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Unconventional Superfluidity in Ultracold Dipolar Gases

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Abstract. In this manuscript, we discuss the emergence of *p*-wave superfluidity in a dipolar Fermi gas confined in a double layer array of parallel optical lattices in two dimensions. The dipole moments of the molecules placed at the sites of the optical lattices, separated a distance L and pointing in opposite directions produce an effective attractive interaction among them, except between those dipoles situated one on top of the other. Such interaction between dipoles is precisely the origin of the non-conventional superfluid state. We present the analysis for the ground state of the many-body system within the mean-field scheme. In particular, we study the stable regions, as a function of the system parameters, namely the effective interaction between dipoles and the filling factor n, for which the superfluid state can exist. Following the BKT scheme, we estimate the critical temperature of the superfluid state.

1. Introduction

Several laboratories around the world have gone beyond the realization of quantum degeneracy in ultracold neutral atoms in both bosonic and fermionic species, and, in recent times, macroscopic samples of dipolar gases with large electric dipolar moments in its electronic and vibrational ground states, have been produced. The main motivation behind these efforts is to simulate novel phases of matter such as supersolids and unconventional superfluids as p-wave or d-wave phases among others [1, 2, 3, 4]. In particular, ultracold molecular Fermi gases have attracted the attention of both, theoretical and experimental communities for several years since, because combined with its fermionic nature, the intrinsic long-range character of its dipolar interactions, as well as the possibility of confining such molecules in external potentials, these systems represent suitable candidates to emulate unconventional superfluids. The long-range nature of dipolar interactions gives rise to have contributions of all partial waves at low energies [5, 6, 7, 8], thus enhancing the possibility of generating BCS paring of several types. As previously proposed in Refs. [9, 10], due to the repulsive core between dipoles situated in a bilayer array, the s-wave pairing is suppressed, however, the p-wave or higher partial wave superfluid phases arise in molecules with rotational moments J = 0 and J = 1.

With the purpose of studying p-wave superfluidity, in this manuscript we consider ultracold dipolar Fermi molecules placed in a bilayer array composed of optical lattices in 2D having square symmetry, such that, as schematically depicted in Figure 1, the dipole moments of molecules situated at the lattice sites are oriented in opposite directions. The strong tail-tail repulsion between molecules lying in on-site positions in layers A and B, that is one on top

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of the other, inhibits s-wave pairing, while favoring the formation of Cooper pairs between molecules located at neighboring sites. Superfluidity of molecule paring in such a model can arise as a consequence of the energy saving associated with a reduction of the electrostatic on-site repulsion. In closeness with this aspect of pair formation associated to electrostatic interactions, other systems exhibiting nonconventional superconductivity, and specifically p-wave phases, are the ruthenate composes [11], which as a matter of fact still remain not understood. Particularly the microscopic process responsible for the superconductivity. The main analogy between this kind of superconductors and molecular superfluids here considered is that the frictionless transport of pairs traveling in 2D has the same origin; the strong electrostatic repulsion of fermions situated one on top of each other in different layers together with the long-range attractive interaction of fermions located in other site configurations. Thus, besides the physics of superfluidity that can be addressed, our model can also be used to access the physics of unconventional ruthenate superconductors.

This manuscript is organized as follows. In section 2 we describe our model and present the relevant parameters of our investigation. Then, by adopting the mean-field BCS scheme in section 3 we characterize the unconventional superfluidity. In section 4 we determine the superfluid density tensor with the purpose of establishing the BKT transition temperature, that is to delineate some conclusions regarding the current investigation with experimental systems. Finally, we present our conclusions in section 5.

2. Model

We consider polar Fermi molecules confined in two parallel optical lattices in 2D separated by a distance L. As schematically shown in Figure 1, the layers labeled with letters A and B are the energy landscape where the molecules are confined. The lattices have a square geometry with lattice constant a. The dipoles are oriented perpendicularly to the layers and in opposite directions in different layers. This configuration can be achieved by confined polar molecules with rotational moments J = 0 and J = 1 in layers A and B respectively [10]. Then, by applying an ac electric field, oriented perpendicularly to the lattices, gives rise to having effective dipole moments pointing in opposite directions [12]. In this scenario, the resulting interaction between the molecules in different layers is:

$$V_{dip}(r) = -d^2 \frac{(r^2 - 2L^2)}{(r^2 + L^2)^{5/2}},$$
(1)

where $-d^2$ is the scalar product of the effective dipole moments in the layers, L and r are the inter-layer and intra-layer separations respectively [13]. Molecules are allowed to move through sites in a given layer, but not between different layers.

