeds the leading short-range ($r \lesssim r^*$) contribution which is related to the p-wave scattering and is $\propto k^2$ away from p-wave resonances. Thus, omitting second order corrections, a detailed behavior of the potential $V_0(r)$ at distances $r \lesssim r^*$, drops out and the only important length scale is r^*.

In our analysis of the superfluid phase, we confine ourselves to the BCS weak coupling regime, where $k_F r^* \ll 1$ with $k_F = \sqrt{4\pi n}$ being the Fermi momentum and n the gas density. (We consider a uniform 2D gas; the effects of a trap can be included within the local density approximation.) The regularized gap equation is obtained expressing the interaction potential through the zero-energy vertex function $\Gamma(\boldsymbol{k},\boldsymbol{q})$ governed by [19]

$$\Gamma(\boldsymbol{k},\boldsymbol{q}) = V_0(\boldsymbol{k}-\boldsymbol{q}) - \int \frac{d^2\boldsymbol{q}'}{(2\pi)^2}\frac{\Gamma(\boldsymbol{k},\boldsymbol{q}')V_0(\boldsymbol{q}-\boldsymbol{q}')}{E_{q'}}, \quad (5)$$

with $E_q = \hbar^2q^2/2M$ and $V_0(\boldsymbol{q})$ being the Fourier transform of $V_0(\boldsymbol{r})$. The gap equation then reads [2,20,21]:

$$\Delta_{\boldsymbol{k}} = -\int \frac{d^2\boldsymbol{q}}{(2\pi)^2}\Gamma(\boldsymbol{k},\boldsymbol{q})\frac{\Delta_q}{2}\left[\frac{\tanh(\epsilon_q/2T)}{\epsilon_q} - \frac{1}{E_q}\right], \quad (6)$$

where $\epsilon_q = \sqrt{(E_q-\mu)^2 + |\Delta_q|^2}$ is the energy of single-

particle excitations and $\mu > 0$ is the chemical potential which is equal to the Fermi energy $E_F = \hbar^2 k_F^2/2M$. To first order, we replace $\Gamma(\boldsymbol{k}, \boldsymbol{q})$ in Eq. (6) with $V_0(\boldsymbol{k} - \boldsymbol{q})$. At $T = 0$, we put $\tanh(\epsilon_{\boldsymbol{q}}/2T) = 1$ and perform an analytical analysis assuming that in the weak coupling limit the main contribution to the integral in Eq. (6) comes from momenta q close to k_F. It shows that the dominant pairing instability is in the channel with orbital angular momentum $l = 1$. The most stable low-temperature phase has $p_x \pm ip_y$ symmetry, following from the fact that this phase fully gaps the Fermi surface, in contrast to competing phases [22]. A full numerical solution of the regularized gap equation confirms this analysis. It further shows that $|\Delta_{\boldsymbol{k}}|$ rises linearly for $k \lesssim k_F$ and approaches a constant $\sim E_F \exp(-3\pi/4k_F r^*)$ for $k \gtrsim k_F$.

In the 2D geometry that we consider, the critical temperature T_c of a Fermi gas is set by the Kosterlitz-Thouless transition. However, in the weak coupling limit, the Kosterlitz-Thouless temperature is very close to T_c obtained in the BCS approach [23]. For $T \to T_c$, we omit $|\Delta_{\boldsymbol{q}}|$ in the expression for $\epsilon_{\boldsymbol{q}}$ in Eq. (6) and obtain

$$T_c \approx E_F \exp(-3\pi/4k_F r^*), \tag{7}$$

where the numerical prefactor is of order of unity [24]. Thus, to obtain an achievable value of T_c, one requires $k_F r^*$ to be not much smaller than unity. The BCS approach assumes that the exponential factor in Eq. (7) is small and $T_c \ll E_F$. A limitation on the strength of the attractive interaction is set by the condition of stability to phase separation (collapse to a high-density gas). A full calculation of this limit requires a strong-coupling theory. However, estimates (provided by Hartree-Fock theory) suggest that the compressibility is positive for $k_F r^* < 3.7$. Thus, the regime of moderately strong interactions $k_F r^* \sim 1$ is accessible.

