Singlet and triplet Bardeen-Cooper-Schrieffer pairs in a gas of two-species fermionic polar molecules

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Taking into account the deformation of the Fermi surface, we investigate the spin-singlet and -triplet BCS pairings in a mixture of fermionic polar molecules with two different hyperfine states. In particular, we explore the relation between the critical temperatures and the Fock-exchange interaction. We also show that, by tuning short-range interaction between interspecies molecules, the singlet- and triplet-paired superfluids may coexist.

I. INTRODUCTION

Following the rapid experimental developments in making ultracold gases of fermionic polar molecules [1–4], there has been growing interest in studying the properties of dipolar Fermi gases. Of particular interest, the partially attractive electric dipole-dipole interaction (EDDI) provides a mechanism to form an anisotropic BCS pair. You and Marinescu [5] first realized that the p-wave paired BCS states could be achieved for fermionic atoms inside an external dc field. Baranov *et al.* further studied the BCS pairing in a homogeneous gas of the spin-polarized dipolar fermions [6]. Compared to the s-wave pairs in nondipolar Fermi gases, the anisotropic dipolar interaction makes the order parameter the superposition of all odd partial waves. Subsequently, the critical temperature of the superfluid transition and its relation to the trap geometry were investigated [6]. In those studies, the Fermi surface (FS) of system was assumed to be a sphere. However, it was found via the variational method that the Fock-exchange interaction deformed the FS [7], which was also confirmed by both numerical [8,9] and perturbation calculations [8,10]. Very recently, the role played by Fock-exchange interaction in BCS pairing has been considered [11].

All the mentioned theoretical work has focused on the spinless dipolar fermions. By adding the spin degree of freedom, an ultracold gas of polar molecules may offer even richer physics. When loaded into an optical lattice, spin-$\frac{1}{2}$ polar molecules can be used as a toolbox for lattice spin models [12]. It was also shown that a two-component dipolar Fermi gas may have a ferro-nematic ground state [13]. More interestingly, Samokhin and Mar'enko studied the nonuniform mixed-parity superfluid states in two-component dipolar Fermis gases with population imbalance [14]. They focused particularly on the weak dipolar interaction (compared to the contact interaction) limit; in addition, the effect of the Fock-exchange interaction on pairing was ignored.

In this work, we study the BCS pairing in a mixture of fermionic polar molecules with two different hyperfine states, $\sigma = \uparrow$ and $\downarrow$. The electric dipole moments d of all molecules are orientated along the z axis such that the spin-independent EDDI becomes $V_d(\mathbf{r}) = C_d r^{-3}(1 - \frac{3z^2}{r^2})$ with $C_d = d^2/(4\pi\varepsilon_0)$. We assume that interspecies molecules also interact via short-range interaction $V_0(\mathbf{r}) = C_0\delta(\mathbf{r})$, where $C_0 = (4\pi\hbar^2 a_s)m$ with a_s being the s-wave scattering length and m the mass of the molecule. The total interaction

potential $V = V_d + V_0$ conserves the number of particles in the individual spin component. As shown, this system supports both the spin-singlet even partial wave and the spin-triplet odd partial wave BCS pairs [14]. In addition, we find that the Fock-exchange interaction always enhances the triplet pairing by increasing the corresponding critical temperature. However, when contact interaction dominates, the Fock-exchange interaction may weaken the singlet pairing. We also point out that, by tuning the contact interaction, the transition between single- and triplet-paired superfluids can be realized. Very recently, Wu *et al.* [15] studied the same system. In particular, they show the existence of the mixed triplet and singlet pairings, which spontaneously breaks the time-reversal symmetry.

II. GAP EQUATION

We consider a homogeneous gas of two-species fermionic polar molecules with total number density $2n$. For simplicity, we assume that $n_\uparrow = n_\downarrow = n$. In momentum space, the second quantized Hamiltonian reads

$$
\begin{aligned}
H = &\sum_{\mathbf{k}\sigma} \left(\frac{\hbar^2\mathbf{k}^2}{2m} - \mu\right) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \\
&+ \frac{1}{2\mathcal{V}} \sum_{\mathbf{kpq},\sigma\sigma'} \widetilde{V}(\mathbf{q}) c^\dagger_{\mathbf{k}+\mathbf{q}\,\sigma} c^\dagger_{\mathbf{p}-\mathbf{q}\,\sigma'} c_{\mathbf{p}\sigma'} c_{\mathbf{k}\sigma},
\end{aligned}
$$

where $\mu = \mu_\uparrow = \mu_\downarrow$ is the chemical potential, $\mathcal{V}$ is the volume of the system, and $\widetilde{V} = \widetilde{V}_d + \widetilde{V}_0$ is the Fourier transform of the interaction potential. One should keep in mind that, in Eq. (1), contact interaction only exists between $\uparrow$ and $\downarrow$ molecules.

