States of fermionic atoms in an optical superlattice across a Feshbach resonance

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We investigate states of fermionic atoms across a broad Feshbach resonance in an optical superlattice which allows interaction only among a small number of lattice sites. The states are in general described by superpositions of atomic resonating valence bonds and dressed molecules. As one scans the magnetic field, level crossing is found between states with different symmetry properties, which may correspond to a quantum phase transition in the many-body case.

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I. INTRODUCTION

The past several years have seen many new developments in ultracold atomic physics \[1,2\]. Two experimental control techniques have played a critical role in these advances: the use of optical lattices to produce diverse interaction configurations \[3\], and Feshbach resonance to control the strength of the interactions between atoms \[4\]. This has motivated significant interest in combining these two techniques \[5,6,7,8\].

Close to a broad Feshbach resonance, one then has a typical wide Feshbach resonance such as with \[9\]. As one scans the magnetic field, level crossing is found between states with different symmetry properties, which may correspond to a quantum phase transition in the many-body case.

We investigate states of fermionic atoms across a broad Feshbach resonance in an optical superlattice. The two-body physics on a single site has been solved exactly in \[8\] under typical experimental configurations \[9\]. Two experimental control techniques have played a critical role in these advances: the use of optical lattices to produce diverse interaction configurations \[3\], and Feshbach resonance to control the strength of the interactions between atoms \[4\]. This has motivated significant interest in combining these two techniques \[5,6,7,8\].

In this paper, we make use of the above effective Hamiltonian \(H_{\text{eff}}\) to study the physics of this strongly correlated system with interactions among a few lattice sites. In particular, we focus on investigation of the states of a single plaquette, which is a basic unit of the two-dimensional square lattice. This study has two purposes. First, understanding the states of atoms at a single plaquette is a necessary step towards the challenging goal of understanding the physics of this strongly interacting gas in a quasi-two-dimensional optical lattice. It is shown in \[8\] that for the case of a multiple-site lattice, one needs to take into account the direct collision interactions between the neighboring sites, as the magnitude of this interaction is larger than the atom tunneling rate for a typical wide Feshbach resonance such as with \(^{40}\text{K}\) or \(^{6}\text{Li}\) atoms. An effective two-body theory through the contractor renormalization procedure \(\[10\]\) will provide the basic entries for an effective many-body theory through the contractor renormalization procedure (a real-space renormalization group method for high dimensions) \(\[13,14\]\). We will see that even for a single plaquette, the behavior of the states has been pretty rich. The eigenstates involve resonating valence bonds and superposition of dressed molecules, and are highly entangled over different lattice sites. With variation of the parameters in the Hamiltonian \(H_{\text{eff}}\), there are sev-
eral level crossings for the lowest eigenstate with change of the state symmetry properties, which may correspond to a quantum phase transition for larger systems.

Second, the study of the physics of a single plaquette is also of practical relevance. For atoms in an optical superlattice, the physics can be dominated by the interactions within single plaquettes. A simple optical superlattice can be formed by adding two standing wave laser beams with commensurate wave vectors \(|\mathbf{k}_1|, |\mathbf{k}_2|\). The potential, say, along the \(x\) direction, has the form \(V(x) = -\left[ V_1 \sin^2 \left( \frac{\pi x}{L} \right) + V_2 \sin^2 \left( \frac{2\pi x}{L} \right) \right] \). If we choose the wave vector \(k_2 = 2k_1 = 2\pi/L\) and require \(0 < V_1 < 4V_2\), then we have potential barriers of two different heights (see FIG. 1). The minima occur at \(x = nL \pm x_0\) (for integer \(n\)), where

\[
x_0 = \frac{L}{2\pi} \cos^{-1} \left( \frac{-V_1}{4V_2} \right)
\]

The lower and higher potential barriers \(V_{\text{low}}\) and \(V_{\text{high}}\) are given respectively by

\[
V_{\text{low}} = \left( 1 - \frac{V_1}{4V_2} \right)^2 V_2
\]
\[
V_{\text{high}} = \left( 1 + \frac{V_1}{4V_2} \right)^2 V_2.
\]

