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Feshbach resonant scattering of three fermions in one-dimensional wells

T. Đurić,[1] A. F. Ho,[2] and D. K. K. Lee[1]
[1]*Blackett Laboratory, Imperial College London, Prince Consort Road, London SW7 2AZ, United Kingdom*
[2]*Department of Physics, Royal Holloway University of London, Egham, Surrey TW20 0EX, United Kingdom*
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We calculate the spectrum for three atoms in a one-dimensional harmonic well near an *s*-wave Feshbach resonance using a two-channel model to describe the Feshbach physics. This is relevant to the study of cold ^{40}K atoms trapped in a one-dimensional optical lattice. 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 nonuniform 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 ultracold atom experiments, thanks to the spectacular progress in trapping cold fermions in optical lattices at degeneracy temperatures [1]. This 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, ^{40}K 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 theoretical effort [1]. In particular, it was recognized 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 multiband systems[9,10] may lead to richer phases, by analogy with multiorbital systems in solid state materials.

While the ultracold atoms parameters of the one-band Hubbard model have been derived right from the beginning [11], the parameters for the multiband generalization have only more recently received some attention [7,8,12–16]. Motivated by the experiments of Köhl *et al.* [6] 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 ^{40}K atoms in the two lowest internal states trapped in a deep optical lattice close to an interspecies *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 three-dimensional (3D) optical lattice, $V(\vec{r})=V_{0x}\sin^2 k_x x+V_{0y}\sin^2 k_y y+V_{0z}\sin^2 k_z z$, by adjusting the laser amplitudes so that $V_{0z}\ll V_{0x}=V_{0y}$ [17,18]. 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, $V_{ho}=\Sigma_{i=x,y,z}\mu\omega_i^2/2$ 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 tunneling 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 [13,16] 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. We note here (and see below in Sec.

IV) that such qualitative differences occur already for two-fermion scattering and appears to be specific to the 1D geometry here.

II. TWO-CHANNEL MODEL FOR THREE ATOMS IN A WELL

When $V_{0z} \ll V_{0x}=V_{0y}$, 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 $\omega_z \to 0$ as presented in [19]. We concentrate on the weak tunneling limit and calculate the local spectrum when there are three atoms in two different internal states in the well.

The ^{40}K atoms are assumed to be trapped in the two lowest hyperfine energy states $|F_1,m_{F_1}\rangle=|9/2,-9/2\rangle$ and $|F_2,m_{F_2}\rangle=|9/2,-7/2\rangle$. The interatomic interaction potential, $U(\vec{r}_1-\vec{r}_2)=U_c(\vec{r}_1-\vec{r}_2)+U_s(\vec{r}_1-\vec{r}_2)\vec{S}_1\cdot\vec{S}_2$, depends only on electronic spins of atoms and preserves the total angular momentum projection of the two colliding atoms, $m_F=m_{F_1}+m_{F_2}$. Then, for the two ^{40}K atoms in the two lowest internal states that constitute the open entrance channel, $|\alpha_1,\alpha_2\rangle=|9/2,-9/2;9/2,-7/2\rangle$, the only closed-channel coupled to this state is $|9/2,-9/2;7/2,-7/2\rangle$. For simplicity, we will use here the notation $|9/2,-9/2\rangle\equiv|\uparrow\rangle$, $|9/2,-7/2\rangle\equiv|\downarrow\rangle$, and $|7/2,-7/2\rangle\equiv|\circ\rangle$. In this notation, the Feshbach physics relies on the scattering between the states:

$$|\uparrow\downarrow\rangle \leftrightarrow |\uparrow\circ\rangle \tag{1}$$

where the final closed-channel state is a tightly bound $|\uparrow\circ\rangle$ dimer. We are interested in a regime near a Feshbach resonance so that the Feshbach-induced interaction is strong. We will therefore neglect for simplicity the direct s-wave scattering of the open-channel states.

In this section, we will focus on the case where there are two atoms of the species $\uparrow$ and one atom of the species $\downarrow$ in the well. (We will comment on the case of one $\uparrow$ and two $\downarrow$ atoms at the end of the section.) We will calculate how the open-channel levels $|\uparrow,\uparrow,\downarrow\rangle$ (i.e., atoms 1 and 2 are $\uparrow$ and atom 3 is $\downarrow$) become coupled together with levels involving a pair of atoms in the closed channel $|\uparrow,\uparrow,\circ\rangle$.