Under Hartree-Fork approximation, Eq. (1) becomes

$$
H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2}\sum_{\mathbf{k},\sigma\sigma'} \Delta_{\sigma\sigma'}(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c^\dagger_{-\mathbf{k}\sigma'} + \text{H.c.}, \quad (1)
$$

where the dispersion relation is $\varepsilon_{\mathbf{k}\sigma} = \{(\hbar^2\mathbf{k}^2)/2m\} - \varepsilon_F - \Sigma_\sigma(\mathbf{k})$ with $\varepsilon_F \equiv \mu - nC_0 = (\hbar^2/2M)(6\pi^2 n)^{2/3}$ being the Fermi energy and $\Sigma_\sigma(\mathbf{k}) = \mathcal{V}^{-1}\sum_{\mathbf{q}} \widetilde{V}_d(\mathbf{k}-\mathbf{q}) f_{\mathbf{q}\sigma}$ being the self-energy. To the lowest order, we choose the Fermi occupation number $f_{\mathbf{q}\sigma} = \langle c^\dagger_{\mathbf{q}\sigma} c_{\mathbf{q}\sigma} \rangle$ to be that at zero temperature. As a result, dispersion relations become spin independent, denoted as $\varepsilon_{\mathbf{k}}$. In addition, the Fock-exchange interaction deforms the FS such that it is now describes by an ellipsoid of the form $\alpha^{-1}(k_x^2 + k_y^2) + \alpha^2 k_z^2 = k_F^2$ [7], where $\hbar k_F = \sqrt{2m\varepsilon_F}$

is the Fermi momentum and α represents the deformation parameter. The value of α ($\leqslant 1$) can be obtained through either variational [7] or numerical calculation [8,9]. Moreover, at the weak interaction limit

$$D \equiv nC_d/\varepsilon_F \ll 1, \tag{2}$$

the perturbation calculation yields $\alpha = 1 - \frac{2\pi}{3}D$ [8,10], where D is the dimensionless dipole interaction strength. For simplicity, the variational result of α is adopted in this work.

The order parameters for the BCS states in the Hamiltonian (1) are defined as

$$\Delta_{\sigma\sigma'}(\mathbf{k}) = \mathcal{V}^{-1} \sum_{\mathbf{q}} \widetilde{V}(\mathbf{k} - \mathbf{q}) \langle c_{-\mathbf{q}\sigma'} c_{\mathbf{q}\sigma} \rangle. \tag{3}$$

Using either Bogoliubov transformation [16] or the standard Green's function method [17], we obtain

$$\langle c_{-\mathbf{q}\sigma'} c_{\mathbf{q}\sigma} \rangle = -\frac{\Delta_{\sigma\sigma'}(\mathbf{q})}{2E_{\mathbf{q}\sigma}} \tanh\left(\frac{1}{2}\beta E_{\mathbf{q}\sigma}\right), \tag{4}$$

where $E_{\mathbf{k}\sigma} = \sqrt{\varepsilon_{\mathbf{k}}^2 + \sum_{\zeta} |\Delta_{\sigma\zeta}(\mathbf{k})|^2}$ is the energy of single-particle excitation and $\beta = 1/(k_B T)$ is the inverse temperature. To obtain $E_{\mathbf{k}\sigma}$, we have assumed that $\Delta_{\sigma\zeta}^{\dagger} \Delta_{\zeta\sigma'}$ is a diagonal matrix. Substituting Eq. (4) into Eq. (3), one finds a set of self-consistent equations for order parameters

$$\Delta_{\sigma\sigma'}(\mathbf{k}) = -\int \frac{d\mathbf{q}}{(2\pi)^3} \widetilde{V}(\mathbf{k} - \mathbf{q}) \frac{\tanh\left(\frac{1}{2}\beta E_{\mathbf{q}\sigma}\right)}{2E_{\mathbf{q}\sigma}} \Delta_{\sigma\sigma'}(\mathbf{q}); \tag{5}$$

here the order parameters corresponding to different BCS paired states are coupled. Similar gap equations also appear in a superfluid ^{3}He system [16]. The integral in Eq. (5) formally diverges. To regularize the interaction, we follow the standard renormalization procedure [6], which, to the first Born approximation, leads to the gap equations

$$\Delta_{\sigma\sigma'}(\mathbf{k}) = -\int \frac{d\mathbf{q}}{(2\pi)^3} \widetilde{V}(\mathbf{k} - \mathbf{q}) \Delta_{\sigma\sigma'}(\mathbf{q})$$
$$\times \left[\frac{\tanh\left(\frac{1}{2}\beta E_{\mathbf{q}\sigma}\right)}{2E_{\mathbf{q}\sigma}} - \frac{m}{\hbar^2 \mathbf{q}^2}\right]. \tag{6}$$

We emphasize that these equations are only valid in weak interaction regime Eq. (2), as we have ignored the higher order contributions from the interaction.

