BCS-BEC Crossover in Two-Dimensional Attractive Hubbard Model under Magnetic Field

Atsushi Tsuruta\textsuperscript{1}, Satoshi Hyodo\textsuperscript{1}, and Kazumasa Miyake\textsuperscript{2}

\textit{1}Division of Materials Physics, Department of Materials Engineering Science
Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan
\textit{2}Toyota Physical and Chemical Research Institute, Nagakute, Aichi 480-1192, Japan

(Received December 11, 2014)

The Bardeen-Cooper-Schrieffer (BCS)-Bose-Einstein condensation (BEC) crossover in the two-dimensional attractive Hubbard model under the magnetic field is discussed at the half-filling at $T = 0$ K on the basis of the formalism of Eagles and Leggett. It is shown that the so-called Fulde-Ferrel-Larkin-Ovchinikov (FFLO)-like state with a non-zero center-of-mass wave vector $q \neq 0$ is not stabilized in the weak-coupling (BCS) region, while such a state with $q \neq 0$ is stabilized against that with $q = 0$ even in a wide strong-coupling (BEC) region where di-fermion molecules are formed. The physical implication of this surprising result is discussed.

The problem of the Bardeen-Cooper-Schrieffer (BCS)-Bose-Einstein condensation (BEC) crossover has long been discussed after the BCS theory was established as the theory of superconductivity. The description of the crossover between these ground states is relatively simple in both three\textsuperscript{1–3} and two\textsuperscript{4, 5} dimensions. However, the crossover of the transition temperature $T_c$ is much more strongly involved because one has to properly take into account the center-of-mass (COM) degrees of freedom of pairs, as first discussed by Nozières and Schmitt-Rink.\textsuperscript{6}

In this decade, this problem has been revived in the context of research on cold atoms,\textsuperscript{7–9} after almost two decades since great interest was devoted to it in relation to high-$T_c$ cuprate superconductors, which were thought to be in the crossover region owing to the shortness of the Cooper pair size.\textsuperscript{10–13}

The purpose of this Letter is to clarify how the crossover of the ground state occurs under the magnetic field in the case of the attractive Hubbard model in two dimensions as a general problem that is not necessarily related to cold-atom systems. Namely, we discuss the crossover of the so-called Fulde-Ferrel-Larkin-Ovchinikov (FFLO)-like state. At first sight, the FFLO-like state is destabilized in the BEC limit where the tight di-fermion molecule is expected to be formed and to exhibit BEC with the zero COM wave vector at least in the free space. However, it is a nontrivial problem whether the COM wave vector of the di-fermion molecule is zero in the attractive Hubbard model on the square lattice near the half-filling owing to the cooperative effects of the lattice periodicity and the magnetic field.
The Hamiltonian of the attractive Hubbard model under the magnetic field used in the grand canonical ensemble is

\[ H = \sum_{\sigma} \left[ -t \sum_{(i,j)} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - \sum_i (\sigma H + \mu) c_{i\sigma}^\dagger c_{i\sigma} \right] - U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}, \tag{1} \]

where \( \mu \) is the chemical potential and \( \langle i, j \rangle \) means that the summation is taken over the nearest-neighbor pairs on the square lattice. In the \( k \)-representation, Eq. (1) is given in the form

\[ H = \sum_{\sigma} \sum_k (\xi_k - \sigma H) c_{k\sigma}^\dagger c_{k\sigma} - \frac{U}{N_L} \sum_k \sum_{k'} c_{k+q/2\uparrow}^\dagger c_{k+q/2\uparrow} c_{-k+q/2\downarrow}^\dagger c_{-k+q/2\downarrow}, \tag{2} \]

where \( N_L \) is the number of lattice points, and \( \xi_k \) is the kinetic energy of fermions measured from the chemical potential \( \mu \),

\[ \xi_k = -2t(\cos k_x a + \cos k_y a) - \mu, \tag{3} \]

where \( a \) is the lattice constant. The mean-field Hamiltonian for Eq. (2) is given in a generalized BCS formula as discussed in the FFLO problem: \(^{14,15}\)