The barrier \(V_{\text{high}}\) can be significantly larger than \(V_{\text{low}}\) if we choose \(V_1\) close to \(4V_2\), and such a high barrier turns off the interactions except for the ones between the sites separated by \(V_{\text{low}}\). If we apply this optical superlattice potential along both the \(x\) and \(y\) directions and a deep lattice potential along the \(z\) direction, we then have interactions dominantly within the single plaquettes in the \(x\)-\(y\) plane. With strongly interacting atoms in this optical superlattice potential, one can test the predictions from the effective Hamiltonian \(H_{\text{eff}}\), and detect the exotic entangled states emerging from the ground state configurations of \(H_{\text{eff}}\).

We should also point out that the effective Hamiltonian \(H_{\text{eff}}\) includes the Hubbard model as a particular case.

The Hubbard model is given by the Hamiltonian

\[
H_{Hub} = -t \sum_{<i,j>,\sigma} (a_i^\dagger \sigma a_j + H.c.) + U \sum_i n_i^\uparrow n_i^\downarrow,
\]

where \(n_i^\sigma = a_i^\dagger \sigma a_i\). Specifically, \(H_{\text{eff}}\) can be written in the form of \(H_{Hub}\) if we substitute \(d_i^\dagger a_i + H.c.\) and make a particular choice of the parameters in \(H_{\text{eff}}\) with \(t_a = -t, t_{da} = t, g = t, t_g = 0\), and \(\Delta = U\). So, one can see that \(H_{\text{eff}}\) extends the well-known Hubbard model \(H_{Hub}\) in a nontrivial way. Note that for strongly interacting atoms near a broad Feshbach resonance, the parameters \(g\) and \(t_{da}\) are significantly different from the atomic tunneling rate \(t\) due to the multi-band populations and the direct neighboring collisions. From the expressions of these parameters in Ref. [6], we estimate that typically \(|t_{da}| \ll |t_a| \ll |t_{da}| \sim |g|\). This is because \(t_a\) corresponds to atomic tunneling in the single lowest band, whereas \(t_{da}\) and \(g\) correspond to interactions involving the dressed molecule states (which are superpositions of states in multiple upper bands). For the numerical calculations in this work, we typically take \(t_{d} \sim 0, -t_a \sim 0.1|g|-0.3|g|\), and \(t_{da} \sim |g|-2|g|\). (Note from the form of \(H_{\text{eff}}\) that the sign of \(g\) is essentially irrelevant, as it can be incorporated into the definition of \(d_i^\dagger\).) The parameter \(\Delta\) is sensitive to the external magnetic field, and can be scanned from the value much smaller than \(-|g|\) to the value much larger than \(|g|\).

The atomic states within each plaquette critically depend on the atom number and the spin configuration in that plaquette. In the following, we will consider all the different nontrivial cases with different numbers of spin \(\uparrow\) and \(\downarrow\) atoms occupying the four-site plaquette.

II. FOUR ATOMS PER PLAQUETTE: TWO \(\uparrow\), TWO \(\downarrow\)

Over most of the typical range of the parameter values, the plaquette occupied by two \(\uparrow\) and two \(\downarrow\) atoms has two distinct types of ground states, with a level crossing occurring at some critical value of \(\Delta\). These two types of states can be distinguished by how they transform under a 90° rotation in the plane of the plaquette. Under such a rotation, the ground state wavefunction for \(\Delta\) less than (greater than) the critical value is multiplied by a factor of +1 (−1). Thus, we say that the phase on the negative side of the transition has s-wave symmetry, and that on the positive side has d-wave symmetry.

