Molecular wavefunction and tunneling properties of a bound pair of Fermi atoms in an optical lattice

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Abstract. We investigate tunneling properties of a bound pair of Fermi atoms in an optical lattice. Including a realistic cosine-shape optical lattice potential, we calculate the molecular wavefunction $\Psi$. Starting from the weak-coupling regime, we show how $\Psi$ shrinks as one increases the strength of a pairing interaction between atoms. When the molecular size becomes comparable to the lattice constant in the intermediate coupling regime, we find from the spatial structure of $\Psi$ that the molecular tunneling between lattice sites is accompanied by virtual dissociation. This phenomenon is shown to be suppressed in the strong-coupling regime due to very strong binding energy. We point out that, while the molecular tunneling accompanied by virtual dissociation can be described by the Hubbard model, it cannot describe the molecular tunneling with no virtual dissociation in the strong-coupling regime.

1. Introduction

Recently, cold atom gases loaded on optical lattices have attracted much attention[1]. In an optical lattice produced by standing wave of laser light, atoms feel a cosine-shape periodic potential. Since this system is close to the Hubbard model, where particles are hopping between lattice sites interacting with each other when they meet at the same site, this system is also expected to be useful for the study of strongly-correlated systems, such as high-$T_c$ cuprates.

Another advantage of cold atom gases is the tunable interaction associated with a Feshbach resonance[2]. Using this unique technique, the BCS-BEC crossover[3, 4, 5, 6] has been realized in the absence of optical lattice[7, 8, 9, 10]. Thus, it is an interesting problem how the BCS-BEC crossover phenomenon is modified by optical lattice. In this regard, we note that the superfluid state has been recently realized in a $^6$Li lattice Fermi gas[11].

In the strong-coupling BEC regime of an attractive Hubbard model, Nozi`eres and Schmitt-Rink[4] showed that the hopping of tightly bound molecule between lattice sites is accompanied by virtual dissociation. This leads to the enhancement of effective molecular mass as $M \sim U_H/t^2$, as well as the suppression of superfluid phase transition temperature as $T_c \sim t^2/U_H$[12] (where $U_H$ and $t$ are an attractive on-site interaction and atomic nearest-neighbor hopping, respectively). On the other hand, Orso and co-workers[13, 14] considered a bound state problem in a cosine-shape periodic potential, and showed that $M$ approaches a constant value in the strong-coupling limit. Their result implies that the simple Hubbard model (consisting of $t$ and $U_H$) cannot describe the strong-coupling regime of a superfluid Fermi gas in an optical lattice.

In this paper, we investigate tunneling properties of a bound pair of Fermi atoms in an optical lattice. Including a realistic cosine-shape periodic potential, we calculate the molecular
wavefunction $\Psi$. We examine whether or not the virtual dissociation predicted in the Hubbard model occurs in the case of cosine-shape periodic potential. We also calculate the effective molecular mass $M$ and compare it with the result obtained based on the Hubbard model. Throughout this paper, we set $\hbar = 1$.

2. Formulation

We consider a bound state of attractively interacting two Fermi atoms in different hyperfine states described by pseudospin $\sigma = \uparrow, \downarrow$. We assume a three dimensional system with a one-dimensional optical lattice in the $x$-direction. We also assume the $s$-wave pairing interaction $-U\delta(r_1 - r_2)$, so that the singlet bound state $|S = 0, S_z = 0\rangle$ is possible. The Hamiltonian is given by

$$H_0(r) = \frac{\hat{P}^2}{2m} + \frac{E_s}{2}(1 - \cos\left(\frac{2\pi}{l}x\right)).$$  \hspace{1cm} (1)

Here, $m$ is the atomic mass and $l$ is the lattice constant. The potential height ($E_s$) is measured in terms of the atomic recoil energy $E_s \equiv \pi^2/2ml^2$. In this model, the spatial part of the bound state wavefunction has the form

$$\Psi_q(r_1, r_2) = \sum_{p, n_1, n_2} g_{p, n_1, n_2} \phi_{p + q/2}(r_1)\phi_{p + q/2}(r_2),$$  \hspace{1cm} (2)

where $\phi_p(x) \equiv e^{ip\cdot x}u_p(x)$ is a Bloch function of $H_0(r)$ with the energy $\varepsilon_p = \varepsilon_{p_x} + (p_y^2 + p_z^2)/2m$. $u_p(x)$ satisfies $u_p(x + l) = u_p(x)$. For the center of mass momentum $q$, since we are interested in the motion in the $x$-direction, we set $q = (q, 0, 0)$. Substituting Eq. (2) into the Schrödinger equation $H\Psi_q = E_q\Psi_q$, we obtain the eigenvalue equation

$$f_{p, n_1, n_2}^{n_1, n_2} = \sum_{p_y, p_z} g_{p, n_1, n_2} U \sum_{x} \varepsilon_{p + q/2}^{-n_1} + \varepsilon_{p - q/2}^{-n_2} - E_q \int dx u_{p_x + q/2}(x)u_{p_x - q/2}(x)u_{k_x + q/2}(x)u_{k_x - q/2}(x) f_{k_x}^{n_1, n_2}.$$  \hspace{1cm} (3)