Consider first the states in the open channel in the absence of Feshbach scattering. Since we are ignoring direct s-wave scattering in the open channel, atoms in the open-channel states are noninteracting and they will have a Hamiltonian h^{op} that consists only of the potential of the harmonic trap h^{trap}.

We will work in the centre-of-mass frame of this three-body system because the motion of the centre of mass can be factored out completely for a single harmonic well. We denote the positions of the atoms $\uparrow,\uparrow,\downarrow$ with $\vec{r}_1=r_1\hat{z}$, $\vec{r}_2=r_2\hat{z}$, and $\vec{r}_3=r_3\hat{z}$, respectively. It is conventional to describe the relative degrees of freedom of the system using the Jacobi coordinates: $x_1=2[r_3-(r_1+r_2)/2]/\sqrt{3}$ and $x_2=r_2-r_1$. We find that it is more convenient for the evaluation of our formulae to use a rotated version of these coordinates:

$$x=\frac{x_1-x_2}{\sqrt{2}}=\frac{1}{\sqrt{6}}[2r_3+(\sqrt{3}-1)r_1-(\sqrt{3}+1)r_2]$$

$$y=\frac{x_1+x_2}{\sqrt{2}}=\frac{1}{\sqrt{6}}[2r_3-(\sqrt{3}+1)r_1+(\sqrt{3}-1)r_2]. \tag{2}$$

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

$$h^{\mathrm{op}}=h^{\mathrm{trap}}(x,y)=-\frac{\hbar^2}{2\mu}(\nabla_x^2+\nabla_y^2)+\frac{\mu\omega^2}{2}(x^2+y^2) \tag{3}$$

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 $d_r=(\hbar/\mu\omega)^{1/2}$ 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 ($\uparrow$), i.e., under the exchange $r_1 \leftrightarrow r_2$ which corresponds to $x \leftrightarrow y$. Therefore, the eigenstates are

$$|k,l\rangle=\frac{[u_k(x,d_r)u_l(y,d_r)-u_k(y,d_r)u_l(x,d_r)]}{\sqrt{2}}|\uparrow,\uparrow,\downarrow\rangle \tag{4}$$

for non-negative integers $k \neq l$ and

$$u_p(s,d)=\frac{e^{-s^2/2d^2}}{(\pi d^2)^{1/4}(2^p p!)^{1/2}}H_p\left(\frac{s}{d}\right) \tag{5}$$

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 $\uparrow$ state and atom 3 in the $\circ$ state. They will have an energy relative to the open channel of δ_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 $|\uparrow\circ\rangle$ dimer essential for Feshbach physics. Therefore, the closed-channel Hamiltonian h^{cl} is given by

$$h^{\mathrm{cl}}=h^{\mathrm{trap}}+V^{\mathrm{cl}}(r_+)+V^{\mathrm{cl}}(r_-)+\delta_B \tag{6}$$

where $r_\pm=r_3-r_{1,2}$ represent the relative coordinates between atom 3 (in $\circ$ state in the closed channel) and each of the other two $\uparrow$ 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 $\uparrow\circ$ atoms to form a dimer while leaving the other $\uparrow$ atom as a spectator. Let h_+^{cl} provide an attraction between atoms 1 and 3, leaving atom 2 as a spectator and h_-^{cl} provide an attraction between atoms 2 and 3, leaving atom 1 as a spectator. These truncated dimer-spectator Hamiltonians are:

$$h_\pm^{\mathrm{cl}}=-\frac{\hbar^2}{2\mu}(\nabla_{s_\pm}^2+\nabla_{r_\pm}^2)+\frac{\mu\omega^2}{2}(s_\pm^2+r_\pm^2)+V^{\mathrm{cl}}(r_\pm)+\delta_B \tag{7}$$

where $s_\pm=[r_{1,2}+r_3-2r_{2,1}]/\sqrt{3}$ are proportional to the distances between the centre of mass of the dimer and the spectator. The eigenstates of these truncated Hamiltonians Eq. (7) are atom-dimer states of the form $u_n(s_\pm,d_r)\chi(r_\pm,d_m)$. The first part, u_n, represents the oscillation in the relative dis-

placement between the spectator and the dimer with energy $(n+1/2)\hbar\omega+\delta_B$. The second part, $\chi(r_\pm,d_m)$, is the wavefunction for the bound state formed due to the attractive interaction $V^{\rm cl}$