The ground states of each of these two types change smoothly with changes in the parameter \(\Delta\). Thus, we can identify particular energy eigenstates as the “s-wave state” and the “d-wave state” over the full range of \(\Delta\), even as the exact form of the eigenstate changes. (Note that these are not the only eigenstates with s-wave and d-wave symmetry – here we use these terms to refer solely to those states which are the ground states when the system is in the corresponding parameter regions.) The
energies of the s-wave and d-wave states can be easily
calculated through exact diagonalization, and they are plotted
in FIG. 2(a), which illustrates the crossover between them.
(For this figure, we scan $\Delta$ and set the other pa-
rameters of $H_{\text{eff}}$ to their typical values with $t_{\text{da}} = 1.5|g|$ and $t_a = 0.2|g|$.) The energy gap between the ground
state and 1st excited state is shown in FIG. 2(b)).

To understand the properties of the ground state, it is
important to have its explicit expression. Although one
can calculate this explicit expression through numerical
exact diagonalization, the state is in general a superposi-
tion of many basis-vectors (36 vectors in this case), with
all the superposition coefficients varying with $\Delta$. It is
troublesome to understand the state’s properties from
this lengthy expression. To overcome this problem, we
describe the s-wave and d-wave states more compactly,
in a way that illustrates their rotational symmetry, by
means of a pictorial representation which we define here.

The four sites of a plaquette we label as: 3 4. We place
various pictures on these sites corresponding to creation
operators applied at those sites. The whole picture repres-
ents the product of these operators, applied to the vac-
uum state $|0\rangle$. For instance, $\uparrow$ placed on two sites (either
horizontally, vertically, or diagonally) represents a nor-
malized singlet between those two sites. So, if the sites
are labeled $i$ and $j$, this represents
\[
\frac{1}{\sqrt{2}} (a_i^\dagger a_j - a_i a_j^\dagger).
\]
(Note that the order of $i$ and $j$ does not matter, as the
anti-commutation of $a_i^\dagger$ and $a_j^\dagger$ makes the singlet sym-
metric under exchange of $i$ and $j$.) $\otimes$ represents a
dressed molecule. (I.e., if located at site $i$, this pic-
ture corresponds to $d_i^\dagger$.) $\otimes$ represents an unoccupied site.
The creation operators that make up a singlet are always
grouped together; other than that, the order of the oper-
ators is irrelevant, as the singlets and dressed molecules
commute. As an example, the picture $\uparrow$\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure2.png}
\caption{Energy vs. $\Delta$ for a plaquette occupied by two $\uparrow$ and
two $\downarrow$ atoms. Other parameters are $t_{\text{da}} = 1.5|g|$, $t_a = -0.2|g|$,
and $t_d = 0$ (a): Eigenenergies of the s-wave ($\circ$) and d-wave ($\times$)
states. (b): Energy difference (gap) between ground state
and first excited state. The gap vanishes at the level crossing
point. Because the eigenenergies vary smoothly with $\Delta$, the
curve is smooth except at the level crossing points for the
ground state (where the gap is zero) and for the first excited
state (indicated by arrows).
\end{figure}

Thus the s-wave and d-wave ground states, respectively, are:

\[ |\psi\rangle_s = s_1 |1\rangle_s + s_2 |2\rangle_s + s_3 |3\rangle_s + s_4 |4\rangle_s, \quad (5) \]
\[ |\psi\rangle_d = d_1 |1\rangle_d + d_2 |2\rangle_d + d_3 |3\rangle_d, \quad (6) \]

They are superpositions of many different distribution patterns of the dressed molecules and the atomic valence bonds (spin singlets). The values of the superposition coefficients are shown in FIG. 3 as a function of the ratio \( \Delta/|g| \). Note that in the limiting case \( \Delta/|g| \gg 1 \), the effective Hamiltonian \( H_{\text{eff}} \) reduces to the t-J model. Indeed, one can see from FIG. 3 that the state \( |\psi\rangle_d \) in that limit tends to the ground state \( |3\rangle_d \) of the t-J model on a plaquette.