III. SYMMETRIES OF THE ORDER PARAMETERS

Up to now, we have expressed the order parameters

$$\mathbf{\Delta} = \begin{pmatrix} \Delta_{\uparrow\uparrow} & \Delta_{\uparrow\downarrow} \\ \Delta_{\downarrow\uparrow} & \Delta_{\downarrow\downarrow} \end{pmatrix}$$

in the uncoupled spin space. While in the basis of coupled spin $\{|SM\rangle\}$, one will have singlet and triplet pairs corresponding to total spin $S = 0$ and 1, respectively. Singlet pairing requires the gap parameter to be antisymmetric such that

$$\mathbf{\Delta}_s = \Delta_s i\boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & \Delta_s \\ -\Delta_s & 0 \end{pmatrix},$$

where σ_2 is the second Pauli matrix. Obviously, $\Delta_s(-\mathbf{k}) = \Delta_s(\mathbf{k})$, and as we show, it is a superposition of even partial waves, that is, $\Delta_s(\mathbf{k}) = \sum_{\text{even } l} \Delta_l^{(s)}(k) Y_{l0}(\hat{\mathbf{k}})$.

Following the convention of ^{3}He [16], we may define a vector $\mathbf{d}(\mathbf{k})$ in spin space by combining three spin components ($M = 0, \pm 1$) of the triplet pair:

$$\mathbf{\Delta}_t = \sum_{\mu=1,2,3} d_\mu(\boldsymbol{\sigma}_\mu i\boldsymbol{\sigma}_2) = \begin{pmatrix} -d_1 + id_2 & d_3 \\ d_3 & d_1 + id_2 \end{pmatrix},$$

where $\boldsymbol{\sigma}_\mu$ are Pauli matrices. It can be easily seen that $\Delta_{t,1} = \Delta_{\uparrow\uparrow} = -d_1 + id_2$, $\Delta_{t,-1} = \Delta_{\downarrow\downarrow} = d_1 + id_2$, and $\Delta_{t,0} = \Delta_{\uparrow\downarrow} = \Delta_{\downarrow\uparrow} = d_3$. In momentum space, $\Delta_{t,M}(\mathbf{k})$ are superpositions of odd partial waves, that is, $\Delta_{t,M}(\mathbf{k}) = \sum_{\text{odd } l} \Delta_{M,l}^{(t)}(k) Y_{l0}(\hat{\mathbf{k}})$.

IV. SPIN-SINGLET PAIRING

For a deformed FS, we introduce the rescaled momentum $\bar{\mathbf{k}}$ such that $\bar{k}_{x/y} = \alpha^{-1/2} k_{x/y}$ and $\bar{k}_z = \alpha k_z$. Moreover, we define $\xi_{\bar{\mathbf{k}}} \equiv \hbar^2 \bar{\mathbf{k}}^2/(2M) - \varepsilon_F$, which allows us to rewrite the order parameter as $\Delta_s(\bar{\mathbf{k}}) \equiv \Delta_s(\xi_{\bar{\mathbf{k}}}, \mathbf{n}_{\bar{\mathbf{k}}})$ with $\mathbf{n}_{\bar{\mathbf{k}}} = \bar{\mathbf{k}}/\bar{k}$ being an unit vector. Using the fact that the pairing is mainly contributed by states near FS, we introduce a characteristic energy $\overline{\omega}_s$ (of the order of ε_F) to single out the contribution from $-\overline{\omega}_s \leqslant \xi_{\bar{\mathbf{k}}} \leqslant \overline{\omega}_s$ [6]. In a weak coupling regime, we have $\overline{\omega}_s \gg |\Delta_s|, k_B T_c^{(s)}$. The value of $\overline{\omega}_s$ is determined self-consistently. After some tedious calculations, we obtain from Eq. (6) that