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2_{r_\pm}+\frac{\mu\omega^2}{2}r_\pm^2+V^{\rm cl}(r_\pm)\right]\chi(r_\pm)=\epsilon_b\chi(r_\pm) \tag{8}$$

with energy ϵ_b. We cannot solve the bound-state equation in general. We will simply assume that χ is a tightly bound s-wave state much smaller in size than the characteristic trap oscillation amplitude d_r: $\chi(r_\pm,d_m)\simeq u_0(r_\pm,d_m)$ with $d_m\ll d_r$.

However, the eigenstates of $h^{\rm cl}_\pm$ 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 χ. 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 $u_n(s_+,d_r)$ part of the wavefunctions indicates that atoms 1 and 2 are separated at a distance of the order of $(3n)^{1/2}d_r/2$. 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 $V^{\rm cl}$ 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 $h^{\rm cl}$ are antisymmetrized combinations of the two possible spectator-dimer states

$$|\chi_n\rangle=\frac{[u_n(s_+,d_r)\chi(r_+,d_m)-u_n(s_-,d_r)\chi(r_-,d_m)]}{\sqrt{2}}|\uparrow,\uparrow,\circ\rangle \tag{9}$$

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

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:

$$\hat{H}^{\uparrow\uparrow\downarrow}=[|\uparrow,\uparrow,\downarrow\rangle \quad |\uparrow,\uparrow,\circ\rangle]\begin{bmatrix}h^{\rm op} & W\\ W & h^{\rm cl}\end{bmatrix}\begin{bmatrix}\langle\uparrow,\uparrow,\downarrow|\\ \langle\uparrow,\uparrow,\circ|\end{bmatrix}$$

$$W=\alpha(r_+)+\alpha(r_-) \tag{10}$$

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 Eq. (10) are now superpositions of the open and closed-channel states:

$$|\psi^{\uparrow\uparrow\downarrow}\rangle=\sum_{\substack{kl\\k<l}}a_{kl}|kl\rangle+\sum_n b_n|\chi_n\rangle \tag{11}$$

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

$$\frac{1}{2}\sum_{kl}\alpha_{kln}a_{kl}+b_n(\varepsilon_n+\bar{\nu})=Eb_n,$$

$$\sum_n\alpha_{kln}b_n+(\varepsilon_k+\varepsilon_l)a_{kl}=Ea_{kl}, \tag{12}$$

where $\varepsilon_n=(n+1/2)\hbar\omega$, $\alpha_{kln}=\langle kl|W|\chi_n\rangle$ is the Feshbach scattering matrix element, and $\bar{\nu}=\delta_B+\epsilon_b$ 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 $\epsilon_b+\delta_B$ coincides in energy with the zero-momentum scattering state (energy zero) in the open channel. This corresponds to $\bar{\nu}=0$. In the presence of the harmonic trap, the Feshbach scattering may cause resonances whenever the open and closed-channel states are degenerate

$$(k+l+1)\hbar\omega=\bar{\nu}+(n+1/2)\hbar\omega \tag{13}$$

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

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

$$(E-\varepsilon_n)b_n+\sum_m M_{nm}(E)b_m=\bar{\nu}b_n, \tag{14}$$

where

$$M_{nm}(E)=\frac{1}{2}\sum_{kl}\frac{\alpha_{kln}\alpha_{klm}}{\varepsilon_k+\varepsilon_l-E}. \tag{15}$$

The matrix M_{nm} can be interpreted as representing an effective scattering of the closed-channel state $|\chi_m\rangle$ to $|\chi_n\rangle$ *via* the virtual state $|kl\rangle$ in the open channel. We solve Eq. (14) numerically by treating it, at any given E, as a matrix eigenvalue problem for eigenvalue $\bar{\nu}$.