Projected onto these subspaces, \( H_{\text{eff}} \) (with \( t_d \simeq 0 \)) expressed in terms of the bases shown above becomes:

\[
H_s = \begin{pmatrix}
2\Delta & -2\sqrt{3}g & 0 \\
-2\sqrt{3}g & \Delta & -2g \\
0 & \sqrt{2}(t_a + t_{da}) & \Delta \\
0 & 0 & 0
\end{pmatrix} \quad (7)
\]

for the s-wave state, and:

\[
H_d = \begin{pmatrix}
2\Delta & -2g & 0 \\
-2g & \Delta & -2\sqrt{3}g \\
0 & 0 & 0
\end{pmatrix} \quad (8)
\]

for the d-wave state. The lowest energy eigenstates of these two Hamiltonians are the s-wave and d-wave states (respectively) of the full Hamiltonian \( H_{\text{eff}} \). (See solid lines on FIG. 3.)

For a small portion of the range of the parameter values \( t_{da}/|g| \) and \( t_a/|g| \) there is another type of ground state, which occurs for \( \Delta \) between the s-wave and d-wave states above. For this type, the ground state also has s-wave rotational symmetry. However, the states \( \uparrow \) and \( \downarrow \) are in a triplet configuration, rather than the singlet occurring in the other two types of states \( |\psi\rangle_s \) and \( |\psi\rangle_d \).

The region of the parameter space for which this triplet phase occurs is shown in FIG. 4. The eigenenergies of the s-wave singlet, s-wave triplet, and d-wave singlet states are shown in FIG. 4(a) for \( t_{da} = 2|g|, t_a = -0.3|g| \) (which is within the range where the triplet ground state occurs.) The gap between the ground state and first excited state for \( t_{da} = 2|g|, t_a = -0.3|g| \) is shown in FIG. 4(b).

The s-wave triplet state can be written as a linear combination of three states:

\[
|1\rangle_{\text{trip}} = \frac{1}{2\sqrt{2}} \left( \begin{array}{c}
\ast \\
\ast \\
\ast \\
\ast
\end{array} \right)
\]

\[ |2\rangle_{\text{trip}} = \frac{1}{\sqrt{2}} \left( \begin{array}{c}
\ast \\
\ast \\
\ast \\
\ast
\end{array} \right)
\]
FIG. 5: Energy vs. $\Delta$ for a plaquette occupied by two $\uparrow$ and two $\downarrow$ atoms. Other parameters are $t_{da} = 2|g|$, $t_a = -0.3|g|$, $t_d = 0$ (a): Eigenenergies of the s-wave singlet ($\circ$), d-wave singlet ($\times$), and s-wave triplet ($+$) states. (b): Energy difference between ground state and first excited state. Crossovers in the first excited state are indicated by arrows.

Here, the triplet wave function is given by:

$$|3\rangle_{\text{trip}} = \frac{1}{2\sqrt{2}} \left( \begin{array}{c} \bigcirc \bigcirc \bigcirc \bigcirc \\ \bigcirc \bigcirc \bigcirc \bigcirc \\ \bigcirc \bigcirc \bigcirc \bigcirc \end{array} \right)$$

where $i$ is the site of the black-filled circle, and $j$ is the site of the white-filled circle. Note that unlike the singlet, the triplet is not symmetric under exchange of $i$ and $j$:

$$\frac{1}{\sqrt{2}} \left( a_{i\uparrow}^{\dagger} a_{j\downarrow}^{\dagger} + a_{j\uparrow}^{\dagger} a_{i\downarrow}^{\dagger} \right) = -\frac{1}{\sqrt{2}} \left( a_{j\downarrow}^{\dagger} a_{i\uparrow}^{\dagger} + a_{i\downarrow}^{\dagger} a_{j\uparrow}^{\dagger} \right)$$

Projected onto the basis $\{ |1\rangle_{\text{trip}}, |2\rangle_{\text{trip}}, |3\rangle_{\text{trip}} \}$, $H_{\text{eff}}$ (with $t_d \approx 0$) becomes:

$$H_{\text{trip}} = \begin{pmatrix} \Delta & \sqrt{2}(t_{da} - t_a) & -2\sqrt{2}g \\ \sqrt{2}(t_{da} - t_a) & \Delta & 0 \\ -2\sqrt{2}g & 0 & 0 \end{pmatrix}$$

and the ground state of this Hamiltonian is the s-wave triplet state. It should also be noted that the s-wave triplet state is the first excited state of $H_{\text{eff}}$ in the limit of large positive $\Delta$.