The $p_x + ip_y$ phase spontaneously breaks time-reversal invariance (the phase $p_x - ip_y$ is its degenerate time-reversed partner) [25]. It can be viewed as a state in which the Cooper pairs have an orbital angular momentum of $\hbar$ with respect to the z axis. The $p_x + ip_y$ phase can exist in one of two topologically distinct phases, depending on the sign of the chemical potential [4]. The phase at $\mu < 0$ may be continuously deformed to the vacuum state; the phase at $\mu > 0$ is topologically distinct from the vacuum and has several very interesting properties. Most notably, the vortices of this phase carry localized zero-energy states, described by a Majorana fermion on each vortex core. These lead to non-Abelian exchange statistics [5,6] and possible applications for topologically protected quantum information processing [7]. The superfluid of dipolar interacting spinless fermions that we describe above has $\mu > 0$ and is in the relevant topological phase.

The typical interatomic potential between atoms or molecules (without the MW dressing field) has a short range $R_0 \sim 1$–10 nm. Thus, in 2D the scattering phase shift is $\sim(k_F R_0)^2$ so that $T_c \sim E_F \exp[-1/(k_F R_0)^2]$ is vanishingly small. If the interaction strength is tuned close to a Feshbach resonance [3] such that the transition temperature strongly increases, then the particles have a significant probability to be inside of the centrifugal barrier at separations of the order of R_0. Under these conditions, the system is very susceptible to rapid losses arising from collisional relaxation into deep bound states [8,9].

In contrast, for MW dressed molecules interacting via the potential $V_0(r)$, the contribution $k_F r^*$ to the attractive coupling strength provides a significant transition temperature T_c even far from the resonance associated with the presence of a two-molecule bound state. Given that the molecules have a small probability to be at separations $\sim r_\delta$, in this BCS regime one anticipates that the superfluid phase is not susceptible to relaxation losses.

The dominant loss mechanism is from binary inelastic collisions between $|+\rangle$ molecules, in which one or both are transferred to the state $|-\rangle$ or $|1, -1\rangle$, which (since $\delta > 0$) lie lower in energy than $|+\rangle$. For $\Omega_R \lesssim \delta$, the released kinetic energy is $\sim\hbar\delta$ and can cause both molecules to escape from the sample. The kinetic energy release requires a momentum transfer of $\sim\hbar/\lambda_\delta$ with $\lambda_\delta \equiv \sqrt{\hbar/M\delta}$. For $\lambda_\delta/r_\delta \ll 1$, the particles cannot approach each other sufficiently closely to allow the required momentum exchange, and one anticipates a reduction in the loss rate. The same condition can be derived semiclassically as the condition of adiabatic motion in the potential. To go beyond this limit and determine the loss rate for $\lambda_\delta \sim r_\delta$, we have solved the full two-body scattering problem involving states of even parity which, at infinite separation, are $(|+\rangle, |+\rangle)$, $(|+\rangle, |-\rangle)$, $(+\rangle, |1, -1\rangle)$, $(|-\rangle, |-\rangle)$, and $(|-\rangle, |1, -1\rangle)$ [the state $(|1, -1\rangle, |1, -1\rangle)$ is decoupled]. We calculate (numerically) the probabilities P_l that two $|+\rangle$-state molecules with relative angular momentum l are scattered into *any* outgoing channel in which at least one of them is in the state $|-\rangle$ or $|1, -1\rangle$. This corresponds to nonadiabatic transitions from the potential $V_0(r)$ to the other potentials shown in the inset to Fig. 1 [26].

