Feshbach resonant scattering of three fermions in one-dimensional wells

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We study the weak-tunnelling limit for a system of cold 40K atoms trapped in a one-dimensional optical lattice close to an s-wave Feshbach resonance. We calculate the local spectrum for three atoms at one site of the lattice within a two-channel model. Our results indicate that, for this one-dimensional system, one- and two-channel models will differ close to the Feshbach resonance, although the two theories would converge in the limit of strong Feshbach coupling. We also find level crossings in the low-energy spectrum of a single well with three atoms that may lead to quantum phase transition for an optical lattice of many wells. We discuss the stability of the system to a phase with non-uniform density.

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I. INTRODUCTION

Quantum simulation of strongly correlated models of condensed matter systems has become one of the most exciting goals in ultra-cold atom experiments, thanks to the spectacular progress in trapping cold fermions in optical lattices at degeneracy temperatures [1]. This new system goes beyond traditional experiments in solids, because it is readily possible to tune independently the hopping amplitude and interaction strength. In particular, by changing the external magnetic field that tunes the relative Zeeman energy between the scattering state and a closed (bound state) channel, one can reach a particular Feshbach resonance between two hyperfine states of, for example, 40K where the scattering length between these states becomes very large and positive [2]. This then allows one to tune the on-site two-body interaction to be strongly repulsive. With this, the fermionic Mott insulator, where interaction driven locking of fermions into a crystalline structure, has been demonstrated in two recent experiments [3, 4].

Currently, there are great experimental interests to reach ordered phases in these systems, in order to understand the phase diagram of the two-dimensional single-band Hubbard model, a model that has been hypothesized to be the minimal model for the high temperature superconductors [5]. Indeed, the unprecedented experimental possibility of studying extremely strong repulsion has spurred on much new theoretical effort [1]. In particular, it was recognised that, close to a Feshbach resonance, the strongly enhanced two-body interaction leads to states with occupation of multiple Bloch bands of the optical lattice, both in experimental [6] and theoretical studies [7] [8]. These multi-band systems [9] [10] may lead to richer phases, by analogy with multi-orbital systems in solid state materials.

While the ultra-cold atoms parameters of the one-band Hubbard model have been derived right from the beginning [11], the parameters for the multi-band generalisation have only more recently received some attention [7] [8] [12] [13] [14] [15]. Motivated by the experiments of Köhl et al. [8] where the average filling per lattice site is about two fermions or slightly more, we study here the energy spectra when two or three fermions interact near a Feshbach resonance within a site of the deep optical lattice, using a two-channel description of the Feshbach resonance. This is then the first step towards deriving from microscopic physics, the effective model and its parameters for a system of strongly interacting fermions in an optical lattice.

In this paper, we consider a system of cold fermionic 40K atoms in the two lowest internal states trapped in a deep optical lattice close to an inter-species s-wave Feshbach resonance. We assume a lattice with average filling of two atoms per site with an equal mix of the two internal states. For simplicity, we consider only a one-dimensional (1D) system. In experiments with cold atoms in optical lattices, a set of quasi-1D tubes can be obtained from a 3D optical lattice, \( V(\vec{r}) = V_{0z} \sin^2 k_x x + V_{0y} \sin^2 k_y y + V_{0z} \sin^2 k_z z \), by adjusting the laser amplitudes so that \( V_{0x} \ll V_{0x} = V_{0d} \) [16] [17]. We concentrate on the weak tunnelling limit (deep lattice), in which experiments with lattice fermions across a Feshbach resonance are usually performed [6], and approximate the optical lattice potential at each lattice site by a harmonic well, \( V_{ho} = \sum_{x,y,z} \mu \omega_i^2 / 2 \) with \( \mu \omega_i^2 / 2 = 2k_i^2V_{0i} \). The local spectrum and eigenstates for two and three atoms at a lattice site provide then a microscopic basis for the model of such lattices found by Ho [10] where a weak tunnelling is introduced perturbatively.

The spectrum for two atoms in a harmonic well close to a s-wave Feshbach resonance was previously studied in e.g. [7] within the one-channel model for the harmonic confinement in one, two and three dimensions and in [8] within the two-channel model for a three dimensional harmonic trap. However, the spectrum for three atoms in a well was previously studied only within the one-channel model (e.g. for 3D harmonic confinement [12]), quasi-1D confinement [13] and fermions at unitarity [14] [15]. Here, we calculate the spectrum within the two-channel model and examine the ground state for our system across the resonance. We find the level crossings in the low energy spectrum that may lead to quantum phase transition when multiple wells form an optical lattice. Similar features were found in the spectrum for a 3D system in [12] within the one-channel model. However, we find that there are quantitative differences between our two-channel and their one-channel results at and near the Feshbach resonance.
II. TWO-CHANNEL MODEL FOR THREE ATOMS IN A WELL

When $V_{0c} \ll V_{0r} = V_0$, the system can be described by an effective 1D Hamiltonian. The effective 1D parameters can be related to the physical 3D parameters in the limit $\omega \rightarrow 0$ as presented in [13]. We concentrate on the weak tunnelling limit and calculate the local spectrum when there are three atoms in two different internal states in the well.

The $^{40}\text{K}$ atoms are assumed to be trapped in the two lowest hyperfine energy states $|F_1, m_{F_1}⟩ = |9/2, -9/2⟩$ and $|F_2, m_{F_2}⟩ = |9/2, -7/2⟩$. The interatomic interaction potential, $U(r_1 - r_2) = U_c(r_1 - r_2) + U_s(r_1 - r_2)\hat{S}_1 \cdot \hat{S}_2$, depends only on electronic spins of atoms and preserves the total angular momentum projection of the two colliding atoms, $\hat{s}$, the only closed channel with atoms 1 and 2 in the $|↑↓⟩$ state.