$$\Delta_s(\xi_{\bar{\mathbf{k}}}, \mathbf{n}_{\bar{\mathbf{k}}}) = -\int \frac{d\mathbf{n}_{\bar{\mathbf{q}}}}{4\pi} W(T, \mathbf{n}_{\bar{\mathbf{q}}}) \mathcal{R}_s(\xi_{\bar{\mathbf{k}}}, \mathbf{n}_{\bar{\mathbf{k}}}; 0, \mathbf{n}_{\bar{\mathbf{q}}}) \Delta_s(0, \mathbf{n}_{\bar{\mathbf{q}}})$$
$$+ \frac{1}{2} \int \frac{d\mathbf{n}_{\bar{\mathbf{q}}}}{4\pi} \int_{-\varepsilon_F}^{\infty} d\xi_{\bar{\mathbf{q}}} \ln\left(\frac{|\xi_{\bar{\mathbf{q}}}| + \eta_{\bar{\mathbf{q}}}}{2\overline{\omega}_s}\right) \frac{d}{d|\xi_{\bar{\mathbf{q}}}|}$$
$$\times \mathcal{R}_s(\xi_{\bar{\mathbf{k}}}, \mathbf{n}_{\bar{\mathbf{k}}}; \xi_{\bar{\mathbf{q}}}, \mathbf{n}_{\bar{\mathbf{q}}}) \Delta_s(\xi_{\bar{\mathbf{q}}}, \mathbf{n}_{\bar{\mathbf{q}}}) - \frac{1}{2} \int \frac{d\mathbf{n}_{\bar{\mathbf{q}}}}{4\pi}$$
$$\times \ln \frac{|\varepsilon_F|}{\overline{\omega}_s} \mathcal{R}(\xi_{\bar{\mathbf{k}}}, \mathbf{n}_{\bar{\mathbf{k}}}; -\varepsilon_F, \mathbf{n}_{\bar{\mathbf{q}}}) \Delta_s(-\varepsilon_F, \mathbf{n}_{\bar{\mathbf{q}}}), \tag{7}$$

where $W(T, \mathbf{n}_{\bar{\mathbf{q}}}) = \int_0^{\overline{\omega}_s} d\xi_{\bar{\mathbf{q}}} \eta_{\bar{\mathbf{q}}}^{-1} \tanh[\eta_{\bar{\mathbf{q}}\sigma}/(2k_B T)]$ and $\eta_{\bar{\mathbf{k}}} = \sqrt{\xi_{\bar{\mathbf{k}}}^2 + |\Delta_s(0, \mathbf{n}_{\bar{\mathbf{k}}})|^2}$. Furthermore, the integration kernel takes the form

$$\mathcal{R}_s(\xi_{\bar{\mathbf{k}}}, \mathbf{n}_{\bar{\mathbf{k}}}; \xi_{\bar{\mathbf{q}}}, \mathbf{n}_{\bar{\mathbf{q}}})$$
$$= \frac{m\bar{q}}{2\pi^2} \widetilde{V}(\mathbf{k} - \mathbf{q}) \left[\frac{\eta_{\bar{\mathbf{q}}}}{E_{\mathbf{q}}} \frac{\tanh\left(\frac{1}{2}\beta E_{\mathbf{q}}\right)}{\tanh\left(\frac{1}{2}\beta \eta_{\bar{\mathbf{q}}}\right)} - \frac{2M\eta_{\bar{\mathbf{q}}}}{\mathbf{q}^2 \tanh\left(\frac{1}{2}\beta \eta_{\bar{\mathbf{q}}}\right)}\right].$$

Close to the critical temperature $T_c^{(s)}$, the gap goes to zero and $\eta_{\bar{\mathbf{q}}} \to |\xi_{\bar{\mathbf{q}}}|$. For the first term in the right-hand side of Eq. (7), we have $\mathcal{C} \equiv W(T_c^{(s)}, \mathbf{n}_{\bar{\mathbf{k}}}) = \ln[2e^\gamma \overline{\omega}_s/(\pi k_B T_c^{(s)})]$, with $\gamma = 0.5772$ being the Euler constant. In contrast, the last two terms in Eq. (7) do not contain the large logarithm $\ln(\overline{\omega}_s/k_B T_c^{(s)})$, indicating that they are only important for the pre-exponential factor in the expression of critical temperature [6]. For the purpose of determining $T_c^{(s)}$, they are neglected such that we find on the FS

$$\Delta_s(0, \mathbf{n}_{\bar{\mathbf{k}}}) = -\mathcal{C} \int \frac{d\mathbf{n}_{\bar{\mathbf{q}}}}{4\pi} \mathcal{R}_s(0, \mathbf{n}_{\bar{\mathbf{k}}}; 0, \mathbf{n}_{\bar{\mathbf{q}}}) \Delta_s(0, \mathbf{n}_{\bar{\mathbf{q}}}), \tag{8}$$

which is essentially an eigenvalue equation of integral operator with kernel $\mathcal{R}_s(0, \mathbf{n}_{\bar{\mathbf{k}}}; 0, \mathbf{n}_{\bar{\mathbf{q}}})$. Finding the highest critical temperature is equivalent to finding the lowest negative eigenvalue of this eigenvalue equation. Even in the case $\alpha \neq 1$, it can be

shown that the eigenstate corresponding to lowest eigenvalue is independent of the azimuthal angle of $\mathbf{n}_{\bar{\mathbf{k}}}$ [6]. This observation allows us to integrate over the azimuthal variable of Eq. (8) to obtain the eigenvalue equation

$$\int_{-1}^{1} dy \, \mathcal{K}_s(x,y)\phi(y) = \lambda\phi(x), \tag{9}$$

where $x = \cos\theta_{\mathbf{n}_{\bar{\mathbf{k}}}}$, $y = \cos\theta_{\mathbf{n}_{\bar{\mathbf{q}}}}$, and $\mathcal{K}_s(x,y) = [3l_\alpha(x,y)\,|x-y|-1] + k_F a_s/(\pi^2 D)$ with $l_\alpha \equiv \{4\alpha^3 + (1 - \alpha^3)[(x-y)^2 - \alpha^3(x+y)^2]\}^{-1/2}$. Clearly, the first term in $\mathcal{K}_s$ originates from EDDI, while the second one corresponds to contact interaction.