The aim of this manuscript is to study the emergence of p-wave superfluidity as a consequence of the attractive interaction between dipoles confined in different layers, situated in neighboring positions one respect to the other. From the expression for the interaction potential, equation (1), one can notice that for values of the interlayer separation satisfying the condition $\Lambda = L/a < 0.5$, the effective interaction for particles lying in layers A and B is attractive except for r = 0. In this manuscript, all the numerical calculations were performed with $\Lambda = 0.2$ while the dimensionless dipole-dipole interaction strength $\chi = m_{eff}d^2/a\hbar^2$, with $m_{eff} = \hbar^2/2ta^2$ the effective mass, and the filling factor n of the lattices were allowed to vary within reasonable experimental values.

3. *p*-wave superfluidity

Our starting point is the effective Hamiltonian that represents the dipolar Fermi system described in section 2. To set this model Hamiltonian we should take into account the prescriptions



Figure 1. Schematic representation of the dipolar Fermi gas confined in a bilayer array of parallel optical lattices in two dimensions.

imposed by the two-body physics of particles interacting through the potential (1), lying in a bilayer lattice potential. Namely, the analysis of the microscopic precursors of both, BEC and BCS states that emerge in the lattice bilayer, associated with the attractive dipolar interaction. This study, previously addressed in ref. [14], analyzes the formation of bound molecules and scattered pairs of molecules as a function of the effective interaction strength parameter χ described above. With this information in mind, we are able to establish the many-body Hamiltonian that describes the fermionic system. It reads as follows,

$$H = -J\sum_{\langle \mathbf{i},\mathbf{j}\rangle} (a^{\dagger}_{\mathbf{i}}a_{\mathbf{j}} + b^{\dagger}_{\mathbf{i}}b_{\mathbf{j}} + h.c) + \sum_{\mathbf{i}\neq\mathbf{j}} V_{dip}(\mathbf{i}-\mathbf{j})a^{\dagger}_{\mathbf{i}}b^{\dagger}_{\mathbf{j}}b_{\mathbf{j}}a_{\mathbf{i}} - \mu\sum_{\mathbf{i}} (a^{\dagger}_{\mathbf{i}}a_{\mathbf{i}} + b^{\dagger}_{\mathbf{i}}b_{\mathbf{i}}),$$
(2)

where J is the nearest-neighbor tunneling strength, $a_{\mathbf{i}} (a_{\mathbf{i}}^{\dagger})$ and $b_{\mathbf{i}} (b_{\mathbf{i}}^{\dagger})$ are the operators that annihilate (create) Fermi molecules at site \mathbf{i} in layers A and B respectively, and μ is the chemical potential. Assuming pairing between \mathbf{k} and $-\mathbf{k}$ states, the mean-field Hamiltonian in momentum representation becomes

$$H = \sum_{\mathbf{k}} \xi_{\mathbf{k}} (a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}) + \Delta_{\mathbf{k}}^{*} b_{-\mathbf{k}} a_{\mathbf{k}} + \Delta_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} b_{-\mathbf{k}}^{\dagger}, \qquad (3)$$

here, $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu + nV_{dip}(\mathbf{k} = 0)$ with $\epsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a)$ the kinetic energy dispersion of molecules in the 2D lattice, and $\Delta_{\mathbf{k}}$ is the superfluid order parameter that must be selfconsistently determined,

$$\Delta_{\mathbf{k}} = \frac{1}{\Omega} \sum_{\mathbf{k}'} V_{dip}(\mathbf{k} - \mathbf{k}') \langle b_{-\mathbf{k}'} a_{\mathbf{k}'} \rangle.$$
(4)

The Hamiltonian in equation (3) can be diagonalized by means of a Bogoliubov transformation which leads to the coupled equations for the energy gap $\Delta_{\mathbf{k}}$ and the filling factors n_A and n_B . We should point here that since the system under study is a balanced mixture of particles in layers A and B, we have $n = n_A = n_B$. Thus, instead of having equations for n_A , n_B , and the energy gap $\Delta_{\mathbf{k}}$, the coupled mean field equations are just for $\Delta_{\mathbf{k}}$ and n,

$$\Delta_{\mathbf{k}} = -\frac{1}{\Omega} \sum_{\mathbf{k}'} V_{dip}(\mathbf{k} - \mathbf{k}') \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{\beta E_{\mathbf{k}'}}{2}\right),\tag{5}$$

$$n = n_A = n_B = \frac{1}{2} \left[1 - \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}'}}{2}\right) \right],\tag{6}$$

where the quasiparticle excitation energy is $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$ and $\beta = 1/(k_B T)$, with k_B the Boltzmann constant. In our calculations, we numerically solve self-consistently the gap equation 5 and the number equation 6 as a function of the effective dipole-dipole interaction χ and the filling factor n in a lattice with $\Omega = 121 \times 121$ sites.