\[ H_{\text{MF}} = \sum_k \left[ (\xi_k + q/2 - H) c_{k+q/2\uparrow}^\dagger c_{k+q/2\uparrow} + (\xi_{-k+q/2} + H) c_{-k+q/2\downarrow}^\dagger c_{-k+q/2\downarrow} \
- \Delta_q c_{-k+q/2\downarrow}^\dagger c_{k+q/2\uparrow} - \Delta_q c_{k+q/2\uparrow}^\dagger c_{-k+q/2\downarrow} + \Delta_q (c_{k+q/2\uparrow}^\dagger c_{-k+q/2\downarrow}) \right], \tag{4} \]

where \( \langle \cdots \rangle \) is the grand canonical ensemble average concerning the mean-field Hamiltonian Eq. (4) itself, and the gap \( \Delta_q \) satisfies the self-consistent equation

\[ \Delta_q = \frac{U}{N_L} \sum_k \langle c_{-k+q/2\downarrow}^\dagger c_{k+q/2\uparrow} \rangle. \tag{5} \]

The eigenvalue problem of this Hamiltonian is solved independently for each wave vector \( k \) and the COM wave vector \( q \) following the method adopted by Leggett in Ref. 16. In the Hilbert space with a fixed \( k \) and a fixed \( q \), eigenvalues are given as

\[ E_{\text{GP}} = \frac{1}{2} \left( \xi_{k+q/2} + \xi_{-k+q/2} \right) - \sqrt{(\xi_{k+q/2} + \xi_{-k+q/2})^2 + 4\Delta_q^2}, \tag{6} \]
\[ E_{\text{EP}} = \frac{1}{2} \left( \xi_{k+q/2} + \xi_{-k+q/2} \right) + \sqrt{(\xi_{k+q/2} + \xi_{-k+q/2})^2 + 4\Delta_q^2}, \tag{7} \]
\[ E_{\text{BP}^+} = \xi_{k+q/2} - H, \tag{8} \]
\[ E_{\text{BP}^-} = \xi_{-k+q/2} + H. \tag{9} \]

The energy level scheme under the magnetic field \( H \) is shown in Fig. 1. The ground state in this restricted Hilbert space is the ground-pair (GP) state if \( (\xi_{-k+q/2} - H) > \Xi_{k,q} \) and the broken-pair (BP\(^+\)) state with the up spin if \( (\xi_{-k+q/2} - H) < \Xi_{k,q} \). Taking this fact into
account, the gap equation at $T = 0$ is given as

$$\Delta_q = \frac{U}{N_L} \sum_k \frac{\Delta_q}{\sqrt{(\xi_{k+q/2} + \xi_{-k+q/2})^2 + 4\Delta_q^2}} \theta(\xi_{k+q/2} - H - \Xi_{k,q}).$$

(10)

where $\theta$ is the Heaviside function. Similarly, the total number of fermions per site at $T = 0$ is given as

$$N = \frac{1}{N_L} \sum_k \left[ 1 - \frac{\xi_{k+q/2} + \xi_{-k+q/2}}{\sqrt{(\xi_{k+q/2} + \xi_{-k+q/2})^2 + 4\Delta_q^2}} \right] \theta(\xi_{k+q/2} - H - \Xi_{k,q})$$

$$+ \frac{1}{N_L} \sum_k \left[ 1 - \theta(\xi_{k+q/2} - H - \Xi_{k,q}) \right] \theta(H - \xi_{k+q/2}).$$

(11)

Equation (11) determines the chemical potential $\mu$ as a function of $U$. Then, Eqs. (10) and (11) should be solved simultaneously as in the theoretical framework of Eagles$^2$ and Leggett$^3$.

With the use of thus-determined $\Delta_q$ and $\mu$, the ground-state energy per site with a fixed $q$ is given as

$$E_0 = \frac{1}{N_L} \sum_k \left[ \Xi_{k,q} + \frac{\Delta_q^2}{\sqrt{(\xi_{k+q/2} + \xi_{-k+q/2})^2 + 4\Delta_q^2}} \right] \theta(\xi_{k+q/2} - H - \Xi_{k,q})$$

$$+ \frac{1}{N_L} \sum_k (\xi_{k+q/2} - H) \left[ 1 - \theta(\xi_{k+q/2} - H - \Xi_{k,q}) \right] \theta(H - \xi_{k+q/2}).$$

(12)

The true ground-state energy is determined so that the energy given by Eq. (12) becomes minimum with the relaxation of the COM wave vector $q$.