The Feshbach physics relies on the scattering between the states: $|↑↓⟩ ↔ |↑◦⟩$ for non-negative integers $k \neq l$ and $u_p(s, d) = e^{-i^2/2d}((\pi d)^{1/4}(2^p p!)^{1/2}) H_p(\frac{s}{d})$ with $H_p$ being the Hermite polynomials of order $p = 0, 1, \ldots$. These states have energy $(k + l + 1)\hbar \omega$. Note that Pauli exclusion is enforced in that the wavefunction vanishes unless $k \neq l$.

Having found basis states for the open channel, we can do the same for the closed channel with atoms 1 and 2 in the $↑$ state and atom 3 in the $⊙$ state. They will have an energy relative to the open channel of $\delta_B$ which is tunable by an external magnetic field $B$. Moreover, there is an additional attractive interaction $V^{cl}$ in the closed channel that creates the $|↑⊙⟩$ dimer essential for Feshbach physics. Therefore, the closed-channel Hamiltonian $h^{cl}$ is given by:

$$h^{cl} = h^{trap} + V^{cl}(r_1) + V^{cl}(r_3) + \delta_B$$

where the coordinates $r_3 = r_1 - r_{1,2}$ represent distances between atom 3 (in $⊙$ state in the closed channel) and each of the other two $↑$ atoms.

To find the eigenstates of this closed-channel Hamiltonian $h^{cl}$, it is useful to identify parts of $h^{cl}$ which provide an attractive interaction between one pair of $↑⊙$ atoms to form a dimer while leaving the other $↑$ atom as a spectator. Let $h^{cl}_d$ provide an attraction between atoms 1 and 3, leaving atom 2 as a spectator and $h^{cl}_s$ provide an attraction between atoms 2 and 3, leaving atom 1 as a spectator.

These truncated dimer-spectator Hamiltonians are:

$$h^{cl}_d = -\frac{\hbar^2}{2\mu} (\nabla^2 r_1 + \nabla^2 r_3) + \frac{\mu \omega^2}{2} (s_x^2 + r_x^2) + V^{cl}(r_3) + \delta_B$$

where $s_x = [r_{1,2} + r_3 - 2r_{2,1}] / \sqrt{3}$. The first part, $u_r$, represents the oscillation in the relative displacement between the spectator and the dimer with energy $(n+1/2)\hbar \omega + \delta_B$. The second part, $\chi(r_3, d_{3m})$, is the wavefunction for the bound state formed due to the attractive interaction $V^{cl}$:

$$\chi(r_3) = e^{i\delta}(r_3) \chi(r_3)$$

where $\delta = \frac{\hbar^2}{2\mu} (\nabla^2 r_3 + \frac{\mu \omega^2}{2} r_x^2 + V^{cl}(r_3)) \chi(r_3)$

The potential of the harmonic trap is separable in these coordinates:

$$h^{trap} = \hbar^{trap}(x, y) = -\frac{\hbar^2}{2\mu} (\nabla^2_x + \nabla^2_y) + \frac{\mu \omega^2}{2} (x^2 + y^2)$$

where $\mu = m/2$ is the reduced mass for the relative motion of two atoms. The characteristic length of the oscillations in the harmonic trap is $d_c = (\hbar/\mu \omega)^{1/2}$ in the centre-of-mass frame.

The eigenstates of this Hamiltonian must have wavefunctions which are antisymmetric under the exchange of two fermions in the same internal state ($↑$), i.e., under the exchange $r_1 ↔ r_2$ which corresponds to $x ↔ y$. Therefore, the eigenstates are $|κ, l⟩$. From these basis states, we can do the same for the closed channel.
with energy $\epsilon_0$. We cannot solve the bound-state equation in general. We will simply assume that $\chi$ is a tightly bound s-wave state much smaller in size than the characteristic trap oscillation amplitude $d$; $\chi(r_s, d_m) \approx u_0(r_s, d_m)$ with $d_m \ll d$.

However, the eigenstates of $\hat{h}^{cl}$ are not exact eigenstates of the total closed channel because they do not include the interaction of the spectator atom with the dimer in the state $\chi$. Nevertheless, in the regime of a tightly bound dimer, this residual atom-dimer interaction is expected to be small due to Pauli suppression. Suppose that atoms 1 and 3 have formed a dimer and atom 2 is the $\uparrow$ spectator. The $u_n(s_1, d_r)$ part of the wavefunctions indicates that atoms 1 and 2 are separated at a distance of the order of $\langle 3n \rangle^{1/2}d_r/2$. Moreover, since they are fermions, Pauli exclusion means that their relative wavefunction must have a node at $r_1 = r_3$, so that $u_n$ remains small until they are separated by a length scale set by the trap length $d_r$. Since atom 3 stays close to atom 1 in a tight dimer, this means that atoms 2 and 3 also stay apart at a distance of the order of $d_r$ where the interaction $\chi^{cl}$ between them is weak. Therefore, we can, to a first approximation, neglect this spectator-dimer interaction so that approximate eigenstates for the closed-channel Hamiltonian $\hat{h}^{cl}$ are antisymmetrised combinations of the two possible spectator-dimer states:

$$\left| \chi_n \right> = \frac{[u_n(s_1, d_r)\chi(r_s, d_m) - u_n(s_2, d_r)\chi(r_s, d_m)]}{\sqrt{2}} | \uparrow, \uparrow, \uparrow, \uparrow, \uparrow, \rangle$$

for $n = 0, 1, \ldots$, with energies $(n + 1/2)\hbar \omega + \epsilon_0 + \delta_B$.