III. FOUR ATOMS PER PLAQUETTE: THREE $\uparrow$, ONE $\downarrow$

The plaquette occupied by three $\uparrow$ and one $\downarrow$ atoms has only one type of ground state over the full range of $\Delta$. The ground state has s-wave symmetry (i.e. it is unchanged under 90° rotations in the plane of the lattice). The ground state energy is plotted in FIG. 6(a), and the energy difference between the ground state and the first excited state is shown in FIG. 6(b). For this figure the other parameters were $t_{da} = 1.5|g|$ and $t_a = -0.2|g|$. The ground state can be represented compactly in the pictorial representation introduced above. Here we add an additional symbol to represent a single atom in the $\uparrow$ state. Because the order of the fermionic creation operators matters, we use $\uparrow$ to represent the left creation operator and $\uparrow$ to represent the right creation operator.
The ground state of this Hamiltonian is the ground state of the full Hilbert space with basis vectors $|\uparrow \uparrow \rangle$, $|\uparrow \downarrow \rangle$, $|\downarrow \uparrow \rangle$, and $|\downarrow \downarrow \rangle$.

The ground state is:

$$|\psi\rangle_S = C_1 |1\rangle_S + C_2 |2\rangle_S + C_3 |3\rangle_S,$$

where

$$|1\rangle_S = \frac{1}{2\sqrt{2}} \begin{pmatrix} \uparrow \uparrow \\ \uparrow \downarrow \\ \downarrow \uparrow \\ \downarrow \downarrow \end{pmatrix},$$

$$|2\rangle_S = \frac{1}{2} \begin{pmatrix} \uparrow \uparrow + \uparrow \downarrow + \downarrow \uparrow + \downarrow \downarrow \\ \uparrow \uparrow + \uparrow \downarrow + \downarrow \uparrow + \downarrow \downarrow \end{pmatrix},$$

$$|3\rangle_S = \frac{1}{2\sqrt{2}} \begin{pmatrix} \uparrow \uparrow + \uparrow \downarrow + \downarrow \uparrow + \downarrow \downarrow \\ \uparrow \uparrow + \uparrow \downarrow + \downarrow \uparrow + \downarrow \downarrow \end{pmatrix}.$$

The values of the coefficients $C_1$, $C_2$, $C_3$ are shown in FIG. 7.

Projected onto the three-dimensional subspace of the full Hilbert space with basis vectors $|1\rangle_S$, $|2\rangle_S$, $|3\rangle_S$, $H_{eff}$ (for $t_d \approx 0$) is:

$$H_S = \begin{pmatrix} \Delta & \sqrt{2}(t_a - t_d) & -2\sqrt{2}g \\ \sqrt{2}(t_a - t_d) & \Delta & 0 \\ -2\sqrt{2}g & 0 & 0 \end{pmatrix}.$$

Thus, the ground state of this Hamiltonian is the ground state of $H_{eff}$. (See solid lines in FIG. 8.)

It should also be noted that the s-wave ground state for 3 $\uparrow$, 1 $\downarrow$ atoms per plaquette is degenerate with the triplet state for 2 $\uparrow$ and 1 $\downarrow$ atoms described in the previous section. In fact, the 2 $\uparrow$, 1 $\downarrow$ triplet state is identical to the ground state for 3 $\uparrow$ and 1 $\downarrow$ atoms and for 1 $\uparrow$ and 3 $\downarrow$ atoms, except that the triplet $\frac{1}{\sqrt{2}} (a_{i\uparrow}^\dagger a_{j\downarrow}^\dagger + a_{i\downarrow}^\dagger a_{j\uparrow}^\dagger)$ is replaced with $a_{i\uparrow}^\dagger a_{j\downarrow}^\dagger$ in the 3 $\uparrow$, 1 $\downarrow$ case, and with $a_{i\downarrow}^\dagger a_{j\uparrow}^\dagger$ in the 1 $\uparrow$, 3 $\downarrow$ case.