3.1. $p_x + ip_y$ paring

At zero temperature, we find a solution for the energy gap $\Delta_{\mathbf{k}}$ that exhibits an antisymmetric behavior, thus resembling the pure l = 1 angular momentum form for the energy gap, that is, $\Delta_{\mathbf{k}} \propto \sin k_x a + i \sin k_y a$. For illustration purposes in Figure 2 we show the obtained gap parameter for a coupling strength $\chi = 0.4$ and a filling factor of n = 0.16. Solid and dashed lines correspond respectively to the real and imaginary parts of $\Delta_{\mathbf{k}}$ plotted as a function of $k_x a$ and $k_y a$. In the upper figure we consider $k_y a = 0$, while in the lower figure its is plotted $\Delta_{\mathbf{k}}$ as a function of $k_x a = 0$.



Figure 2. Gap parameter $\Delta_{\mathbf{k}}$ as a function of \mathbf{k} for a filling factor n = 0.16, an interaction strength $\chi = 0.4$ and a temperature T = 0. Upper and lower panels correspond to $k_y a = 0$ and $k_x a = 0$ respectively.

Also, in order to exhibit the full dependency of the gap parameter $\Delta_{\mathbf{k}}$ as a function of the **k** values in the first Brillouin zone, in Figure 3 we show a density plot of $\Delta_{\mathbf{k}}$ as a function of $k_x a$ and $k_y a$. As can be appreciated from these figures, our model supports a solution characterized by a gap with $p_x + ip_y$ symmetry. As found by [15] the $p_x + ip_y$ solution is the appropriate candidate for the most stable p-wave pairing, in contrast to the p_z symmetry. Moreover, the $p_x + ip_y$ pairing breaks the time-reversal symmetry and can be classified as a class D topological superfluid [16, 17].

A conclusion that we reach directly from our calculations is that the p-wave superfluid becomes unstable towards phase separation when the interaction strength or the filling factor is large enough. To illustrate this behavior in Figure 4 we plot the chemical potential μ as a function of the filling factor n for an interaction strength $\chi = 0.4$ at zero temperature. As one can notice from the curve μ/t vs n, there is a region in which the chemical potential is a monotonically decreasing function of the filling factor. Such a behavior exhibits an inconsistency with the second law of thermodynamics since it that region the compressibility $\kappa = 1/n^2(\partial n/\partial \mu)$ is negative, thus indicating that the $p_x + ip_y$ superfluid state is dynamically unstable. Precisely, **1540** (2020) 012002 doi:10.1088/1742-6596/1540/1/012002



Figure 3. Gap parameter $\Delta_{\mathbf{k}}$ as a function of \mathbf{k} for a filling factor n = 0.16, an interaction strength $\chi = 0.4$, and a temperature T = 0. (a) real part of $\Delta_{\mathbf{k}}$ (b) imaginary part of $\Delta_{\mathbf{k}}$.

the arrows in Figure 4 indicate the range of values of n for which the system is unstable. The phase separation region can be recognized from the Maxwell construction of equal areas, which, due to the particle-hole symmetry, give rise to have phase separation regions symmetric with respect to the half-filling point. In particular, the construction simplifies to determine the filling factor n_1 , which satisfies the following conditions, $\mu(n_1) = \mu(n = 0.5) = \mu(1 - n_1)$. The orange shaded region in Figure 4 indicates the Maxwell construction of equal areas. Solid black lines separate stable and metastable SF phases, that is, within the region labeled PS -phase separation- the system becomes a mixture of SF phases at different densities.



Figure 4. Dimensionless chemical potential as a function of the filling fraction n at zero temperature. Vertical black lines separate stable from metastable p-wave superfluid phases. Arrows indicate the values of the filling fractions associated to unstable superfluids (area inside the arrows).