For singlet pairing, we focus on the subspace of the eigenstates with even parity, that is, $\phi(x) = \phi(-x)$. Assuming that λ_s is the lowest eigenvalue of Eq. (9) corresponding to an even eigenstate $\phi_s(x)$, the critical temperature can then be expressed as

$$k_B T_c^{(s)} = \frac{2e^\gamma \overline{\omega}_s}{\pi} \exp\left(-\frac{1}{\pi D |\lambda_s|}\right). \tag{10}$$

In addition, at $T_c^{(s)}$, the order parameter on the FS becomes $\Delta_s(0,\mathbf{n}_{\bar{\mathbf{k}}}) = \Delta_{s0}\phi_s(\cos\theta_{\mathbf{n}_{\bar{\mathbf{k}}}})$, where $\phi_s(\cos\theta_{\mathbf{n}_{\bar{\mathbf{k}}}})$ represents the angular dependence of the order parameter on FS.

If the Fock-exchange interaction is ignored, we have exactly $\phi_s(x) = \mathcal{N}\cos(x\sqrt{3/|\lambda_s|})$, where $\mathcal{N}$ is a normalization constant and $|\lambda_s|$ is the largest positive root of the equation $t\cos\sqrt{3/t} + \{1 + [(2k_F a_s)/(\pi^2 D)]\}\sqrt{t/3}\sin\sqrt{3/t} = 0$. It can be shown that λ_s (<0) is a decreasing function of $k_F a_s/D$. For negative $k_F a_s$, our result reduces to that for s-wave pairing when $D = 0$. In the case $\alpha \neq 1$, λ_s and ϕ_s can only be determined numerically. As shown in Fig. 1, λ_s is an increase of α for $k_F a_s = 0$, indicating that, in the absence of contact interaction, the Fock-exchange interaction enhances singlet BCS pairing.

Next, we compute the characteristic energy $\overline{\omega}_s$. Following the standard BCS mean-field approach [6], we obtain

$$\ln\frac{\overline{\omega}_s}{\varepsilon_F} = \lim_{\delta\to 0^+}\ln\delta + \frac{1}{2\pi D\lambda_s}\int\frac{d\mathbf{n}_{\bar{\mathbf{k}}}}{4\pi}\int\frac{d\mathbf{n}_{\bar{\mathbf{q}}}}{4\pi}\phi_s(\mathbf{n}_{\bar{\mathbf{k}}})$$
$$\times \int_{-\varepsilon_F}^{\infty}\frac{d\xi_{\bar{\mathbf{q}}}}{|\xi_{\bar{\mathbf{q}}}|}\mathcal{R}_s(0,\mathbf{n}_{\bar{\mathbf{k}}};\xi_{\bar{\mathbf{q}}},\mathbf{n}_{\bar{\mathbf{q}}})\frac{\Delta_s(\xi_{\bar{\mathbf{q}}},\mathbf{n}_{\bar{\mathbf{q}}})}{\Delta_0}, \tag{11}$$

where the order parameter, at $T_c^{(s)}$, satisfies the equation

$$\frac{\Delta_s(\xi_{\bar{\mathbf{k}}},\mathbf{n}_{\bar{\mathbf{k}}})}{\Delta_{s0}} \simeq \frac{1}{\pi D\lambda_s}\int\frac{d\mathbf{n}_{\bar{\mathbf{q}}}}{4\pi}\mathcal{R}_s(\xi_{\bar{\mathbf{k}}},\mathbf{n}_{\bar{\mathbf{k}}};0,\mathbf{n}_{\bar{\mathbf{q}}})\phi_s(\cos\theta_{\bar{\mathbf{q}}}). \tag{12}$$
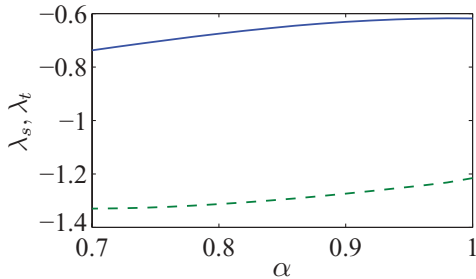
FIG. 1. (Color online) The α dependence of λ_s for $k_F a_s = 0$ (solid line) and λ_t (dashed line).
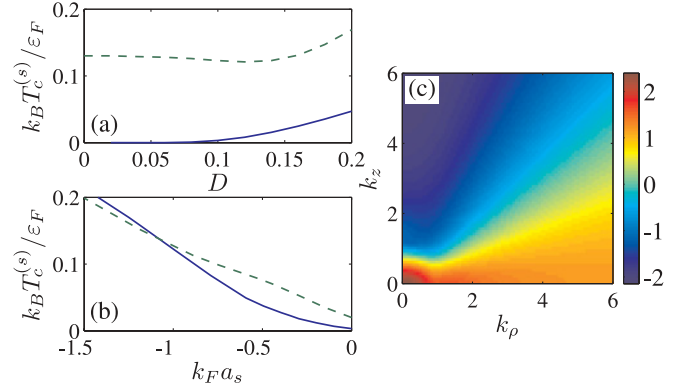