We need to evaluate the Feshbach matrix elements α_{kln}. 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 $\alpha(r_\pm)\chi(r_\pm,d_m)$. 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 [8,20]: $\alpha(r)\chi(r,d_m)\to\alpha\delta(r)$. This leaves α as a single parameter controlling the strength of the Feshbach interaction. There is also an exchange term involving $\alpha(r_\mp)u_n(s_\pm,d_r)\chi(r_\pm,d_m)$. This term is only large when all three atoms are very close to each other. These terms can be neglected due to Pauli suppression by the same argument that we neglected atom-dimer interactions in the closed

channel: the range of the Feshbach scattering is much smaller that the typical separation ($\sim d_r$) of two atoms in the same hyperfine state.

With this approximation of a short-ranged Feshbach interaction, the matrix elements $M_{nm}(E)$ can be written in terms of the Green's functions of the system

$$M_{nm}(E) = \frac{\alpha^2}{4}\int dxdx'dydy'\psi_n(x,y)\psi_m(x',y') \times [G^{(2)}(x,y;x',y';E) - G^{(2)}(x,y;y',x';E)] \tag{16}$$

where $\psi_n = u_n(s_+,d_r)\delta(r_+) - u_n(s_-,d_r)\delta(r_-)$ and $G^{(2)}$ is the two-particle Green's function of noninteracting atoms in a 1D harmonic well

$$G^{(2)}(x,y;x',y';E) = \sum_{kl}\frac{u_k(x,d_r)u_l(y,d_r)u_k(x',d_r)u_l(y',d_r)}{\varepsilon_k+\varepsilon_l-E}. \tag{17}$$

We notice [12] that the harmonic oscillator Hamiltonian h^{trap} is invariant under rotations in the x-y plane and that the $(r_\pm,s_\pm)$ are both related to (x,y) by such a rotation: $r_\pm = [(\sqrt{3}\mp 1)x + (\sqrt{3}\pm 1)y]/2\sqrt{2}$ and $s_\pm = [(1\pm\sqrt{3})x + (1\mp\sqrt{3})y]/2\sqrt{2}$. Therefore, $G^{(2)}(x,y;x'y';E) = G^{(2)}(r_\pm,s_\pm;r'_\pm,s'_\pm;E)$. 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

$$M_{nm}(E) = \alpha^2\left\{G^{(1)}(0,0;E-\varepsilon_n)\delta_{n,m} - \int ds G^{(1)} \times\left(\frac{\sqrt{3}s}{2},0;E-\varepsilon_n\right)u_n\left(-\frac{s}{2},d_r\right)u_m(s,d_r)\right\}, \tag{18}$$

where $G^{(1)}$ is the single-particle Green's function $G^{(1)}(x,x';E) = \Sigma_n u_n(x,d_r)u_n(x',d_r)/(\varepsilon_n - E)$. The advantage of expressing the matrix in this form is that we know the quantities we need analytically [21]

$$G^{(1)}(x,0;E) = \frac{\Gamma\left(-\frac{E}{\hbar\omega}+\frac{1}{2}\right)}{\sqrt{\pi}d_r\hbar\omega}D_{E/\hbar\omega-1/2}\left(\frac{\sqrt{2}|x|}{d_r}\right)D_{E/\hbar\omega-1/2}(0), \tag{19}$$

where $D_\nu(x)$ is the parabolic cylinder function with $D_\nu(|y|) = 2^{\nu/2}e^{-y^2/4}U(-\nu/2,1/2,y^2/2)$ where U is the confluent hypergeometric function and $D_\nu(0) = 2^{\nu/2}\sqrt{\pi}/\Gamma[(1-\nu)/2]$.