3.2. Phase diagram

In Figure 5 we summarize the full information obtained in our calculations. In particular, in a T = 0 phase diagram, we show the couples of the effective coupling interaction χ , and the filling factor n, for which a stable superfluid p-wave phase can exist. Also, the values of χ and n associated with superfluid phases composed by a mixture of superfluids at different densities are recognized. In this figure, the stable superfluid phases and those with two definite densities are plotted in blue and beige colors respectively. At a critical interaction of $\chi \approx 0.494$, the phase separation takes place between n = 0 and n = 1. When the interaction is above this critical value the system becomes a mixture of n = 0 and n = 1 densities, and no superfluid phases

occur since the stable states are the zero particle or zero hole densities which are insulating states. On the other hand, when the interaction strength is below the critical value the phase separation region shrinks giving rise to bigger stable superfluid regions.



Figure 5. Phase diagram of the *p*-wave superfluid phases at zero temperature in terms of the dimensionless interaction coupling parameter χ and the filling factor *n*. Beige shaded regions identify stable superfluid phases, while blue surface indicates the values of χ and *n* for which the system becomes phase separated and thus a coexistence of superfluids at two densities.

4. Critical Temperature of the $p_x + ip_y$ superfluid phase

Since the system under study is a quantum fluid confined in the 2D space, the emergence of the p-wave superfluid transition necessarily is of BKT type, that is, the interacting gas become a superfluid via the BKT mechanism [18, 19, 20]. As well established, 2D systems with continuous order parameter indeed exhibit a transition, which is typically captured by the behavior of the density-density correlation function that shows an algebraic dependence instead of the classical exponential decaying associated to systems with no phase transition [18, 19, 20]. As we expose at the end of this section, once that a proper analysis for the superfluid in terms of χ and n is done, we will be able of calculating the value of the critical temperature at which the dipolar Fermi system becomes a BKT superfluid. To determine such a superfluid density, we proceed as delineated in Ref. [21], by performing a gauge transformation on the operators that create and annihilate particles at the lattice sites in both layers,

$$\begin{split} &(a_{\mathbf{i}}^{\dagger},a_{\mathbf{i}}) \rightarrow (a_{\mathbf{i}}^{\dagger}e^{i\Theta\cdot\mathbf{r}_{\mathbf{i}}},a_{\mathbf{i}}e^{-i\Theta\cdot\mathbf{r}_{\mathbf{i}}}) \\ &(b_{\mathbf{i}}^{\dagger},b_{\mathbf{i}}) \rightarrow (b_{\mathbf{i}}^{\dagger}e^{i\Theta\cdot\mathbf{r}_{\mathbf{i}}},b_{\mathbf{i}}e^{-i\Theta\cdot\mathbf{r}_{\mathbf{i}}}), \end{split}$$

being $\Theta = (\Theta_x/(aN_x), \Theta_y/(aN_y))$. Through this procedure, the system becomes composed of a mixture of both, the normal and the superfluid components. Then, the superfluid density can be determined by first constructing the free energy of the system and then, taking the difference between the normal and superfluid free energies as dictated by the following equations,

$$\rho_{\alpha,\alpha'} = \lim_{\Theta \to 0} \frac{1}{\Omega t} \frac{F_{\Theta} - F_0}{\Theta_{\alpha} \Theta_{\alpha'}} = \frac{1}{\Omega t} \frac{\partial^2 F_{\Theta}}{\partial \Theta_{\alpha} \partial \Theta_{\alpha'}}, \ \alpha = \{x, y\}.$$
(7)

The explicit expression for the full free energy F_{Θ} is obtained by expanding it up to second order for the order parameter Δ , and thus incorporating the phase as $\Delta_{\mathbf{i}} = \Delta_0 e^{i\Theta\cdot\mathbf{r}_i}$, being Θ

