Vortex state in a superfluid Fermi gas near a Feshbach resonance

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We consider a single vortex in a superfluid Fermi gas in the BCS-BEC crossover regime near a Feshbach resonance. The effect of the molecular Bose-Einstein condensate upon the vortex structure is discussed within the mean field approximation at zero temperature. Using the self-consistent Bogoliubov-de Gennes equation of the fermion-boson coupled model, we calculate density distributions of atoms and molecules. As the number of the molecules increases, both atomic and molecular density changes from BCS-like distribution to BEC-like. We also study the change of the vortex core size in the crossover regime.

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I. INTRODUCTION

The evidence of fermionic superfluidity in trapped atomic gases has been clearly shown in the recent experiments [1, 2, 3, 4, 5]. The significant feature of these systems is that the strength of the inter-atomic interaction is manipulated via a Feshbach resonance (FR) phenomena. The crossover, which has been discussed several decades ago [6, 7, 8], between a weak coupling Bardeen-Cooper-Schrieffer (BCS) superfluid and a Bose-Einstein condensate (BEC) of pre-formed pairs can be realized in these systems.

The FR phenomena involve the scattering of atoms from open channel states into a molecular bound state formed from neighboring closed channel states. The so-called “pre-formed pair” in the conventional BCS-BEC crossover theory is here equivalent to the substantial molecule in the closed channel, which has been observed as a BEC on the one side of the FR.

In this paper we discuss the property of a single vortex in the BCS-BEC crossover regime at zero temperature. Since the vortex states in BCS superfluids and in BECs are significantly different in their distributions of particles, observing a vortex state in a Fermi gas provides the information about superfluidity in the crossover regime. In the case of a vortex in the BCS state, the energy gap is suppressed at the vortex core, and therefore the particle-hole symmetrical modes, which are localized at the vortex core, exist in the vicinity of the Fermi surface [9]. Therefore, the atomic density is finite at the center of the vortex core. On the other hand, the particle density in a BEC vanishes at the vortex core, directly reflecting a singularity of the order parameter.

We are also interested in the vortex core size in the crossover regime. The core size in a BCS superfluid is given by $\xi_{\text{BCS}} \sim \hbar v_F / \Delta$, where $v_F$ is the Fermi velocity and $\Delta$ is the energy gap. As the attractive interaction becomes strong, the growth of the energy gap makes the core size smaller [10]. As for a molecular BEC, the core size is written by $\xi_{\text{BEC}} \sim \sqrt{1/8\pi n_M a_M}$, where $n_M$ is the number density of molecules and $a_M$ is the s-wave scattering length of a molecule, which diverges at resonance as well as that of an atom [11, 12]. So $\xi_{\text{BEC}}$ also becomes small near the resonance. Then, how does the core size change in the crossover regime?

There are several theoretical papers concerning vortex states in Fermi gases [13, 14, 15, 16, 17]. These papers, however, deal with only Fermi gases of which interaction strength is manipulated, and the effect of a molecular BEC is not considered. In this paper, we start with an atom-molecule coupled model [18, 19, 20], and calculate density distributions and order parameters of both atoms and molecules. We use the mean field approximation to simply deal with the effect of a molecular BEC.

II. FORMALISM

We consider atomic gases of two atomic hyperfine states (labeled by $\sigma = \uparrow, \downarrow$), which are coupled to a molecular two-particle bound state. The energy of a bare molecule relative to that of two bare atoms is denoted by $2\nu$. The model Hamiltonian of the fermion-boson coupled system is given by

$$\hat{H} = \int dr \left[ \sum_{\sigma} \hat{\psi}_{\sigma}^\dagger(\vec{r}) \hat{H}_A(\vec{r}) \hat{\psi}_{\sigma}(\vec{r}) + \hat{\phi}^\dagger(\vec{r}) \{ \hat{H}_M(\vec{r}) + 2\nu \} \hat{\phi}(\vec{r}) + g \left\{ \hat{\phi}^\dagger(\vec{r}) \hat{\psi}_A(\vec{r}) \hat{\psi}_B(\vec{r}) + \text{h.c.} \right\} \right], \quad (1)$$

where $\hat{\psi}_\sigma$, $\hat{\phi}$ are the field operators of atoms and molecules, respectively. The first and second terms in the integration represent the bare Hamiltonian of atoms and molecules, respectively, where $\hat{H}_A(\vec{r}) = -\hbar^2/2m \nabla^2 + V_A(\vec{r})$, $\hat{H}_M(\vec{r}) = -\hbar^2/4m \nabla^2 + V_M(\vec{r})$, $m$ is the atomic mass and $V_{A,M}(\vec{r})$ are the trapping potential for atoms and molecules, respectively. The last term in Eq. (1) represents the atom-molecule coupling associated with FR.
Its contribution to the effective atom-atom interaction is $-g^2/2\nu$. This means that the interaction is manipulated by changing $\nu$. So we investigate the $\nu$ dependence of this system, especially at around $\nu = 0$. Although there exist non-resonant inter-atomic and intermolecular interactions, we assume that the effect of the resonant process is so dominant that the other processes are negligible.