We can now discuss the full Hamiltonian with Feshbach scattering between the open and closed channels. The Hamiltonian for the three atoms is given (in the centre-of-mass frame) by:

$$\hat{H}^\uparrow = \left[ \begin{array}{ccc} | \uparrow, \uparrow, \downarrow \rangle & | \uparrow, \uparrow, \uparrow \rangle \\ | \downarrow, \uparrow, \uparrow \rangle & | \chi \rangle \end{array} \right] \left[ \begin{array}{cc} h^{op} & W \\ W & \hat{h}^{cl} \end{array} \right] \left[ \begin{array}{c} | \uparrow, \uparrow, \downarrow \rangle \\ | \uparrow, \uparrow, \uparrow \rangle \end{array} \right]$$

W = \alpha(r_s) + \alpha(r_\uparrow)$

where $\alpha(r)$ describes the coupling between the open and closed channels for two atoms at a distance of $r$. The eigenstates of this Hamiltonian (10) are now superpositions of the open and closed channel states:

$$| \phi^{\uparrow} \rangle = \sum_{\alpha \delta} a_{\alpha \delta} | k \rangle + \sum_n b_n | \chi_n \rangle$$

where the first term represents the three atoms in the open channel in terms of the basis set (4) and the second term represents the atom-dimer states in terms of the basis set (9). An eigenstate with energy $E$ obeys the Schrödinger equation: $\hat{H}^{\uparrow} | \phi^{\uparrow} \rangle = E| \phi^{\uparrow} \rangle$. This requires

$$\frac{1}{2} \sum_{\alpha \delta} \alpha_{\alpha \delta} a_{\alpha \delta} + b_n(\epsilon_0 + \tilde{\nu}) = E b_n,$$

$$\sum_n \alpha_{\alpha \delta} b_n + (\epsilon_0 + \tilde{\nu}) a_{\alpha \delta} = E a_{\alpha \delta},$$

where $\epsilon_0 = (n + 1/2)\hbar \omega$, $\alpha_{\alpha \delta} = \langle k \rangle \chi_n$ is the Feshbach scattering matrix element, and $\tilde{\nu} = \delta_B + \epsilon_0$ is a detuning parameter which sweeps across the Feshbach resonance as a function of applied magnetic field.

In the absence of the confinement potential, the resonance occurs when the atom-dimer state of energy $\epsilon_0 + \delta_B$ coincides in energy with the zero-momentum scattering state (energy zero) in the open channel. This corresponds to $\tilde{\nu} = 0$. In the presence of the harmonic trap, the Feshbach scattering may cause resonances whenever the open and closed channel states are degenerate:

$$(k + l + 1)\hbar \omega = \tilde{\nu} + (n + 1/2)\hbar \omega$$

for non-negative integers $k, l(\neq k)$ and $n$. A non-zero Feshbach coupling will lift the degeneracy and one will find a level anti-crossing in the energy spectrum as a function of $\nu$. We will see in section III that there are level crossings allowed by selection rules.

To simplify our calculation, we can eliminate the open-channel coefficients $a_{\alpha \delta}$ using the second equation in (12). Then, we obtain a matrix equation for just the atom-dimer components, $b_n$, of the eigenstate:

$$(E - \epsilon_0) b_n + \sum_m M_{nm}(E) b_m = \epsilon b_n,$$

where

$$M_{nm}(E) = \frac{1}{2} \sum_{\alpha \delta} \alpha_{\alpha \delta} \alpha_{\alpha m} - \epsilon_n - \epsilon_l - E.$$

The matrix $M_{nm}$ can be interpreted as representing an effective delta-function coupling between the open and virtual state $| k \rangle l$ via the virtual state $| k \rangle$. We solve equation (14) numerically by treating it, at any given $E$, as a matrix eigenvalue problem for eigenvalue $\tilde{\nu}$.

We need to evaluate the Feshbach matrix elements $\alpha_{\alpha \delta}$. We will assume that it only occurs when two atoms are close together at a scale much smaller than the trap length $d_r$. We see that there are direct and exchange terms in this matrix element. The direct term involves $\alpha(r_s)\chi(r_s, d_m)$. For a tightly-bound dimer in the closed channel, we can reduce this to an effective delta-function coupling between the open and closed channel $\delta_{\alpha \delta}$ numerically by treating it, at any given $E$, as a matrix eigenvalue problem for eigenvalue $\tilde{\nu}$.

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where $\psi_n = u_n(s, d_r) \delta(r_s) - u_n(s, d_r) \delta(r_s)$ and $G^{(2)}$ is the two-particle Green’s function of non-interacting atoms in a 1D harmonic well

$$G^{(2)}(x, y; \alpha, \beta; E) = \sum \frac{u_\alpha(x, d_r)u_\beta(y, d_r)u_\alpha(x', d_r)u_\beta(y', d_r)}{\epsilon_k + \epsilon_l - E}$$

We notice [12] that the harmonic oscillator Hamiltonian $h^{\text{hop}}$ is invariant under rotations in the $x$-$y$ plane and that the $(r_s, s_s)$ are both related to $(x, y)$ by such a rotation: $r_s = [(\sqrt{3} \pm 1)x + (\sqrt{3} \pm 1)yi]/2\sqrt{2}$ and $s_s = [(1 \pm \sqrt{3})x + (1 \pm \sqrt{3})yi]/2\sqrt{2}$. Therefore, $G^{(2)}(x, y; \alpha, \beta; E) = G^{(2)}(r_s, s_s; r_\alpha, s_\beta; E)$. This allows us to express all the integrations in terms of $r$ and $s$ variables. We find that the matrix elements $M_{nm}(E)$ can be written in the final form

$$M_{nm}(E) = a^2 \left \{ G^{(1)}(0, 0; E - \epsilon_n) \delta_{nm} - \int ds G^{(1)} \left \{ \frac{\sqrt{2} \sqrt{x}}{2}, 0; E - \epsilon_n \right \} u_n(s, d_r) u_m(s, d_r) \right \},$$

where $G^{(1)}$ is the single-particle Green’s function $G^{(1)}(x, x'; E) = \sum u_n(x, d_r)u_n(x', d_r)/(\epsilon_n - E)$. The advantage of expressing the matrix in this form is that we know the quantities we need analytically [20]:

$$G^{(1)}(x, 0; E) = \frac{\Gamma(\frac{E - \epsilon_n + \frac{1}{2}}{\hbar \omega})}{\sqrt{\pi} \sqrt{d_r} \hbar \omega} \frac{\sqrt{2} \sqrt{|x|}}{d_r} D_{\epsilon_n - \frac{1}{2}}(0),$$

where $D_r(x)$ is the parabolic cylinder function with $D_r(|y|) = 2^{1/2} e^{-y^2/4} U(-1/2, 1/2, y^2/2)$ where $U$ is the confluent hypergeometric function and $D_r(0) = 2^{-1/2} \sqrt{\pi} \Gamma(1 - \nu)/2$. The delta functions in the $\psi_n d_\alpha$ factors in the form [16] indicate which particles are interacting via the Feshbach scattering. The two $G^{(2)}$ terms come from the fact the virtual excitation via an open-channel state involves a direct process and an exchange process. The direct process gives the first term in [18] which requires $r_e = r_s - r_l = 0$ or $r_e = r_s - r_l = 0$: it involves only the interaction of one pair of atoms while the third atom remains a spectator. The exchange process involves the virtual dissociation of a dimer into $\uparrow$ and $\downarrow$ atoms in open-channel followed by the $\downarrow$ atom recombining with a different $\uparrow$ atom to form a new dimer. This gives the second term in [18] which is a term present in the three-body problem but not in a two-body problem.

Before proceeding to discuss our results, we should point out the difference between $|\uparrow, \uparrow, \downarrow \rangle$ and $|\downarrow, \downarrow, \uparrow \rangle$ states. Since the Feshbach interaction only affects the $\downarrow$ state in the open channel, there is no symmetry under the operation $\uparrow \leftrightarrow \downarrow$. The difference is that, in the $\downarrow \uparrow \downarrow$ case, there is no residual interaction between the $|\downarrow \rangle$ atom in the dimer and the spectator $\downarrow$ atom: the closed-channel attraction $V_{cl}$ only acts on a $|\uparrow \downarrow \downarrow \rangle$ pair. However, we have already dropped this interaction within our approximation of a tightly bound dimer state. Therefore, our results should apply also to the $\downarrow \downarrow \uparrow$ case. More explicitly, for the $\downarrow \downarrow \uparrow$ case, the Hamiltonian for the relative degrees of freedom is of the form

$$H^{1\uparrow} = V \cdot \begin{pmatrix} h^{op} & W & W_+ \\ W_+ & h^d & 0 \\ W_- & 0 & h^cl \end{pmatrix} \cdot V^\dagger,$$

where $W \pm = \alpha(r_s)$. $V = [(\downarrow, \downarrow, \uparrow) |\uparrow, \downarrow, \downarrow \rangle |\downarrow, \downarrow, \uparrow \rangle |\downarrow, \downarrow, \uparrow \rangle]$, and $h^d$ and $h^cl$ have been defined in [7]. Now, the wavefunctions $u_n(s, d_r)\chi(r_s, d_m)\alpha, \downarrow, \uparrow \rangle$ and $\uparrow, \downarrow, \downarrow \rangle$ are exact eigenstates of the closed-channel part of the Hamiltonian.

### III. SELECTION RULES

We can take advantage of selection rules for the Feshbach coupling. In the pseudospin language of $\uparrow$ and $\downarrow$ states of the open channel, we are discussing the three-atom states with $S_z = +1/2$. If we completely antisymmetrise the wavefunction of the three atoms [21]:

$$|\psi(1, 2, 3)\rangle_A = |\psi(1, 2, 3)\rangle + |\psi(2, 3, 1)\rangle + |\psi(3, 1, 2)\rangle,$$

we can classify the three-atom states as $S = 3/2$ or $1/2$. The $S = 3/2$ spin wavefunction is totally symmetric under exchange and so its spatial part is totally antisymmetric under exchange, leading to a node at $r_1 = r_2$. Therefore, this state is unaffected by the $s$-wave Feshbach scattering. On the other hand, the $S = 1/2$ states have mixed exchange symmetry (see for example [21]) and Feshbach scattering is allowed. To see exactly how in this explicit way, we can write the open-channel part of the Hamiltonian in terms of the form $1/2$.

In addition to exchange symmetry, we note that the system is symmetric under inversion $(r_1, r_2, r_3, r_4) \rightarrow (r_4, r_3, r_2, r_1)$. This means that the eigenstates of the system must be even or odd under inversion. In terms of the matrix equation [14], the solutions divide into two sectors, one for $b_n$ with even $n$ and one for $b_n$ with odd $n$. More precisely, the matrix elements $a_{klm}$ are non-zero only if $k + l$ and $n$ are both even or both odd.

There are also other matrix elements $a_{klm}$ which vanish between the open and closed channels: it can be shown that $a_{klm}$ vanish when $n > k + l$. This can be proved using the fact that $\int x e^{-x^2} H_n(x) dx = 0$ for $r < n$ [24]. In other words, atom-dimer states with energy $\tilde{\nu} + (n + 1/2)\hbar \omega$ do not couple directly to the three-atom states with the relative energy $(k + l + 1)\hbar \omega$ when $n > k + l$, even if they are degenerate (possible when $\tilde{\nu} < \hbar \omega$). However, they can be coupled by multiple Feshbach scattering. Therefore, we expect avoided level crossings for such levels but the splitting at the anti-crossing point will be smaller in size than the level splittings at anti-crossing points for levels coupled directly by a non-zero matrix element $a_{klm}$. This is because the splitting will be higher order in $\alpha$. 
In this section, we will outline the results for the Feshbach resonances of two atoms in a 1D harmonic well. This will be useful for the discussion of our results for three atoms. These results are analogous to the 3D results of Diener and Ho [8]. Our calculation differs from [8] in the lower dimensionality and also in the fact that we have factored out the motion of the centre of mass.