FIG. 2. (Color online) (a) The D dependence of $T_c^{(s)}$ for $k_F a_s = 0$ (solid line) and -1 (dashed line). (b) $T_c^{(s)}$ as a function of $k_F a_s$ for $D = 0.1$ (solid line) and 0.15 (dashed line). (c) $\Delta_s(k_\rho,k_z)/\Delta_{s0}$ at critical temperature for $k_F a_s = 0$ and $D = 0.1$, where $k_\rho = (k_x^2 + k_y^2)^{1/2}$.

The term $\overline{\omega}_s$ can be obtained by substituting Eq. (12) into Eq. (11). We remark that, in the right-hand side of Eq. (11), the second term also contains a divergent term which cancels the divergence from the first term. In general, $\overline{\omega}_s$ is a function of both D and $k_F a_s$, indicating that it also implicitly depends on α. For simplicity, we use $\alpha = 1$ to calculate $\overline{\omega}_s$, which yields $\overline{\omega}_s \simeq 0.36\varepsilon_F$ for $k_F a_s = 0$ and $\overline{\omega}_s \simeq 0.54\varepsilon_F$ for $D = 0$. The latter is exactly the value for s-wave pairing.

In Fig. 2(a), we present the D dependence of the critical temperature for singlet pairing. For $k_F a_s = 0$, only the dipolar interaction is responsible for pairing; therefore, $T_c^{(s)}$ is a monotonically increasing function of D. However, for $k_F a_s = -1$, $T_c^{(s)}(D)$ becomes a concave curve. This result suggests that even though both attractive contact interaction and dipolar interaction contribute to pairing, they also compete with each other. In fact, the deformed FS makes it difficult for contact interaction to form s-wave pairs, which is responsible for the drop of $T_c^{(s)}$ at small D. When dipolar interaction dominates, $T_c^{(s)}$ becomes an increasing function of D again. We also verify that if the FS deformation is ignored, $T_c^{(s)}$ would always be an increasing function of D. Figure 2(b) shows the $k_F a_s$ dependence of $T_c^{(s)}$ for given D. As α is fixed by D, $T_c^{(s)}$ always increases as one increases the strength of contact interaction. In addition, when short-range interaction dominates, the one with smaller FS deformation (smaller D) will eventually have a higher critical temperature. Finally, the angular dependence of the order parameter for a spin-singlet pair at critical temperature is presented in Fig. 2(c).

V. SPIN-TRIPLET PAIRING

At critical temperature, the order parameters for triplet pairs $\Delta_{t,M}$ are decoupled. In addition, they satisfy gap equations with exactly the same form. Therefore, we denote the triplet order parameter as Δ_t. Since the critical temperature and order parameters can be obtained by following the same procedure as that for singlet pairing, here we only present our results.

The critical temperature $T_c^{(t)}$ for triplet pairing can be expressed as $k_B T_c^{(t)} = [(2e^\gamma\overline{\omega}_t)/\pi]\exp(-\frac{1}{\pi D|\lambda_t|})$, where λ_t is
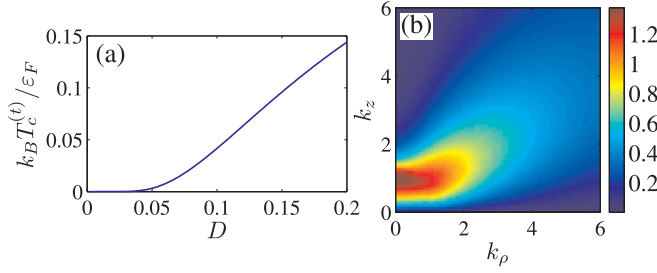
FIG. 3. (Color online) (a) The D dependence of $T_c^{(t)}$. (b) $\Delta_t(k_\rho, k_z)/\Delta_{t0}$ at critical temperature for $D = 0.1$.