We numerically solve Eq. (3) to determine $E_q$ and $f_{p, n_1, n_2}^{n_1, n_2}$. As usual, Eq. (3) involves the ultraviolet divergence originating from the contact interaction $U\delta(r_1 - r_2)$. We eliminate this singularity by introducing the two-body atomic $s$-wave scattering length $a_s$ given by $4\pi a_s/m = -U/(1 - U\sum_p m/p^2)$. The molecular binding energy $E_{\text{bind}}$ is given by $E_{\text{bind}} = |E_q = 0\rangle$. The effective molecular mass $M$ is calculated from $M^{-1} \equiv (\partial^2 E_q/\partial q^2)_{q=0}$. For the molecular wavefunction, to see the spatial variation in the $x$-direction, we set $y_1 = y_2 \equiv y$ and $z_1 = z_2 \equiv z$ in Eq. (2). Introducing $R \equiv (x_1 + x_2)/2$ and $x \equiv x_2 - x_1$, we have

$$\Psi_q(R, x) \equiv \Psi_q(x_1, y, z; x_2, y, z) = e^{iqR} \sum_{p_s, n_1, n_2} f_{p_s, n_1, n_2}^{n_1, n_2} u_{p_s + q/2}(R - x/2)u_{p_s - q/2}(R + x/2).$$  \hspace{1cm} (4)

3. Molecular wavefunction and effective mass

Figure 1 shows the calculated molecular wavefunction $\Psi_{q=0}(R, r)$. When the interaction is weak (panels (a) and (b)), $\Psi_{q=0}(R, r)$ spreads out due to the weak binding energy $E_{\text{bind}}[15]$. When we simply substitute this $E_{\text{bind}}$ into the expression for the molecular wavefunction ($\equiv \Psi_{\text{uniform}}(r)$) in the absence of the lattice (dashed line in panel (a)), we find that, apart from the oscillating structure, the overall spatial variation of $\Psi_{q=0}(R, r)$ is well described by $\Psi_{\text{uniform}}(r)$. 

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staying at the bottom of the periodic potential. In the case of Fig. 1(a) (the two, except for the one at the fine structures seen around the motion of molecule is model with the one obtained from the single-band Hubbard model, interaction, the peaks at regime of the Hubbard model[4]. However, when we further increase the strength of the pairing process. (The same result is also obtained when the molecule moves from R = 0. In the relative coordinate, this leads to the peaks at R = x2 − x1 = 0, ±2l, ±4l, · · · , as shown in Fig. 1(a). In the same way, to realize R = 0.5l, one may put two atoms at x1 = jl + l and x2 = −jl, leading to the peaks shown in Fig. 1(b) (r = ±l, ±3l, · · · ). As the pairing interaction becomes strong, the molecular wavefunction shrinks. In Fig. 1(e), only one large peak exists around r = 0, showing that both atoms are localized around x = 0 when R = 0. In contrast, Fig. 1(d) (R = 0.5l) shows peaks at r = ±l in addition to a sharp peak at r = 0. This means that, when one of the two atoms exists around x = 0, the other atom can exist around the bottoms of the periodic potential at x = ±l when R = 0.5l. Namely, when the molecule moves from R = 0 to R = l, it dissociates into two atoms in the tunneling process. (The same result is also obtained when q ̸= 0, although we do not show the result here.) This behavior just corresponds to the virtual dissociation obtained in the strong-coupling regime of the Hubbard model[4]. However, when we further increase the strength of the pairing interaction, the peaks at x = ±l completely disappear, as shown in Fig. 1(f). This indicates that the motion of molecule is not accompanied by dissociation in the strong-coupling regime[13, 14].

To see the validity of the Hubbard model, we compare the molecular mass M in the present model with the one obtained from the single-band Hubbard model,

\[
H_{\text{Hubbard}} = \sum_{p, \sigma} \varepsilon_{p, \sigma} c_{p, \sigma}^\dagger c_{p, \sigma} - U_{H} \sum_{p, p', k} c_{p+\mathbf{k}/2, \uparrow}^\dagger c_{p' - \mathbf{k}/2, \downarrow}^\dagger c_{p'} c_{p}. \tag{5}
\]

Here, c_{p, \sigma}^\dagger is the creation operator of a Fermi atom with pseudospin \( \sigma = \uparrow, \downarrow \). For the kinetic energy, the lowest energy band \( \varepsilon_{p, \sigma}^{\text{p}=1} = \varepsilon_{p, \sigma}^{\text{p}=1} + (p_y^2 + p_z^2)/2m \) obtained from Eq. (1) is used. The value of \( U_{H} \) is determined so that Eq. (5) can reproduce the binding energy \( E_{\text{bind}} \) obtained in the case of cosine-shape periodic potential.
Figure 2. Effective molecular mass $M$ in optical lattice as a function of the pairing interaction. The dashed line shows the molecular mass obtained from the single-band Hubbard model given by Eq. (5).

Figure 2 shows the calculated effective molecular mass $M$ as a function of the pairing interaction. We find that the Hubbard model can reproduce $M$ for $(a_s/l)^{-1} \lesssim 1$. In the strong-coupling regime $(a_s/l)^{-1} \gtrsim 1$, the Hubbard model overestimates the value of $M$, reflecting the fact that it cannot describe the correct molecular tunneling in this regime.

4. Summary
In this paper, we have investigated tunneling properties of a bound pair of Fermi atoms in an optical lattice. We calculated the molecular wavefunction, including a realistic cosine-shape periodic potential. We showed that the molecular tunneling accompanied by virtual dissociation, which has been obtained in the Hubbard model, also occurs in optical lattice in the intermediate coupling regime. This virtual dissociation is, however, suppressed in the strong-coupling regime. We also compared the molecular mass obtained in the present model with that calculated in the single-band Hubbard model. While the Hubbard model can reproduce $M$ in the weak and intermediate coupling regime, it overestimates the value of $M$ in the strong-coupling regime. Our result indicates that an additional term to describe the molecular tunneling without dissociation is necessary in considering the entire BCS-BEC crossover regime of a superfluid Fermi gas in an optical lattice using the Hubbard model.

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[15] In a uniform system, a bound state is possible only when $a_s > 0$. On the other hand, a molecular formation becomes possible even when $a_s < 0$ in the presence of a lattice potential[13, 14].