In the centre-of-mass frame, the energy for two Feshbach interacting atoms in a well within the two-channel model is given by the equation

\[ E - \bar{\nu} = -\frac{\alpha^2}{2\hbar d_1} - \frac{\Gamma \left( \frac{3}{4} - \frac{E}{2\hbar \omega} \right)}{\Gamma \left( \frac{3}{4} - \frac{\hbar \omega}{2\hbar} \right)} \]  

(23)

The lowest-energy solution of this equation has an energy below \( \hbar \omega/2 \) for any value of the detuning parameter \( \bar{\nu} \). Since \( \hbar \omega/2 \) is the lowest energy of the open-channel scattering states, this corresponds to a bound state. The existence of a bound state for any \( \bar{\nu} \) is not unexpected in one dimension.

We can relate our two-channel parameters \( \alpha \) and \( \bar{\nu} \) to the parameters of a one-channel scattering theory in the absence of the trap: \( a_{1D} \), the s-wave scattering length, and \( r_{1D} \), the effective range. These are the physical parameters that can be found experimentally. To do so, we follow the procedure of Diener and Ho [8] and examine the bound state energy of two atoms in the limit of an infinitely shallow well: \( \omega \to 0 \) at a constant negative \( E \). We also need \( |E| \ll \bar{\nu} \) so that the state is clearly separated from dimer states (energy \( \bar{\nu} \)) in the closed channel. In this limit, the equation (23) becomes

\[ \frac{\mu_0^2}{\hbar^2 \bar{\nu}} - \frac{\mu_0^2 |E|}{\hbar^2 \bar{\nu}^2} = \left( \frac{2\mu |E|}{\hbar^2} \right)^{1/2} = 0. \]  

(24)

On the other hand, we find that the energy of a weakly bound state in a homogeneous case with no external confinement is given by the equation \( 1/a_{1D} - \mu |E|/\hbar^2 = 0 \), where \( |E| = \hbar^2 k^2/(2\mu) \) and \( k \ll 1 \) with \( R \) being the range of the scattering potential.

Comparing those two equations, we find

\[ \frac{1}{a_{1D}} = \frac{\mu_0^2}{(\hbar^2 \bar{\nu})}, \quad r_{1D} = \frac{\alpha^2}{\bar{\nu}^2}. \]  

(25)

We see that the effective 1D scattering length \( a_{1D} \) is proportional to the detuning parameter \( \bar{\nu} \) in the regime of a weakly-bound state where \( |E| \ll \bar{\nu} \). In terms of the parameters of the two-channel model, this regime corresponds to a detuning of \( \bar{\nu} \gg \alpha^2/(2\hbar^2)^{1/3} \). Note that this 1D case is very different to the 3D case where \( a_{3D} \sim -1/\bar{\nu} \), see section VI.

We will now discuss our results for the spectrum and eigenstates of the three-body system. As mentioned already, we treat the matrix equation (14) as an eigenvalue problem for the detuning parameter \( \bar{\nu} \) at fixed energies \( E \).

In order to obtain numerical results, we truncate the matrix equation (14) by taking into account only atom-dimer energy levels with \( \epsilon_n < \epsilon_2 \). This should properly reproduce the low-energy behaviour of the system for the few lowest atom-dimer energy levels. Here we choose \( n_c = 20 \). We have checked that the ground and first excited states do not change significantly if we use a higher cutoff \( n_c \).

We will discuss two opposite regimes of weak and strong Feshbach scattering. The kinetic energy of the system is on the energy scale \( \hbar \omega \). This should be compared to the magnitude of the scattering matrix elements \( \alpha_{1dn} \). We note that the oscillator wavefunctions \( \psi_n(x, d_r) \) have a magnitude of the order of \( d_r^{-1/2} \) over a spatial size \( d_r \) so that \( \alpha_{1dn} \sim \alpha/d_r^{1/2} \). Therefore, a dimensionless measure for the strength of the Feshbach scattering is the ratio of these two energy scales:

\[ \tilde{\alpha} = \frac{\alpha}{\hbar \omega d_r^{1/2}}. \]  

(26)

We will consider first the weak-scattering regime, \( \tilde{\alpha} \ll 1 \), where the open and closed channel states are weakly coupled. Then, we will discuss strong scattering, \( \tilde{\alpha} \gg 1 \), relevant to \( ^{40}\)K atoms [18, 23].

We can also obtain a scale for the range of detuning \( \delta \bar{\nu} \) over which the Feshbach scattering significantly affects the atom-dimer energy levels, as governed by (14). This can be estimated by the scale of the elements of \( M_{nm} \sim (\alpha/d_r^{1/2})^2/\hbar \omega \). Therefore, a dimensionless measure of the detuning parameter is \( \tilde{v} \hbar \omega d_r/\alpha^2 \). From the results (25) for the two-body problem, we see that this is also the ratio of the effective 1D scattering length \( a_{1D} \), for states in the open channel (in the absence of a trap) compared to the trap oscillation length \( d_r \):

\[ \frac{a_{1D}}{d_r} = \frac{\bar{\nu} \hbar \omega d_r}{\alpha^2}. \]  

(27)

in the regime of a weak two-body bound state.

We present in figure [1] our results for the spectrum at \( \tilde{\alpha} = 0.5 \). We plot the energy in units of \( \hbar \omega \) versus the dimensionless detuning parameter \( \tilde{\nu} \hbar \omega d_r/\alpha^2 \). The selection rules discussed above are reflected in the energy spectrum as it can be seen in figure [1]. The two graphs, (a) and (b), correspond to the energy levels for states with even and odd inversion symmetry.