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a vector with components Θ_x and Θ_y written above. The final expression for the superfluid density tensor is given as follows,

$$\rho_{\alpha,\alpha'} = \frac{1}{a\Omega} \sum_{\mathbf{k}} \left(n(\mathbf{k}) \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_\alpha \partial k_{\alpha'}} - Y(\mathbf{k}) \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_\alpha} \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_{\alpha'}} \right),\tag{8}$$

where $n(\mathbf{k})$ is the Fermi momentum distribution and $Y(\mathbf{k})$ is the Yoshida distribution defined as $Y = \beta sech(\beta E_{\mathbf{k}}/2)/4$. Since the off-diagonal matrix elements of the superfluid tensor are small, the superfluid density can be approximated as $\rho \approx (\rho_{xx} + \rho_{yy})/2$. In order to determine the critical temperature of the superfluid, one has to impose the BKT condition [21, 22, 23]:

$$T_{BKT} = \frac{\pi}{8k_B} \rho(T_{BKT}). \tag{9}$$



Figure 6. Orange solid line is the superfluid density as a function of temperature obtained from BCS mean-field description. The intersection of the blue dashed line and orange curve corresponds to the critical temperature at which BKT transition occurs for an effective dipole-dipole interaction strength $\chi = 0.4$ and a filling factor n = 0.16

In Figure 6 the orange solid line represents the superfluid density as a function of the temperature, obtained from the BCS mean-field scheme. The blue dashed line corresponds to the BKT treatment that behaves linearly with the temperature. We find that the intersection between both curves takes place at $k_B T_{BKT} = 0.0028t$. For dipolar Fermi molecules of NaK [2] confined in an optical lattice having a wavelength of $\lambda = 1064$ nm and a lattice depth of $V_0 = 5E_r$ [24], the predicted critical transition temperature is $T_{BKT} \approx 0.6$ nK. Certainly, such a temperature is up to now not reachable in current experiments with dipolar samples. However, one way in which such a low temperature can be raised is by increasing the interaction strength. This can be accomplished by externally tuning the electric field up to a certain value at which the dipole moment saturates [25]. In Figure 7 we plot the critical temperature as a function of the dimensionless interaction strength χ for both, the BCS scheme and the BKT formalism. Using the above experimental parameters, the predicted critical BKT temperature is $T_{BKT} \approx 10$ nK. Another alternative to achieve higher temperatures is by means of the use of subwavelength lattices [26, 27, 28], where smaller separation of the layers can be achieved. Considering $L \approx 50$ nm, the critical temperature for a Fermi gas of NaLi molecules, under the same condition $V_0 = 5E_r$ is about $T_{BKT} \approx 4$ nK.

5. Conclusions

In this manuscript, we have studied the emergence of unconventional p-wave pairing in a system of dipolar Fermi molecules confined in two parallel optical lattices in 2D. In particular, we

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Figure 7. Curves for the BCS and BKT critical temperatures as a function of the interaction parameter χ , considering a filling factor of n = 0.16.

proposed a model in which the attractive long-range interactions between the dipoles situated in each layer, was guarantied by imposing a proper constant distance between the layers. The expensive energy cost of having one molecule on top of the other in each lattice, namely molecules placed at the same lattice in different lattices, gives rise to have forbidden s-wave interactions. In contrast, the energy saving associated with interactions between dipoles situated in neighboring sites site is precisely the individual mechanism responsible for the $p_x + ip_y$ superfluid phases exhibited in our model. Based on previous calculations for the scattered and bound states molecules presented in Ref. [14], in terms of the effective interaction strength parameter χ , in this report we determine the presence of p-wave pairing. Specifically, by analyzing the manybody physics through the BCS mean-field scheme, we determine the parameters for which the model shows superfluid states. We summarized the whole results of our calculations in a phase diagram in terms of the effective interaction χ and the filling factor n. Further, we recognize the superfluid density, by performing a gauge transformation of the original creation and annihilation fermionic operators in layers A and B, $(a_i^{\dagger}, b_i^{\dagger}; a_i, b_i)$, after considering a second order expansion for the free energy in terms of the order parameter Δ . This procedure allowed us to establish the link between the BCS prediction with the correct one for systems exhibiting phase transitions in 2D, that is BKT transitions. Considering the recent experimental realization of dipolar ultracold Fermi molecules of NaK we found that our calculations predicts that the transition takes place at $T_{BKT} = 0.6$ nK for $\chi = 0.4$ while $T_{BKT} = 10$ nK for $\chi = 1.0$. Moreover, by using the recently proposed subwavelength lattice technique we obtained temperatures around 4 nK for $\chi = 0.4$. In contrast with other previous p-wave proposals, the model here discussed represents a natural candidate to simulate the physics behind the ruthenates, since it contains the strong on-site repulsion, which is a crucial ingredient in unconventional superconductors. In addition, our model share the peculiarity of being composed of layered structures which are present in ruthenate compounds and unconventional superconductors.

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