the lowest eigenvalue of the equation $\int_{-1}^{1} dy \mathcal{K}_t(x,y)\phi(y) = \lambda\phi(x)$ in the subspace of the eigenstates with odd parity. The integration kernel is $\mathcal{K}_t(x,y) = 3l_\alpha(x,y)|x-y| - 1$, which is essentially $\mathcal{K}_s$ with $k_F a_s = 0$. Assuming that the corresponding eigenstate of λ_t is $\phi_t(x)$, the triplet order parameter on the FS is $\Delta_t(0, \cos\theta_{\mathbf{n}_{\bar{\mathbf{k}}}}) = \Delta_{t0}\phi_t(\cos\theta_{\mathbf{n}_{\bar{\mathbf{k}}}})$. The α dependence of λ_t (Fig. 1) indicates that the critical temperature of the triplet pairing is also enhanced by the Fock-exchange interaction. This enhancement can be attributed to the increase of the density of states near the north and south poles of the stretched (along the z axis) FS, which provides the main contribution to the triplet pairing [11].

The characteristic energy $\overline{\omega}_t$ and the triplet order parameter $\Delta_t(\xi_{\bar{\mathbf{k}}}, \mathbf{n}_{\bar{\mathbf{k}}})/\Delta_{t0}$ at critical temperature satisfy equations similar to Eqs. (11) and (12), except that $\mathcal{R}_s$ is now replaced by $\mathcal{R}_t$ which does not contain the contact interaction. In Fig. 3(a), we plot the dipolar interaction strength dependence of the critical temperature $T_c^{(t)}$, where we have used $\overline{\omega}_t \simeq 0.42\varepsilon_F$, the value corresponding to the $\alpha = 1$ case. We remark that the analytic result for $T_c^{(t)}$ agrees very well with that obtained numerically [18]. The typical order parameter for a triplet pair is plotted in Fig. 3(b). In the case where the FS deformation is ignored, our results for triplet pairing reduce to those obtained by Baranov *et al.* [6].

VI. SINGLET VERSUS TRIPLET PAIRING

For $k_F a_s = 0$, it can be seen from Fig. 1 that we always had $|\lambda_s| < |\lambda_t|$; by further assuming $\alpha = 1$, we also find that $\overline{\omega}_s < \overline{\omega}_t$. These results suggest that, without attractive contact interaction, the critical temperature for singlet pairing is always lower than that for triplet pairing. However, for $k_F a_s < 0$, $T_c^{(s)}$ increases as one increases the strength of the short-range interaction such that beyond a threshold $k_F a_s^*$, we have $T_c^{(s)} > T_c^{(t)}$. The critical s-wave scattering length is determined by equation

$$\pi D \ln \frac{\overline{\omega}_s(k_F a_s^*)}{\overline{\omega}_t} = \frac{1}{\lambda_t} - \frac{1}{\lambda_s(k_F a_s^*)},$$

where we have explicitly expressed $\overline{\omega}_s$ and λ_s as functions of $k_F a_s$. In Fig. 4, we present the D dependence of the critical scattering length. We point out that when $T_c^{(s)} = T_c^{(t)}$, the singlet and triplet pairs may coexist in the system.

One should note that, in our expressions for the critical temperatures, we have ignored the many-body effect on the pre-exponential factor. In a weak interaction limit, a proper treatment of this effect requires the calculations of the
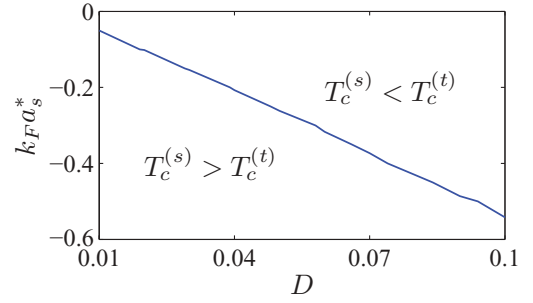

FIG. 4. (Color online) The dipolar interaction strength dependence of the critical scattering length.

second-order corrections of the scattering amplitude between interacting particles [6], which is out of the scope of the present work. However, this effect can be roughly estimated as follows. For triplet pairing, the higher order corrections can be incorporated into the expression for critical temperature as

$$k_B T_c^{(t)} \simeq \frac{2e^\gamma \overline{\omega}_t}{\pi} \exp\left(-\frac{1}{\pi D|\lambda_t| + gD^2 + hD^3 + \cdots}\right)$$
$$\simeq \frac{2e^\gamma \overline{\omega}_t}{\pi} e^{g/(\pi^2 \lambda_t^2)} \exp\left(-\frac{1}{\pi D|\lambda_t|} + \frac{hD}{\pi^2 \lambda_t^2} + \cdots\right),$$

where $g (>0)$ comes from the many-body correction when the Fermi surface is assumed to be spherical and all other higher order corrections originate from the additional effects due to the deformation of the Fermi surface. For small D, the second-order and higher order terms in the exponential function are negligible. Therefore, for triplet pairing, we may adopt the result from Ref. [6], which yields $k_B T_c^{(t)} \simeq 1.44\varepsilon_F e^{-1/(\pi D|\lambda_t|)}$. For the singlet pairing, the situation becomes more complicated due to the interplay of the contact and dipolar interactions. However, we note that the s-partial wave of the singlet pair dominated in the order parameter when λ_s is comparable to λ_t for any given D. Therefore, the main contribution to the many-body correction originates from the contact interaction, such that the critical temperature for singlet pairing can be approximated as $k_B T_c^{(s)} \approx 0.61\varepsilon_F e^{-1/(\pi D|\lambda_s|)}$ [19].