The \( S = 3/2 \) open-channel states which are unaffected by the Feshbach scattering are found at energies \( E/\hbar \omega = 4, 6, \ldots \) At negative detuning and at negative energies, we see the unperturbed atom-dimer states \( |s_n \rangle \), the different diagonal lines corresponding to different atom-dimer oscillations. As we increase \( \tilde{\nu} \), Feshbach interaction with open-channel states become possible near the resonance points given by (13). At the resonances, there are anti-crossings between the three-atom and atom-dimer states. For small \( \tilde{\alpha} \), we can approximate by restricting the matrix equation (14) to just the two open and closed levels near the anti-crossing in question. Then, we see immediately that, for resonances at positive detuning \( \tilde{\nu} \), the size of the splitting at resonance is of the order of the matrix element coupling the two states: \( \alpha_{1sn} \sim \alpha/d_r^{1/2} = \tilde{\alpha} \hbar \omega \).
However, for resonances at negative \( \bar{v} \), the splittings are much smaller. As discussed in the section [11], these are the levels which are only coupled through multiple Feshbach scattering.

![Diagram 1](image1)

**FIG. 1:** Energy levels (in the centre-of-mass frame) versus detuning for three atoms in a harmonic well with \( s \)-wave Feshbach scattering at a dimensionless coupling \( \tilde{a} = 0.5 \). Dashed lines represent total pseudospin \( S = 3/2 \) states which are unaffected by \( s \)-wave Feshbach scattering. Figures (a) and (b) represent eigenstates with odd and even inversion symmetry respectively. Grey circles represent eigenstates in the absence of Feshbach scattering. Black dots represent \( S = 1/2 \) states.

We can now turn to the regime of strong Feshbach scattering. Large coupling strength \( \tilde{a} \) means much stronger level anticrossing than for \( \tilde{a} = 0.5 \) case shown in figure [1]. As an example, we have calculated the spectrum for \( \tilde{a} = 100 \). (We will see later that there is very little admixture of high-energy level in the lowest-energy eigenstates, justifying our use of a relatively low cutoff \( n_c \).) The six levels with the lowest energies are shown in figure [2]. The apparent kink in the highest branch in figures [2] and [3] is due to the level crossing that can be better seen for the small \( \tilde{a} \) case in figure [1]. Again, we see the unperturbed open-channel states at \( 4\hbar\omega \) and \( 6\hbar\omega \) (dashed lines). Note that the lines corresponding to the unperturbed atom-dimer states would be very steep and very close to the vertical axis on this graph.

We find level crossings in the low-energy spectrum between these two sets of states with opposite parity under inversion. This is most easily seen in energy spectrum at weak Feshbach scattering (Fig. [1]). For large positive detuning, the lowest energy states belong to the odd-parity branch that gives the open-channel \( |01 \rangle \) state asymptotically far away from the resonance \( (\bar{v} \to +\infty) \). On the other hand, for large negative detuning, the states of lowest energy belong to the even-parity branch that becomes the \( |y_0 \rangle \) atom-dimer state asymptotically \( (\bar{v} \to -\infty) \). Therefore, the two parity branches must cross as a function of detuning. For weak Feshbach scattering, the crossing for the lowest two parity states occurs at a positive detuning, just below \( E = 2\hbar\omega \). For strong Feshbach scattering, we find that these level crossings have shifted to small negative detuning and negative energies \( (\bar{v}\hbar d_1/\alpha^2 \approx -0.07 \) and \( E \approx -9\alpha/\alpha^{1/2} \) for \( \tilde{a} = 100 \). Similar features were found for the spectrum of three atoms in a 3D harmonic well within the one-channel model [12].

![Diagram 2](image2)

**FIG. 2:** Lowest six energy levels at strong Feshbach coupling: \( \tilde{a} = 100 \). Dashed lines represent total pseudospin \( S = 3/2 \) states. Grey and black dots represent \( S = 1/2 \) states with odd and even inversion symmetry respectively.

The level crossings between the branches of opposite inversion symmetry are best seen if we subtract from the three-body energies \( (E_3) \) both the ground-state energy of two atoms in a well \( (E_2 \) as given by (23)) and the energy of one atom in a separate well \( (\hbar\omega/2) \). This quantity, \( E_3 - E_2 - \hbar\omega/2 \), is plotted in figure [3]. The subtraction does not alter the crossings of the three-body states at any given \( \bar{v} \). In section [11] we speculate that these crossings may lead to quantum phase transitions.

This data allows us to discuss the ground state of the system with three atoms for every two wells. One might ask whether the Feshbach interaction could generate an attraction such that there is a regime where the system would prefer to arrange three atoms in one well and none in the other well. Such a distribution would have an energy of \( E_3 + \hbar\omega/2 \) for the zero-point motion of the centre of mass. We can also have two atoms in one well and one atom in the ground state in the other well. This has energy \( E_2 + \hbar\omega/2 \) for the centre of mass in one well and \( \hbar\omega/2 \) in the other well. Therefore, the energy gap between these two states is \( E_1 - E_2 - \hbar\omega/2 \). From Fig. [3] we see that this gap remains positive for all detunings, suggesting that the ground state of an optical lattice with 3/2 atoms per site to be a phase with uniform density. This energy gap has a minimum as small as \( 0.2\hbar\omega \) at \( \tilde{a} = 100 \). This minimum is due to a reduction in \( E_3 \) compared to \( E_2 \) arising from
exchange processes which do not occur for two atoms, as discussed in previous section\cite{11} after equation (19). We note that this energy gap is much smaller in magnitude than the Feshbach energy scale $\alpha/d^{1/2}$ and the individual energies $E_3$ and $E_2$.

We can similarly ask about the ground state of four atoms in two wells. The evenly-distributed state with two atoms per well is lower in energy because it contains two binding energies $2E_2$ whereas the uneven distribution can only take advantage of Feshbach physics for one pair of atoms in $E_3$.