$q = 0, H = 0$ 

$q \neq 0, H \neq 0$

$\xi_k$ 

$\sqrt{\xi_k^2 + \Delta^2} \quad \sqrt{\xi_k^2 + \Delta^2}$

$E_{EP}$ $E_{BP}^+$ 

$E_{BP}$ $E_{GP}$

$H = 0 \quad H \rightarrow$

Fig. 1. Energy level scheme, Eqs. (6)--(9), under the magnetic field $H$ in the Hilbert space with a fixed $k$ and a fixed $q$.

We solve the self-consistent equations (10) and (11) numerically by dividing the first Brillouin zone up to $1000 \times 1000$ meshes; we then determine the ground-state energy given by Eq. (12) for a fixed COM wave vector $q$. Then, we seek the wave vector $q$ that minimizes $E_0$. 

3/10
given by Eq. (12). The filling of electrons is restricted within the case of half-filling, otherwise stated explicitly. We have verified that the results are essentially independent of the mesh size of the first Brillouin zone even if the mesh size decreases from $900 \times 900$ to $500 \times 500$. Figure 2 shows some examples of the distribution of the ground-state energy $E_0$ in the space of the COM wave vector $q$ for $U = 6t$ and $H/t = 0$ [Fig. 2(a)], $H/t = 1.0$ [Fig. 2(b)], and $H/t = 1.6$ [Fig. 2(c)].

In the case of $U/t = 6$, for the magnetic field $0 < H/t < 2.05$, the COM wave vector minimizing the ground-state energy, Eq. (12), is $q=(q_x, q_y = 0)$ or $q=(q_x = 0, q_y)$. Such $q_x$ is drawn in Fig. 3(a), together with the ground-state energy $E_0/t$ [Fig. 3(b)], and the superconducting gap $\Delta_q/t$ [Fig. 3(c)]. It is remarked that $q_x = 0$ holds up to $H/t = H^*/t \simeq 1.53$ where a first order transition occurs from the state with $q_x = 0$ to that with $q_x \neq 0$. The transition to the normal state at $H/t \simeq 2.05$ is a second order.

We have searched for the COM wave vector minimizing the ground-state energy, Eq. (12), for a series of sets of $U/t$ and $H/t$. The resultant phase diagram in the $U/t$-$H/t$ plane is shown in Fig. 4 where the second-order transition is indicated by the solid lines and the first-order transition by the dashed lines. It is remarkable that the FFLO-like state with $q \neq (0, 0)$ does not exist in the region of attractive interaction $U < U^*, U^*/t \simeq 2.0$, which is a new aspect of issues on the possibility of the FFLO-like state in lattice systems. Indeed, in the ground state of the continuum model, there always exists the FFLO-like state between the conventional pairing state with $q=(0,0)$ and the normal state.$^{14,15,17}$

The reason why the conventional Cooper pair with $q = 0$ is stable against the magnetic field up to $H = H^*$ is understood as follows: In the case of $H = 0$, Cooper pair formation is promoted by the diverging density of states due to the van Hove singularity in addition to the usual Cooper effect, as shown in Fig. 5(a). Even under the weak magnetic field, this additional
Fig. 3. (a) $q_x$, $x$-component of COM wave vector, (b) ground-state energy $E_0/t$ given by Eq. (12), and (c) superconducting gap $\Delta_q/t$ as a function of attractive interaction $H/t$.

The phase diagram in a wider region of parameters $H/U-U/t$ is shown in Fig. 6. Note that there exists a region where the pairing with $q=(\pi, \pi)$ is stabilized in the strong-coupling region $U/t \sim 12$ and $H/U \sim 0.28$. The attractive interaction is larger than the half bandwidth $W/t = 4$ so that the BEC region is realized. At first sight, this is somewhat surprising because it seems difficult for a tightly bound “di-electronic molecule” to acquire the COM wave vector. However, it turns out to be rather natural considering the dispersion of electrons under the strong magnetic field larger than $W$, the half bandwidth, as shown in Fig. 7. Namely, the “molecule” is expected to form between the electron around the $\Gamma$ point $k=(0,0)$ with the
Fig. 4. Phase diagram of the ground state in $U/t-H/t$ plane. The solid and dashed lines represent the second-order and first-order transitions, respectively. The wave vector $q$ in regions I, II, and III are $(\delta_x, 0)$, $(\pi, 0)$ and $(\pi, \delta_y)$, respectively.