The delta functions in the $\psi_n\psi_m$ factors in the form Eq. (16) indicate which particles are interacting via the Feshbach scattering. The two $G^{(2)}$ terms comes 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 Eq. (18) which requires $r_+ = r_3 - r_1 = 0$ or $r_- = r_3 - r_2 = 0$: 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 Eq. (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 $\downarrow\downarrow\uparrow$ case, there is no residual interaction between the $|\circ\rangle$ atom in the dimer and the spectator $\downarrow$ atom: the closed-channel attraction V^{cl} only acts on a $|\uparrow\circ\rangle$ 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

$$H^{\downarrow\downarrow\uparrow} = \mathbf{V}\cdot\begin{bmatrix} h^{\text{op}} & W_+ & W_- \\ W_+ & h_+^{\text{cl}} & 0 \\ W_- & 0 & h_-^{\text{cl}}\end{bmatrix}\cdot\mathbf{V}^\dagger. \tag{20}$$

where $W_\pm = \alpha(r_\pm)$, $\mathbf{V} = [|\downarrow,\downarrow,\uparrow\rangle\ |\circ,\downarrow,\uparrow\rangle\ |\downarrow,\circ,\uparrow\rangle]$, and $h_\pm^{\text{cl}}$ have been defined in Eq. (7). Now, the wavefunctions

$$u_n(s_+,d_r)\chi(r_+,d_m)|\circ,\downarrow,\uparrow\rangle - u_n(s_-,d_r)\chi(r_-,d_m)|\downarrow,\circ,\uparrow\rangle \tag{21}$$

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 antisymmetrize the wavefunction of the three atoms [22]

$$|\psi(1,2,3)\rangle_A = |\psi(1,2,3)\rangle + |\psi(2,3,1)\rangle + |\psi(3,1,2)\rangle, \tag{22}$$

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 $r_3 = r_{1,2}$. 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, [23]) and Feshbach scattering is allowed. To see this explicitly in our formulation of the problem, we can write the open-channel part of the Hamiltonian in terms of the polar coordinates $\zeta = (x^2+y^2)^{1/2}$ and $\phi = \arctan(y/x)$. In this coordinate system, the energies can be written as $(2n_r + m_l + 1)\hbar\omega$ with integers $n_r \geq 0$ and $m_l > 0$. The $S=3/2$ states correspond to $m_l = 0 (\text{mod } 3)$ and these states have zero scattering matrix element to the atom-dimer states. The $S=3/2$ state of lowest energy has energy $4\hbar\omega$.

In addition to exchange symmetry, we note that the system is symmetric under inversion $(r_{1,2,3} \to -r_{1,2,3})$. This means that the eigenstates of the system must be even or odd under inversion. In terms of the matrix Eq. (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 α_{kln} are nonzero only if $k+l$ and n are both even or both odd.

There are also other matrix elements α_{kln} which vanish between the open and closed channels: it can be shown that α_{kln} vanish when $n>k+l$. This can be proved using the fact that $\int_{-\infty}^{\infty} x^r e^{-x^2} H_n(x)dx=0$ for $r<n$ [26]. In other words, atom-dimer states with energy $\bar{\nu}+(n+1/2)\hbar\omega$ 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 $\bar{\nu}<\hbar\omega/2$). However, they can be coupled by *multiple* Feshbach scattering. Therefore, we expect avoided level crossings for such levels but the splitting at the anticrossing point will be smaller in size than the level splittings at anticrossing points for levels coupled directly by a nonzero matrix element α_{kln}. This is because the splitting will be higher order in α.

IV. TWO-ATOM SYSTEM

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

$$E-\bar{\nu}=-\frac{\alpha^2}{2\hbar\omega d_r}\frac{\Gamma\left(\frac{1}{4}-\frac{E}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4}-\frac{E}{2\hbar\omega}\right)}. \tag{23}$$

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 α 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. This provides the parameters for us to compare one-channel and two-channel results in the presence of the trap in Sec. VI. 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 Eq. (23) becomes

$$\frac{\mu\alpha^2}{\hbar^2\bar{\nu}}-\frac{\mu\alpha^2|E|}{\hbar^2\bar{\nu}^2}-\left(\frac{2\mu|E|}{\hbar^2}\right)^{1/2}=0. \tag{24}$$