Having discussed the energy spectrum of the three-body system, we will now examine the wavefunctions of the low-energy eigenstates. The compositions of the ground state and the first excited state (for pseudospin $S=1/2$) are shown at figure 4. Figure 4(a)/(b) presents the composition of the lowest energy state with an odd/even inversion symmetry. As expected, the state in figure (a) becomes the $|\psi_1\rangle$ atom-dimer level at large negative detuning while it is predominately the open-channel $|0,1\rangle$ level at large positive detuning. Near the resonance, there is also a significant admixture of other open-channel levels and a smaller admixture of other atom-dimer levels. The most significant components are shown at the figure. Figure (b) gives the even inversion symmetry. The state is asymptotically the $|\psi_0\rangle$ atom-dimer state at large negative detunings. Closer to the resonance at negative $\bar{\nu}$ there is also a significant $|\psi_{13}\rangle$ component. For positive $\bar{\nu}$, the dominant contributions are from the $|0,2\rangle$ and $|1,3\rangle$ open-channel levels with the $|1,3\rangle$ contribution vanishing far from the resonance.

We notice that, while only $|\psi_1\rangle$ dominates in the lowest energy state with odd inversion symmetry, both $|\psi_0\rangle$ and $|\psi_2\rangle$ are significant for the corresponding state with even inversion symmetry particularly near the resonance. This difference can be traced back to the Feshbach matrix element $\alpha_{3ln}$. As discussed in\cite{11}, the wavefunctions involved should have similar symmetries to ensure a finite value for $\alpha_{3ln}$. Thus, using the rules that $k \neq l$ (Pauli principle) and that $k + l$ and $n$ should be both even or both odd with $n \leq k + l$, the lowest few $\alpha_{3ln}$ that contribute to the lowest energy states are $\alpha_{011}$ and $\alpha_{020}$ for the odd-parity state and $\alpha_{020}$ and $\alpha_{022}$ for the even-parity state. These matrix elements are large only if the quantum numbers $k$ and $l$ are similar to $n$ and so $|\alpha_{011}| \gg |\alpha_{013}|$ and $|\alpha_{020}| \approx |\alpha_{022}|$. In terms of equation (14) for the coupling of the closed-channel amplitudes, the magnitude of $M_{11}$ is big compared to that of $M_{13}$ for the odd case, while both $M_{00}$ and $M_{02}$ are significant for the even case. Hence, both $|\psi_0\rangle$ and $|\psi_2\rangle$ contribute to the lowest energy even sector eigenstate in Fig. 4(b).

These results allow us to understand the validity of our truncation of the matrix equation (16). We see that the admixture of high-energy levels is small. This allows us to ignore the contribution of $|\psi_n\rangle$ levels with $n \geq 2n_C = 40$. For comparison, if we use a smaller cutoff of $n_C = 5$ instead of 20, the value of $\bar{\nu}$ at a given $E$ changes by less than 1% and the ratios between different amplitudes change by less than 10%.
VI. COMPARISON WITH ONE-CHANNEL MODEL

In this paper, we have used a two-channel model for states near the Feshbach resonance. It is often convenient to use a one-channel model in which the Feshbach-induced interaction between open-channel states is modelled by a contact potential: \( V(r) = g\delta(r) \), with a potential strength \( g \) that depends on the detuning \( \hbar \omega \). We discuss now how a one-channel model may be appropriate for the three-body problem in a 1D well.

Physically, we expect that an effective model for just the open channel cannot capture physics involving the details of the dimer state in the closed channel. Therefore, one-channel models can approximate the results of two-channel models only if we focus our attention on scattering states and weakly bound states, neither of which would have a strong admixture of the closed-channel dimer. We have been discussing the branch of bound states induced by Feshbach interaction. In three dimensions without a harmonic trap, these states are weakly bound, with a binding energy that vanishes as we approach the resonance (\( \nu = 0 \)) from negative detuning. In other words, these eigenstates have only a small amplitude in the closed channel dimer state. Therefore, the matching to a one-channel model is best near the resonance. The range of validity of the one-channel model will be wide if the Feshbach coupling is strong.

This comparison between one-channel and two-channel models in 3D has also been studied in the presence of a harmonic trap. At a wide Feshbach resonance (strong coupling between the open and closed channels), the admixture of the closed channel dimer component to the low energy states is very small \( \hbar^2 a^2 \ll \hbar \omega \) and the effective interaction between the atoms close to the resonance can be described by an effective contact potential \( g_{3D} = 2\hbar^2 a_{3D} / \mu \) which diverges as one sweeps the system across the resonance at \( \nu = 0 \). However, there are also narrow resonances where a one-channel model does not apply \[27\] due to the significant admixture of the closed-channel component.

We will now turn to our results in one dimension. We have already studied in section [14] the matching of the two-channel results (for two atoms without a trap) to one-channel scattering parameters for the branch of bound states that develops at energies below the open channel. Note that this branch is not confined to \( \nu < 0 \) (as is the case in 3D without a trap). Instead, it exists for all \( \nu \) with the most weakly bound states at large positive detuning. This is the regime where we expect the one-channel and two-channel models to converge. The weak-binding condition that \( |E| \ll \hbar^2 / 2 \mu a_{1D}^2 \ll \nu \) can be expressed in terms of the dimensionless Feshbach and detuning parameters used in our study \[25\]:

\[
\frac{\nu \hbar \omega}{a^2} \ll \frac{a_{1D}}{d_c} \gg \frac{1}{a^{2/3}}. \tag{28}
\]

We see that this matching applies to positive detuning away from the level anticrossing near \( \nu = 0 \). Note that the regime of validity improves at strong coupling: \( \alpha \to \infty \) so that such a theory may be applicable for realistic \( ^{40} \text{K} \) systems except very close to the resonance. In terms of an effective contact potential strength, we have \( g_{1D} = -\hbar^2 / \mu a_{1D} \) \[27\] so that the regime of validity corresponds to a weak contact potential which traps a bound state for arbitrary weak \( g_{1D} \) in one dimension.