To conserve the total number of particles, we use a single chemical potential $\mu$ and work with $\mathcal{H} = \hat{H} - \mu \hat{N}$, where $\hat{N}$ is the number operator given by

$$\hat{N} = \int dr \left[ \sum_o \hat{\psi}_o^\dagger(r) \hat{\psi}_o(r) + 2\hat{\phi}^\dagger(r) \hat{\phi}(r) \right].$$

Here, we introduce the mean-field order parameters $\mathcal{P}(r) \equiv \langle \hat{\psi}_o(r) \hat{\psi}_o(r) \rangle$ and $\phi(r) \equiv \langle \hat{\phi}(r) \rangle$, which correspond to the Cooper pair amplitude and molecular order parameter, respectively. The number density of molecules are given by $n_M(r) = |\phi(r)|^2$, as usual. Though we neglect the bare atom-atom interaction, the effective interaction via FR supports the pairing of atoms. Since $\phi(r)$ is related to an energy gap as we will show below, the pair amplitude remains finite as long as a molecular BEC exists. The relation between these order parameters is given by the equilibrium condition $i\hbar \langle \partial \phi(r) / \partial t \rangle = \langle [\phi(r), \mathcal{H}] \rangle = 0$, from which it follows that

$$[\mathcal{H}_M(r) + 2\nu - 2\mu] \phi(r) + g \mathcal{P}(r) = 0. \quad (3)$$

As in the case of the well-known mean field BCS theory, the “off-diagonal energy” should be defined as the energy gap, i.e., Eq. (1) implies that $\Delta_{\text{eff}}(r) = g \phi(r)$. Then, the conventional Bogoliubov-de Gennes (BdG) approach is used in a similar manner: the field operator of the atom is transformed with

$$\begin{bmatrix} \hat{\psi}_o(r) \\ \hat{\psi}_o^\dagger(r) \end{bmatrix} = \sum_j \begin{bmatrix} u_j(r) & -v_j(r) \\ v_j(r) & u_j^\dagger(r) \end{bmatrix} \begin{bmatrix} \alpha_j \alpha_j^\dagger \end{bmatrix}, \quad (4)$$

and the BdG equation is obtained by

$$\begin{bmatrix} \mathcal{H}_A(r) - \mu & g \phi(r) \\ g \phi^*(r) & -\mathcal{H}_A(r) + \mu \end{bmatrix} \begin{bmatrix} u_j(r) \\ v_j(r) \end{bmatrix} = \epsilon_j \begin{bmatrix} u_j(r) \\ v_j(r) \end{bmatrix}. \quad (5)$$

In this notation, the pair amplitude and the density at zero temperature are written by $\mathcal{P}(r) = -\sum_j u_j^\dagger(r) v_j(r)$ and $n_A(r) = 2 \sum_j |v_j(r)|^2$, respectively. To avoid the ultraviolet divergence in $\mathcal{P}(r)$, we introduce a cutoff energy $\omega_c$, which is in the order of the Fermi energy, and redefine $\mathcal{P}(r) = -\sum_j u_j^\dagger(r) v_j(r) e^{-\epsilon_j/\omega_c^2}$.

Then, all we have to do is to solve Eqs. (3) and (5) self-consistently. The chemical potential is determined so that the total number of atoms $N_{\text{tot}} = N_A + 2N_M$ is conserved, where $N_{A,M} = \int d\mathbf{r} n_{A,M}(r)$.

## III. VORTEX STATE IN THE CROSSOVER REGIME

We assume a cylindrical optical trap and approximate it with a two-dimensional harmonic potential: $V_A(r) = (1/2)m\omega^2(x^2 + y^2)$ and $V_F(r) = 2V_A(r)$. For simplicity, we neglect the $z$ dependence of the order parameters. When considering the microscopic vortex structure, however, the degree of freedom in $z$ direction is important. So we assume that gases are confined in the length $L_z$, and impose the periodic boundary condition. We have numerically confirmed that the results does not depend on $L_z$ but on $N_{\text{tot}}/L_z$ when $L_z \geq a_{\text{HO}}$, where $a_{\text{HO}} = \sqrt{\hbar/2m\omega}$ is the harmonic oscillator length.

A single particle state of a bare atom in this potential is given by $e^{ikz} e^{i\theta(r/a_{\text{HO}})} \phi(r) = 2 \alpha_{\text{HO}}^{-1/2} e^{-r^2/4\alpha_{\text{HO}}^2}$, where $\alpha_{\text{HO}} = (2\pi a_{\text{HO}}/L_z)^{1/2}$ and the generalized Laguerre polynomial function. The indices specifying the energy are given by $l = 0, \pm 1, \pm 2, \ldots$, $n = 0, 1, 2, \ldots$, and $k\alpha_{\text{HO}} = (2\pi a_{\text{HO}}/L_z) n_k \equiv k n_k$.