IV. TWO ATOMS PER PLAQUETTE: ONE $\uparrow$, ONE $\downarrow$

When occupied by only a single atom of each spin state, the plaquette has a single type of ground state for all values of $\Delta$ (for values of the other parameters within the typical range). This state is symmetric under 90° rotations – i.e., it has s-wave symmetry. The ground state energy of this system is plotted in figure 8(a). Figure 8(b) shows the excitation gap between the ground state and first excited state. Both these figures assume typical values of $t_{da}$ and $t_a$ ($t_{da} = 1.5|g|$, $t_a = -0.2|g|$, $t_d = 0$). (a): Ground state energy (b): Energy difference between ground state and first excited state. The curve is smooth except at a crossover in the first excited state (indicated by an arrow).
introduced above are:

\[ |1\rangle = \frac{1}{2} \left( \begin{array}{c} \Theta \Theta \vdots \vdots \\
\vdots \Theta \Theta \vdots \\
\vdots \vdots \Theta \Theta \\
\vdots \vdots \vdots \Theta \\
\end{array} \right) \]

\[ |2\rangle = \frac{1}{2} \left( \begin{array}{c} \Delta \vdots \\
\vdots \Delta \\
\vdots \vdots \\
\vdots \vdots \\
\end{array} \right) \]

Thus, the ground state is given by: \(|\psi\rangle = c_1 |1\rangle + c_2 |2\rangle + c_3 |3\rangle\), where the values of the coefficients \(c_1, c_2, c_3\) are shown in FIG. 9.

Projected onto this subspace, \(H_{eff}\) (for \(t_d \approx 0\)) expressed in the above basis becomes:

\[
H = \begin{pmatrix}
\Delta & -2\sqrt{2}g & 0 \\
-2\sqrt{2}g & 0 & 2\sqrt{2}t_d \\
0 & 2\sqrt{2}t_d & 0
\end{pmatrix}
\] (11)

Thus, the ground state of this Hamiltonian is the ground state of \(H_{eff}\). (See solid lines on FIG. 9)

V. THREE ATOMS PER PLAQUETTE: TWO \(\uparrow\), ONE \(\downarrow\)

The plaquette with two \(\uparrow\) atoms and one \(\downarrow\) atom has three distinct types of ground states for different values of the parameter \(\Delta\) (with the other parameters in the typical range). However, over a wide range of \(\Delta\) around \(\Delta = 0\) the system is in the same type of ground state. The ground state of this type is two-fold degenerate. (Hence, we will refer to this as the “degenerate state”.) The ground state energy and the gap between the ground state and first excited state are shown in FIG. 10 (For the full range of \(\Delta\) values shown in the figure, the system is in the degenerate state.) The degenerate ground states (which we call \(|\psi\rangle_+\) and \(|\psi\rangle_-\)) can be defined in such a way that they are eigenstates of a \(90^\circ\) rotation in the plane of the plaquette, in which case \(|\psi\rangle_\pm\) gains a factor of \(\pm i\) under such a rotation.

The state \(|\psi\rangle_+\) can be expressed as a vector in a particular six-dimensional subspace of the full Hilbert space. We define the basis vectors of this subspace in the pictorial representation introduced above. However, because the order of the fermionic creation operators matters, we use three symbols \(\uparrow, \uparrow, \wedge\) (\(\downarrow, \downarrow, \vee\)) to represent the first, second, and third creation operator for atoms in the \(\uparrow\) (\(\downarrow\)) state. E.g., \(\downarrow \uparrow \wedge = a_{\downarrow \uparrow}^\dagger a_{\uparrow \wedge}^\dagger |0\rangle\). Represented in this way, the six basis vectors are:

\[|1\rangle_+ = \frac{1}{2} \left[ \left( \begin{array}{c} \Theta \uparrow \uparrow \vdots \\
\vdots \Theta \uparrow \uparrow \\
\vdots \vdots \Theta \uparrow \\
\vdots \vdots \vdots \Theta \\
\end{array} \right) - i \left( \begin{array}{c} \Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\end{array} \right) \right] \]