down spin (the bottom of the minority band) and that around the M point $k=(\pi, \pi)$ with the up spin (the top of the majority band), because the energy difference between the up-spin band and the down-spin band takes a minimum for such a combination of $k$ points, giving $q=(\pi, \pi)$. The FFLO-like state does not exist in the weak-coupling region even in the half-filling case and the case in which the next-nearest-neighbor hopping is finite. Details of effects of the next-nearest-neighbor hopping will be discussed elsewhere.

The Shiba transformation is defined as $^{18}$

$$
b^+_i = c^+_i,
\quad b^+_i = e^{iQ_0 \cdot R_i} c^+_i
\quad Q_0 = (\pi, \pi),
$$

where $R_i$ is the position vector in unit of the lattice constant $a$ of the simple square lattice. By
Fig. 5. (Color) (a) Schematic band dispersion along the wave vector $\Gamma$-X-M $[(k_x, k_y): (0, 0)-(\pi, 0)-(\pi, \pi)]$ without magnetic field, i.e., $H = 0$. The red line indicates the path of Cooper pair formation with $q = 0$. (b) Schematic band dispersion along the wave vector $\Gamma$-X-M $[(k_x, k_y): (0, 0)-(\pi, 0)-(\pi, \pi)]$ with magnetic field, i.e., $H \neq 0$. The red line indicates the path of Cooper pair formation with $q = 0$, while the blue line indicates that with $q \neq 0$.

Fig. 6. (Color) Phase diagram of ground state in $H/U-U/t$ plane.

This transformation, the attractive Hubbard model Eq. (1) is transformed into the repulsive Hubbard model. Adding the magnetic field in Eq. (1) corresponds to changing the chemical potential (the particle number density) in the repulsive Hubbard model. In the transformed world, the BCS state and charge density wave (CDW) state in Eq. (1) are transformed to the transverse spin density wave (SDW) state and longitudinal SDW state, respectively, in the transformed repulsive Hubbard model. The SU(2) symmetry in the repulsive Hubbard model is saved even if we change the chemical potential. Therefore, the degeneracy of the BCS state and CDW state is saved under the magnetic field in the attractive Hubbard model.
Here, we note that the charge density wave (CDW) state is degenerate with the BCS state in the system described by the model Hamiltonian Eq. (1). Therefore, one might wonder how the CDW state is influenced by the magnetic field. This issue is clarified by analysis using the so-called Shiba transformation. In this sense, the magnetic field affects the CDW state in the same manner as in the BCS state. Namely, the incommensurate component in CDW is expected to be induced by the magnetic field. The FFLO-like state with $q = (\pi, \pi)$, which is the yellow region in Fig. 6 corresponds to the Nagaoka ferromagnetic ordered state in the repulsive Hubbard model.

Hirsch$^{19}$ and many theorists investigated the SDW state in the repulsive Hubbard model. Although they did not investigate detailed properties of the SDW state, there exist differences between the results in Ref. 20 for the repulsive Hubbard model in the mean field approximation and our results for the attractive Hubbard model with the same mean field approximation. For example, in the repulsive Hubbard model, the incommensurate SDW state exists even in the weak-coupling region, and the SDW state with $q = (Q, Q) (0 < Q < \pi)$ can be stable near the half filling. On the other hand, in the attractive Hubbard model, the FFLO-like state does not exist in the weak-coupling region, and the FFLO-like state with $q = (\pi - Q, \pi - Q) (0 < Q < \pi)$, which corresponds to $q = (Q, Q) (0 < Q < \pi)$ in the repulsive Hubbard model through the Shiba transformation, is not the ground state in the entire region of the $U - H$ phase diagram. The reason for this difference is not clear at the moment. It is suggestive to note that the theory of Nozière and Schmitt-Rink for the transition temperature $T_c^6$ when applied to the attractive Hubbard model is not equivalent to $T_{SDW}$, the SDW transition temperature, but the equivalency is recovered in the fluctuation exchange (FLEX) approximation, which is applied
to the thermodynamic potential treated by Nozière and Schmitt-Rink. This implies that the equivalency between the attractive and repulsive Hubbard models is not always maintained if some sort of approximation is introduced.