For a vortex state in equilibrium, we assume the form

$$\phi(r) = e^{i\theta}(r), \quad (6)$$

$$u_{kln}(r) = e^{ikz} e^{i(\nu - 1)\theta} u_{kln}(r), \quad (7)$$

$$v_{kln}(r) = e^{ikz} e^{i\theta} v_{kln}(r), \quad (8)$$

where $u_{kln}(r), v_{kln}(r)$ and $\phi(r)$ are real functions, and $n = 0, 1, 2, \ldots$ is the radial quantum number. In the BEC limit, by substituting $g \mathcal{P} = 0$ in Eq. (3) the lowest energy state of a molecular BEC with a single vortex is given by $\phi(r) = \sqrt{N_{\text{tot}}/2\pi \alpha_{\text{HO}} \sqrt{L_z \hbar \omega}} e^{-r^2/2\alpha_{\text{HO}}^2}$.

We consider a gas of $^6$Li atoms in a trap with $\omega = 2\pi \times 300$ Hz and $a_{\text{HO}} = 1.7 \mu m$. The line density are set as $N_{\text{tot}}/L_z = 30 \mu m^{-1}$ and $200 \mu m^{-1}$, leading to $E_F/\hbar \omega$ in the same order. As for the coupling constant, we consider a narrow FR and set $g/v = E_{F} \hbar \omega$ and $3E_{F}$, where $n$ is the mean density of total atoms: $n = N_{\text{tot}}/2\pi \alpha_{\text{HO}} \sqrt{L_z}$.}

Figure 1(a) shows the $\nu$ dependence of the chemical potential. Since we neglect the bare atom-atom and molecule-molecule interactions, the trapped gas behaves as an ideal gas far from the resonance in each side as shown in Fig. 1(a), i.e., in the BCS limit $\mu$ goes to $E_F$, while $\nu \to \nu + \hbar \omega$ in the BEC limit. In Fig. 1(b), the numbers of atoms and molecules are plotted as a function of $\nu$. It is clearly shown that where the crossover occurs
in the parameter space $\nu/E_F$ is determined by the interaction energy $g\sqrt{n}$ relative to $E_F$, while the width of the crossover region depends on the coupling constant $g$.

IV. CORE STRUCTURE

Figure 2 shows the density distributions of (a) atoms and (b) molecules in the case of $E_F = 21\hbar\omega$ and $g\sqrt{n} = 3E_F$. Both profiles are normalized by the corresponding numbers of each species. We also plot the density distribution of a non-interacting BEC, $|f_0(r)|^2$, in both figures. As we mentioned above, the atomic distribution far from resonance in BCS side ($\nu/E_F = 1.5$) has no explicit hole associated with a vortex. The broad distribution in radial direction is also the feature of a fermionic profile. As $\nu$ decreases, however, these fermionic features disappear and the atomic distribution becomes BEC-like, i.e., the cloud becomes narrower in radial direction and, moreover, the hole at the vortex core clearly appears. This result is consistent with that of the one-channel model [14], which argues that the density decreases at the vortex core when a BCS superfluid goes into the BEC regime. Our calculation shows that this density depletion does not merely come from the increase of the molecular fraction. The atomic profile itself also turns into a BEC-like distribution.

The existence of a molecular BEC leads to these changes in atomic distribution. Since the molecular density always vanishes at vortex core as shown in Fig. 2(b), the atomic density is also suppressed there when the number of molecules becomes large. On the other hand, the molecular distributions in the BCS side are also strongly affected by atoms, being broader than those in BEC side. In the crossover regime, atoms and molecules are strongly coupled to each other, and both gradually turn from BCS-like to BEC-like distribution.

Next, we discuss the change of order parameters. Figure 3 shows the $\nu$ dependence of (a) the pair amplitude $\mathcal{P}(r)$ and (b) the molecular order parameter $\phi(r)$, or the effective energy gap. These are also the results of the calculation with $E_F = 21\hbar\omega$ and $g\sqrt{n} = 3E_F$. As $\nu$ decreases, the molecular order parameter monotonically
The core size does not strongly depend on \( \nu \) at a nearly same radius. This means that the core size does not become smaller any more. The core size in this region is determined by the scale of spatial variations of the single-particle wavefunction with the energy \( E_F \), which is in the order of \( a_{HO} \). In the case of free atoms, this size corresponds to the Fermi wave length \( 1/k_F \equiv \hbar/\sqrt{2mE_F} \).

As for the molecular order parameter, the core region of \( \phi(r) \) in BEC limit corresponds to the harmonic oscillator length since we neglect the bare molecule-molecule interaction. In the crossover regime, the atomic pair is expected to affect the core size of the molecular order parameter. It seems, however, that the effect of the change in the \( \mathcal{P}(r) \) on the core size in \( \phi(r) \) is very little in our results.

V. CONCLUSION

We have studied a vortex state in a superfluid Fermi gas near a Feshbach resonance, using the atom-molecule coupled model and the mean field approximation. Coupled to each other, both atomic and molecular density distributions change from BCS-like to BEC-like in the crossover regime. The depletion of the total particle density in BEC side does not merely come from the increase of the number of molecules. Affected by a molecular BEC, a hole at the core in atomic density clearly appears. We have also studied the change of a vortex core size. In the BCS side, the change of the core size is consistent with the BCS theory. But because of the trapping potential, the core size dose not show drastic change in the crossover regime.

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