\[|2\rangle_+ = \frac{1}{2} \left[ \left( \begin{array}{c} \Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\end{array} \right) - i \left( \begin{array}{c} \Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\end{array} \right) \right] \]

\[|3\rangle_+ = \frac{1}{2} \left[ \left( \begin{array}{c} \Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\end{array} \right) - i \left( \begin{array}{c} \Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\Theta \Theta \Theta \Theta \\
\end{array} \right) \right] \]

FIG. 9: Components of the ground state \((c_1: \Theta, c_2: x, c_3: \vee)\) vs. \(\Delta\) for a plaquette occupied by one \(\uparrow\) and one \(\downarrow\) atom. \((t_{da} = 1.5|g|, t_a = -0.2|g|, \ t_d = 0)\) The marked datapoints were computed from the full Hamiltonian \(H_{eff}\), whereas the solid lines were computed from the projected Hamiltonian \(H\).

FIG. 10: Energy vs. \(\Delta\) for a plaquette occupied by two \(\uparrow\) and one \(\downarrow\) atoms. \((t_{da} = 1.5|g|, \ t_a = -0.2|g|, \ t_d = 0)\) (a): Ground state energy (b): Energy difference between ground state and first excited state. Crossovers in the first excited state (at which points the curve is not smooth) are indicated by arrows.
The ground state of $H_{eff}$ is given by:

$$H_{+} = \begin{pmatrix}
\Delta & t_{da} & t_{a} & -ig & ig & 0 \\
-t_{da} & \Delta & -it_{a} & g & 0 & ig \\
t_{a} & it_{a} & \Delta & -2g & g & -ig \\
-ig & g & -2g & 0 & -it_{a} & t_{a} \\
0 & -ig & -t_{a} & 0 & t_{a} & 0 \\
0 & -ig & t_{a} & 0 & -t_{a} & 0
\end{pmatrix}$$

(16)

The ground state of $H_{+}$ is thus $|\psi\rangle_+$. (See solid lines in FIG. 11.) Projected onto the subspace with basis elements $\{1\}_+, \{2\}_+, \{3\}_+, \{4\}_+, \{5\}_+, \{6\}_+$, $H_{eff}$ is given by:

$$H_{-} = H_{+}^* = H_{+}^T$$

(17)

(Note that in this equation $H_{+}$ is still expressed in the basis in which it was defined above.) Thus the ground state of $H_{-}$ is $|\psi\rangle_{+}^* = |\psi\rangle_{-}$.

For $\Delta$ far to the negative side ($\Delta < -92.9 |g|$ for $t_{da} = 1.5 |g|$, $t_a = -0.2 |g|$, $t_d = 0$), the system of two $\uparrow$ atoms and one $\downarrow$ atom on a plaquette has a non-degenerate $d$-wave ground state. This state can be expressed as a vector in a 3-dimensional subspace of the full Hilbert space of this system, with basis vectors:

$$|1\rangle_{left} = \frac{1}{2\sqrt{2}} \begin{pmatrix}
\uparrow \uparrow \uparrow \\
\uparrow \uparrow \downarrow \\
\downarrow \uparrow \uparrow \\
\downarrow \uparrow \downarrow \\
\uparrow \downarrow \uparrow \\
\downarrow \downarrow \downarrow
\end{pmatrix}$$

$$|2\rangle_{left} = \frac{1}{2} \begin{pmatrix}
\downarrow \uparrow \uparrow \\
\uparrow \downarrow \uparrow \\
\downarrow \downarrow \uparrow \\
\downarrow \uparrow \downarrow \\
\uparrow \downarrow \downarrow \\
\downarrow \uparrow \uparrow
\end{pmatrix}$$
The ground state of this Hamiltonian is the ground state of \( H_{\text{eff}} \) in the left-most region \( (\Delta < -92.9 |g|) \).