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 $1/a_{1D}-\mu r_{1D}|E|/\hbar^2-(2\mu|E|/\hbar^2)^{1/2}=0$ where $|E|=\hbar^2\kappa^2/(2\mu)$ and $\kappa R\ll 1$ with R being the range of the scattering potential. Comparing those two equations, we find

$$1/a_{1D}=\mu\alpha^2/\hbar^2\bar{\nu}$$

$$r_{1D}=\alpha^2/\bar{\nu}^2. \tag{25}$$

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 $\bar{\nu}\gg(\mu\alpha^4/2\hbar^2)^{1/3}$. In other words, we can match the two-channel parameters to the one-channel scattering parameters *away* from the resonance at $\bar{\nu}=0$ for positive $\bar{\nu}$. Indeed, this agrees with the work of [7] which showed that the lowest (bound state) branch of the spectrum exists only for $a_{1D}>0$: as $a_{1D}\to 0^+$ at the resonance, the energy diverges as $-1/a_{1D}^2$. This behavior is very different to that of Eq. (23) for the two-channel case in 1D which does not have a divergent energy at the resonance. This peculiarity is specific to 1D, and can be traced ultimately to the fact that the effective potential strength $\sim -1/a_{1D}$ and $\bar{\nu}\sim a_{1D}$; while in 3D, the effective potential strength $\sim a_{3D}$ and $\bar{\nu}\sim -1/a_{3D}$, and the matching using weakly bound states is valid near the resonance at $\bar{\nu}=0$ only in 3D.

V. RESULTS FOR THREE ATOMS

We will now discuss our results for the spectrum and eigenstates of the three-body system. As mentioned already, we treat the matrix Eq. (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 Eq. (14) by taking into account only atom-dimer energy levels with $\varepsilon_n<\varepsilon_{2n_C}$. This should properly reproduce the low-energy behavior 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 α_{kln}. We note that the oscillator wavefunctions $u_n(x,d_r)$ have a magnitude of the order of $d_r^{-1/2}$ over a spatial size d_r so that $\alpha_{kln}\sim\alpha/d_r^{1/2}$. Therefore, a dimensionless measure for the strength of the Feshbach scattering is the ratio of these two energy scales

$$\tilde{\alpha}=\frac{\alpha}{\hbar\omega d_r^{1/2}}. \tag{26}$$

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 [19,24].

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 Eq. (14). This can be estimated by the scale of the elements of M_{nm}

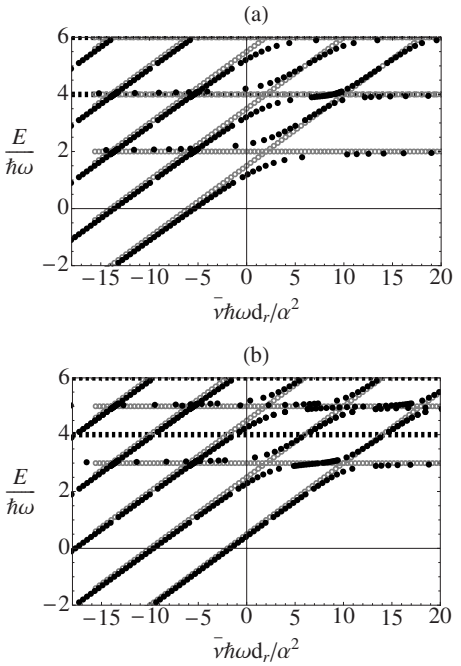

FIG. 1. Energy levels (in the centre-of-mass frame) versus detuning for three atoms in a harmonic well with s-wave Feshbach scattering at a dimensionless coupling $\tilde{\alpha}=0.5$. Dashed lines represent total pseudospin $S=3/2$ states which are unaffected by s-wave Feshbach scattering. Figures (a) 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.

$\sim(\alpha/d_r^{1/2})^2/\hbar\omega$. Therefore, a dimensionless measure of the detuning parameter is $\bar{\nu}\hbar\omega d_r/\alpha^2$. From the results Eq. (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

$$\frac{a_{1D}}{d_r}=\frac{\bar{\nu}\hbar\omega d_r}{\alpha^2} \tag{27}$$

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

We present in Fig. 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 $\bar{\nu}\hbar\omega d_r/\alpha^2$. The selection rules discussed above are reflected in the energy spectrum as it can be seen in Fig. 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 $|\chi_n\rangle$, the different diagonal lines corresponding to different atom-dimer oscillations. As we increase $\bar{\nu}$, Feshbach interaction with open-channel states becomes possible near the resonance points given by Eq. (13). At the resonances, there are anticrossings between the three-atom and atom-dimer states. For small $\tilde{\alpha}$, we can describe each anticrossing approximately by restricting the matrix Eq. (14) to just the two open and closed levels near the anticrossing in question. Then, we see immediately that, for resonances at positive detuning $\bar{\nu}$, the size of the splitting at resonance is of the order of the matrix element coupling the two states: $\alpha_{kln}\sim\alpha/d_r^{1/2}=\tilde{\alpha}\hbar\omega$.