These conclusions about the validity of a one-channel approximation are also consistent with our three-atom results presented above. We can examine directly the degree of the admixture of open- and closed-channel components as a function of detuning. At large negative detuning, the states illustrated in figure [4] are predominantly the closed-channel atom-dimer state and so should have no relation to any model based on open-channel states. The change in the balance between open- and closed-channel components as a function of increasing detuning is clearly seen in figure [4]. Indeed, in our 1D system, there is a significant admixture of the atom-dimer levels close to the resonance even for strong coupling between the open and closed channels (\( \alpha \gg 1 \)). Therefore, we conclude that the system cannot be modelled by a one-channel theory close to the resonance. On the other hand, for large positive detuning, the states are predominantly open-channel states and so can be modelled in an effective theory for the open-channel states.

![FIG. 5: The lowest energy state with odd inversion symmetry for three atoms calculated using the two-channel models (solid circles) and one-channel model (open circles). The horizontal axis is plotted using the correspondence in equation (28). Grey line represents the closed-channel state in the two-channel model in the absence of Feshbach coupling (\( E = \nu + 3\hbar \omega / 2 \)).](#)

Furthermore, we have performed a one-channel calculation for three atoms in a well for our system using an effective \( g_{1D} \) \[28\], following an analogous study for the 3D problem \[12\]. From Fig. 5 we see that the energies calculated for the lowest branch of eigenstates agree in the one-channel and two-channel models at large positive detuning, but they differ significantly close to the resonance. Similar conclusions can be made for the two atoms in a 1D well by comparing one-channel results \[17\] the two-channel result \[23\] \[8\]. We can also confirm that the one- and two-channel calculations give different results when there is a significant admixture of the atom-dimer levels.

Interestingly, we find that the energy difference \( E_3 - E_2 \) are very similar in the one-channel and two-channel models for the whole range of positive detuning at \( \alpha = 100 \).
VII. SUMMARY AND DISCUSSION

We have considered two species of fermionic $^{40}$K atoms at ultra cold temperatures trapped in a 1D optical lattice and close to an inter-species Feshbach resonance. We have concentrated on the zero-tunnelling limit in which the dynamics of the system is well described by the local spectrum of atoms at a lattice site. The calculations are performed within the two-channel model for two and three atoms at a lattice site approximated by a harmonic well.

Close to the resonance, we find a significant admixture of the atom-dimer states to the lowest energy eigenstates of the system. Consequently, the one- and two-channel models must differ close to the resonance for our 1D system since a one-channel theory cannot capture the physics of the dimer state.

The results suggest that the ground state is a state with uniform atom density. In particular, for three atoms in two wells, we compared the energy of all three atoms in one well (3+0) to the energy of two atoms in one well and one atom in the other (2+1). The energy difference can be as small as 0.2$\hbar\omega$ at $\tilde{\alpha} = 100$ which is much smaller than the Feshbach energy scale. However, we note that, for the $S_z = +1/2$ case, we have neglected the residual interaction between the atom and dimer in a $\{k_0\}$ state. There is an attractive component from the closed-channel potential $V_{cl}$ and also a Feshbach scattering term, both of which we argued to be suppressed by fermionic statistics. We can ask whether these additional terms may significantly reduce or even change the sign of the energy difference between 2+1 and 3+0 configurations. In other words, we ask whether there is an instability to a density wave in an optical lattice with a filling close to 3/2 atoms per site.

To obtain a quantitative analysis for such a scenario, we would require a detailed short-distance description of the dimer state. Here, we will limit ourselves to a rough estimate for the lowest-energy state at positive detuning by considering the probability that the spectator atom can be in the vicinity of the dimer.

This state has odd inversion symmetry and the amplitude for the two atoms ($r_1$ and $r_2$) to approach each other is proportional to $(r_1 - r_2)/d_{m}^{1/2}$. So, the probability for the spectator to be in the vicinity of a dimer of size $d_m$ is proportional to $\int_{d_m} \frac{d^2r}{\sqrt{r_1^2 + r_2^2}} \sim (d_m/d_r)^{3/2}$. We estimate the residual attraction $\epsilon_{ad}$ between the atom and the dimer would be of the order of $\sqrt{\frac{V_{cl}}{d_r}}$ where $V_{cl}$ is a measure of the strength $V_{cl}$ experienced by the closed-channel dimer, e.g. the minimum value of the potential. As mentioned above, the minimum energy gap in $E_3 - E_2 - \hbar\omega/2$ is only a fraction of $\hbar\omega$. Therefore, if $V_{cl}$ is sufficiently large compared to $\hbar\omega$, there is a possibility that this additional attraction can favour the 3+0 configuration compared to the 2+1 configuration in two wells. (A similar term in the Feshbach scattering can be absorbed into a renormalised scattering strength $\alpha$, but our results are not sensitive to the value of $\alpha$ in this regime of large $\tilde{\alpha}$.) In fact, the even-symmetry state has a similar but larger correction of $\sqrt{\frac{V_{cl}}{d_r}}$ which could change the ordering in energy of the even and odd branches over a range of detuning. These speculations need to be confirmed by further work.

Note that these hypothetical scenarios rely on the residual interaction between an $\uparrow$ atom (but not a $\downarrow$ atom) with a dimer in the state $| \uparrow \downarrow \rangle$. In other words, such a scenario would reveal the asymmetry of the system under the transformation $\uparrow \leftrightarrow \downarrow$, it would only be a possibility if we have more atoms in the $\uparrow$ open-channel state than in the $\downarrow$ state. The magnitude of this effect depends on the size of the dimer in the closed channel compared to the trap size and therefore depends on the details of the actual Feshbach resonance.

Finally, we discuss briefly the optical lattice with weak tunnelling between a set of wells. Consider the case with three atoms per site on average. From the level crossing we found in figure 5, we see that the ground state would consist of states with odd or even inversion symmetry within each site depending on the detuning parameter. As we sweep past this crossing, this may be a first-order transition. However, it is also possible that a continuous quantum phase transition would occur because an inter-site tunnelling would couple the states of different inversion symmetries. We need to investigate collective quantum fluctuations to study this possibility.

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