For \( \Delta \) far to the positive side \( (\Delta > 97.9 |g|) \) for \( t_{da} = 1.5 |g| \), \( t_a = -0.2 |g| \), \( t_d = 0 \), the system has a non-degenerate s-wave ground state. Furthermore, in this state the ground state wavefunction and energy are constant for changing \( \Delta \). In the pictorial representation this ground state is given by:

\[
|\psi\rangle_{\text{right}} = \frac{1}{\sqrt{6}} \begin{pmatrix}
\uparrow \uparrow + \downarrow \uparrow + \downarrow \downarrow + \\
\uparrow \downarrow + \downarrow \uparrow + \uparrow \uparrow + \\
\uparrow \downarrow + \downarrow \uparrow + \downarrow \uparrow + \\
\end{pmatrix}
\]

The energy of this state is \( H_{\text{right}} = 2t_a \).

It should be noted that the case of 1 \( \uparrow \), 2 \( \downarrow \) atoms on a plaquette is equivalent to the 2 \( \uparrow \), 1 \( \downarrow \) case under exchange of \( \uparrow \) and \( \downarrow \) spins. The Hamiltonian \( H_{\text{eff}} \) is invariant under such a spin exchange, except for a change in the sign of \( g \). This is equivalent to replacing \( d^\dagger \) with \( -d^\dagger \). Thus, the eigenenergies of these two cases are identical, and the eigenstates are identical except for a change in the sign of the components which include a dressed molecule.

**VI. SUMMARY AND DISCUSSION**

In the above, we have investigated the ground state properties of the system with different numbers of spin \( \uparrow \) and \( \downarrow \) atoms occupying the four-site plaquette in an optical superlattice. All the other cases can be reduced to one of the configurations considered above, or to a trivial case, through the particle-hole exchange. (Cases where all particles are in the same spin state are non-interacting, and thus trivial.) For instance, for five atoms with three spin-\( \downarrow \) and two spin-\( \uparrow \), one has two spin-\( \uparrow \) and one spin-\( \downarrow \) holes in that plaquette. So, the states are equivalent to those in the case with two spin-\( \uparrow \) and one spin-\( \downarrow \) atoms, but with exchange of the parameters \( t_{da} \) and \( t_a \) in the effective Hamiltonian \( H_{\text{eff}} \). The sign of \( g \) also changes, but as noted above this is equivalent to replacing \( d^\dagger \) with \( -d^\dagger \). Thus this change has no effect on the eigenenergies, and the eigenstates only experience a change in the sign of those components where the plaquette is occupied by an odd number of dressed molecules. In addition, if particle-hole exchange changes the number of atoms by \( N \), then the eigenenergies are shifted by \( \frac{N}{2} \Delta \).

From this investigation, we have seen that even on a single plaquette, the Hamiltonian \( H_{\text{eff}} \) exhibits a number of different types of ground state configurations, possessing various forms of rotational symmetry (s-wave, d-wave, etc.). There are level crossings between these different types of ground states as the detuning \( \Delta \) is varied. The change of the ground state symmetry from s-wave to d-wave as one scans the parameter \( \Delta \) from negative to positive regions may be a general feature and not limited to a single plaquette. For a large lattice, this symmetry change might correspond to a quantum phase transition from the s-wave to the d-wave superfluidities [13]. The states found in this work on a single plaquette also provide some basic entries for constructing the effective many-body Hamiltonian for atoms in a quasi-two-dimensional optical lattice through the contractor renormalization method [13, 14]. When the average filling number of the lattice is close to a half with hole doping, one expects that the basic degrees of freedom from each plaquette are the ground state configurations specified in Sec. II, the fermionic hole excitations given by the states in Sec. V, the bosonic hole-pair excitations specified in Sec. IV, and the bosonic spin excitations given by the states in Sec. III and II. The effective many-body Hamiltonian will then describe the interaction between these basic degrees of freedom. So, it is our hope that the investigation of the single-plaquette physics here will make it possible to better understand the physics of strongly interacting fermions on larger lattices.

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