VII. CONCLUSION

We have investigated the singlet and triplet BCS pairings in an ultracold gas of two-species fermionic polar molecules. We calculate the critical temperatures and angular dependence of the order parameters. In the absence of the contact interaction, the critical temperature of the triplet pairing is always higher that of the singlet pairing. Moreover, the critical temperature of the singlet pairing can be increased by tuning the s-wave scattering length between interspecies molecules, such that the singlet and triplet pairs may coexist. For singlet pairing, we also show that the inclusion of the Fock-exchange interaction yields lower (higher) critical temperature if the contact (dipolar) interaction dominates. On the other hand, the Fock-exchange interaction always enhances the triplet pairing. Finally, we comment on the experimental realization of the spin-singlet and -triplet pairings in a mixture of polar molecules with two different hyperfine states. It has been demonstrated experimentally that a spin-mixed KRb

molecular gas has a shorter lifetime compared to a pure gas of spin-polarized molecules, as it suffers from the exothermic chemical reaction $KRb + KRb \rightarrow K_2 + Rb_2$ [3]. Since such loss channel is forbidden in RbCs molecular gas [20], it provides a better opportunity to explore the spin-singlet and -triplet BCS pairs in spin-mixed molecular gas.

[1] S. Ospelkaus *et al.*, Nat. Phys. **4**, 622 (2008).

[2] K.-K. Ni *et al.*, Science **322**, 231 (2008); S. Ospelkaus *et al.*, Faraday Discuss. **142**, 351 (2009).

[3] S. Ospelkaus, K. K. Ni, G. Zuemener, B. Neyenhuis, D. Wang, M. H. G. deMiranda, J. L. Bohn, J. Ye, and D. S. Jin, Phys. Rev. Lett. **104**, 030402 (2010); S. Ospelkaus *et al.*, Science **327**, 853 (2010).

[4] J. Deiglmayr, A. Grochola, M. Repp, K. Mortlbauer, C. Gluck, J. Lange, C. Dulieu, R. Wester, and M. Weidemuller, Phys. Rev. Lett. **101**, 133004 (2008).

[5] L. You and M. Marinescu, Phys. Rev. A **60**, 2324 (1999).

[6] M. A. Baranov, M. S. Marenko, V. S. Rychkov, and G. V. Shlyapnikov, Phys. Rev. A **66**, 013606 (2002); M. A. Baranov, L. Dobrek, and M. Lewenstein, Phys. Rev. Lett. **92**, 250403 (2004).

[7] T. Miyakawa, T. Sogo, and H. Pu, Phys. Rev. A **77**, 061603 (2008).

[8] S. Ronen and J. L. Bohn, Phys. Rev. A **81**, 033601 (2010).

[9] J.-N. Zhang and S. Yi, Phys. Rev. A **80**, 053614 (2009); **81**, 033617 (2010).

[10] C.-K. Chan, C. Wu, W. C. Lee, and S. DasSarma, Phys. Rev. A **81**, 023602 (2010).

[11] C. Zhao, L. Jiang, X. Liu, W. M. Liu, X. Zou, and H. Pu, Phys. Rev. A **81**, 063642 (2010).

[12] A. Micheli *et al.*, Nat. Phys. **2**, 341 (2006).

[13] B. M. Fregoso and E. Fradkin, Phys. Rev. Lett. **103**, 205301 (2009).

[14] K. V. Samokhin and M. S. Mar'enko, Phys. Rev. Lett. **97**, 197003 (2006).

[15] C. J. Wu and J. E. Hirsch, Phys. Rev. B **81**, 020508(R) (2010).

[16] D. Vollhardt and P. Wölfle, *The Superfluid Phases of Helium 3* (Taylor & Francis, London, 1990).

[17] See, e.g., E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics Part 2: Theory of the Condensed State* (Pergamon Press, Oxford, 1980).

[18] J.-N. Zhang *et al.* (unpublished).

[19] L. P. Gor'kov and T. K. Melik-Barkhudarov, Zh. Eksp. Teor. Fiz. **40**, 1452 (1961); Sov. Phys. JETP **13**, 1018 (1961).

[20] L. D. Carr, D. DeMille, R. V. Krems, and J. Ye, New J. Phys. **11**, 055049 (2009).