In conclusion, we have investigated the BCS-BEC crossover in the attractive Hubbard model on the square lattice under the magnetic field at the half-filling at $T = 0$ K on the basis of the formalism of Eagles and Leggett. It has been shown that the so-called FFLO-like state with a nonzero center-of-mass wave vector $\mathbf{q} \neq 0$ is not stabilized in the weak-coupling (BCS) region, while such a state with $\mathbf{q} \neq (0, 0)$ is stabilized against that with $\mathbf{q} = 0$ even in a wide strong-coupling (BEC) region. In particular, $\mathbf{q} = (\pi, \pi)$ in the strong coupling limit $U \gg W$.

**Acknowledgments**

One of the authors (K.M.) has benefited from conversations on BCS-BEC crossover with H. Tamaki in the very early stage of this work. This work was supported by a Grant-in-Aid for Scientific Research on Innovative Areas “Topological Quantum Phenomena” (No. 22103003) from the Ministry of Education, Culture, Sports, Science and Technology and by a Grant-in-Aid for Scientific Research (No. 25400369) from the Japan Society for the Promotion of Science.
References

1) Y. Wada, Prog. Theor. Phys. 24, 920 (1960); Y. Wada, Prog. Theor. Phys. 25, 713 (1961); Y. Wada, Prog. Theor. Phys. 26, 321 (1961).
2) D. M. Eagles, Phys. Rev. 186, 456 (1969).
3) A. J. Leggett, Modern Trends in the Theory of Condensed Matter ( Lecture Notes of the 1979 Karpacz Winter School). A. Pekalski and J. Przystawa (Springer-Verlag, Berlin, 1980) p. 14.
4) K. Miyake, Prog. Theor. Phys. 69, 1794 (1983).
5) M. Randeria, J.-M. Duan, and L.-Y. Shieh, Phys. Rev. Lett. 62, 981 (1989).
6) P. Nozières and S. Schmitt-Rink, J. Low Temp. Phys. 59, 195 (1985).
7) Y. Ohashi and A. Griffin, Phys. Rev. Lett. 89, 130402 (2002).
8) See, for example, Q. Chen, J. Stajic, S. Tan, and K. Levin, Phys. Rep. 412, 1 (2005) and references therein.
9) H. Tamaki, Y. Ohashi, and K. Miyake, Phys. Rev. A 77, 063616 (2008).
10) See, for example, R. Micnas, J. Ranninger, and R. Robaszkiewicz, Rev. Mod. Phys. 62, 113 (1990).
11) M. Randeria, in Bose-Einstein Condensation, eds. A. Griffin, D. W. Snoke, and S. Stringari (Cambridge University Press, Cambridge, 1995) p. 355.
12) S. Schmitt-Rink, C. M. Varma, and A. Ruckenstein, Phys. Rev. Lett. 63, 445 (1989).
13) A. Tokumitsu, K. Miyake, and K. Yamada, Phys. Rev. B 47, 11988 (1993).
14) P. Fulde and R. A. Ferrel, Phys. Rev. 135, A550 (1964).
15) A. I. Larkin and Y. N. Ovchinikov, Sov.-Phys. JETP 20, 762 (1965).
16) A. J. Leggett, Rev. Mod. Phys. 47, 331 (1975).
17) See, for example, R. Casalbuoni and G. Nardulli, Rev. Mod. Phys. 76, 263 (2004).
18) H. Shiba, Prog. Theor. Phys. 48, 2171 (1972).
19) J. E. Hirsch, Phys. Rev. B 31, 4403 (1985).
20) P. A. Igoshev, M. A. Timirgazin, A. A. Katanin, A. K. Arzhnikov, and V. Yu. Irkhin, Phys. Rev. B 81, 094407 (2010).
21) H. Tamaki, K. Miyake, and Y. Ohashi, J. Phys. Soc. Jpn. 78, 073001 (2009).