Taking into account that two molecules are lost in each inelastic collision and writing the molecule loss rate as $\dot{n} = -\alpha n^2$, for the 2D inelastic rate constant we obtain $\alpha = 4\hbar/M\sum_l P_l$. For incident energy chosen such that $kR^* \ll 1$, we have $\alpha \propto (kr^*)^2$. The results for this quantity versus r_δ/λ_δ are shown in Fig. 2 for $\Omega/\delta = 0.25$ and $kr^* = 1$. The general trend is a reduction of inelastic losses with increasing r_δ/λ_δ, consistent with the semiclassical expectations. However, in addition there is a dramatic modulation of the inelastic scattering rate, arising from an interference of incoming and outgoing waves in the scattering potential. By tuning to $r_\delta/\lambda_\delta \simeq 10.5$, the rate constant can be suppressed to $\alpha \simeq 4 \times 10^{-4}\hbar/M$.

Thus, at a density $n = (10^8$–$10^9)$ cm^{-2} of, for example, ^{7}Li^{40}K molecules, the lifetime of the gas is $\tau \approx (\alpha n)^{-1} \simeq$ 2–0.2 s. The permanent dipole moment of ^{7}Li^{40}K in the ground state was found to be 3.5 D [27], and for $r_\delta/\lambda_\delta \simeq 10.5$ and $\Omega_R = 0.25\delta$, the length scales are $r_\delta \simeq 30$ nm,

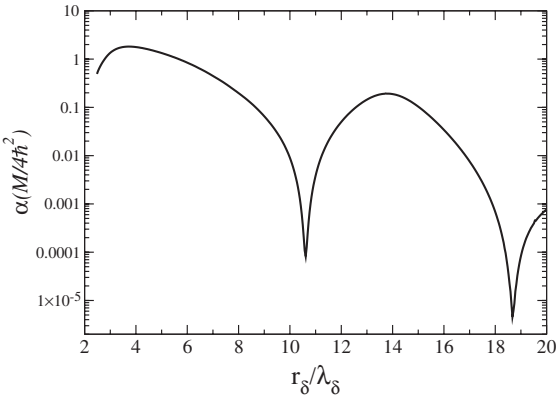

FIG. 2. Inelastic rate constant α as a function of r_δ/λ_δ for $\Omega_R = 0.25\delta$ and $kr^* = 1$ (see text).

$r^* \simeq 200$ nm. For $k_F r^*$ close to unity, we then get $n \simeq 2 \times 10^8$ cm^{-2} and $E_F \simeq 120$ nK so that the transition temperature is $T_c \simeq 10$ nK and the lifetime is ~ 1 s. (For ^{40}K^{87}Rb, the possible r^* is rather small and the high densities required for a sizeable T_c lead to rapid losses. The addition of a shallow optical lattice will increase the effective mass M, allowing $T_c \sim 10$ nK at $n \sim 10^8$ cm^{-2}.)

We should avoid the presence of bound states of two molecules in the potential $V_0(r)$; otherwise, three-body recombination will lead to a rapid decay of the gas on approach to the superfluid transition. A dimensional estimate for the three-body decay rate gives $\tau_{\rm rec}^{-1} \sim (\hbar r^{*2}/M)(k_F r^*)^4 n^2$, which can be large for $k_F r^* \simeq 1$ and reasonable densities. However, for $\Omega_R \simeq 0.25\delta$ (as used above), the potential $V_0(r)$ does not support bound states for $r_\delta/\lambda_\delta \lesssim 14$. Thus, for the considered value $r_\delta/\lambda_\delta \simeq 10.5$, the three-body recombination is absent.

The formation of the $p_x + ip_y$ superfluid phase should be apparent in numerous observables. These include quantities used to detect s-wave pairing in two component Fermi gases, such as the density distribution, collective modes, and rf absorption spectra [1,2]. The most striking new features of the $p_x + ip_y$ superfluid arise in the presence of quantized vortices, which may be generated by rotation of the gas as in usual superfluids. rf absorption will then show evidence for Majorana modes on the vortex cores [28]. Ultimately, one would hope to probe non-Abelian exchange statistics of these vortices [29].

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[26] The outgoing particles are treated as 2D, which is valid both for $\lambda_\delta \gg l_z$ (when the energy release is insufficient to allow occupation of higher subbands) and for $\lambda_\delta \ll l_z$ (when the outgoing particles have a very small angle $\sim \lambda_\delta/l_z$ out of the 2D plane).

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