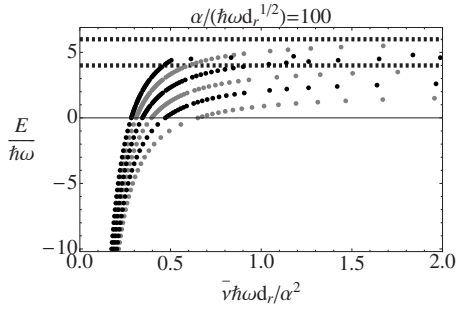

FIG. 2. Lowest six energy levels at strong Feshbach coupling: $\tilde{\alpha}=100$. Dashed lines represent total pseudospin $S=3/2$ states. Grey and black dots represent $S=1/2$ states with odd and even inversion symmetry, respectively.

However, for resonances at negative $\bar{\nu}$, the splittings are much smaller. As discussed in the Sec. III, these are the levels which are only coupled through multiple Feshbach scattering.

We can now turn to the regime of strong Feshbach scattering. Large coupling strength $\tilde{\alpha}$ means much stronger level anticrossing than for $\tilde{\alpha}=0.5$ case shown in Fig. 1. As an example, we have calculated the spectrum for $\tilde{\alpha}=100$. (We will see later that there is very little admixture of high-energy levels in the lowest-energy eigenstates, justifying our use of a relatively low cut-off n_C.) The six levels with the lowest energies are shown in Fig. 2. The apparent kink in the highest branch in Figs. 2 and 3 is due to the level crossing that can be better seen for the small $\tilde{\alpha}$ case in Fig. 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

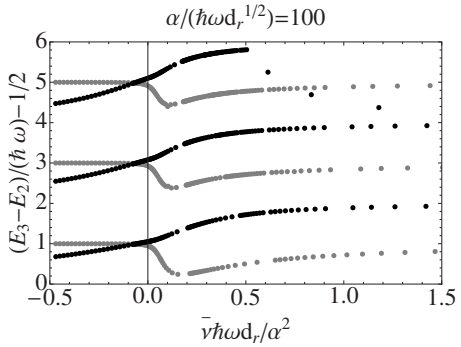

FIG. 3. Difference between the energy of three atoms in a harmonic well and the ground-state energy of two atoms in the well plus the lowest one-atom energy in a separate well. Grey and black dots represent $S=1/2$ states with odd and even inversion symmetry, respectively.

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 ($\bar{\nu}\to+\infty$). On the other hand, for large negative detuning, the states of lowest energy belong to the even-parity branch that becomes the $|\chi_0\rangle$ atom-dimer state asymptotically ($\bar{\nu}\to-\infty$). 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 ($\bar{\nu}\hbar\omega d_r/\alpha^2\simeq-0.07$ and $E\simeq-9\alpha/d_r^{1/2}$ for $\tilde{\alpha}=100$). Similar features were found for the spectrum of three atoms in a harmonic well within a one-channel model in one [16] and three [12] dimensions. Interestingly, qualitatively similar level crossings occur also in 1D in absence of the harmonic trap [25].

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 Eq. (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 Fig. 3. The subtraction does not alter the crossings of the three-body states at any given $\bar{\nu}$. In Sec. VII, 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 plus $\hbar\omega/2$ 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 plus $\hbar\omega/2$ 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 $E_3-E_2-\hbar\omega/2$. 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 $\tilde{\alpha}=100$. 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 Sec. II after Eq. (19). We note that this energy gap is much smaller in magnitude than the Feshbach energy scale $\alpha/d_r^{1/2}$ 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 in Fig. 4. Figures 4(a) and 4(b) present the composition of the lowest-energy state with an odd/even inversion symmetry. As expected, the state in Fig. 4(a) becomes the $|\chi_1\rangle$ atom-dimer

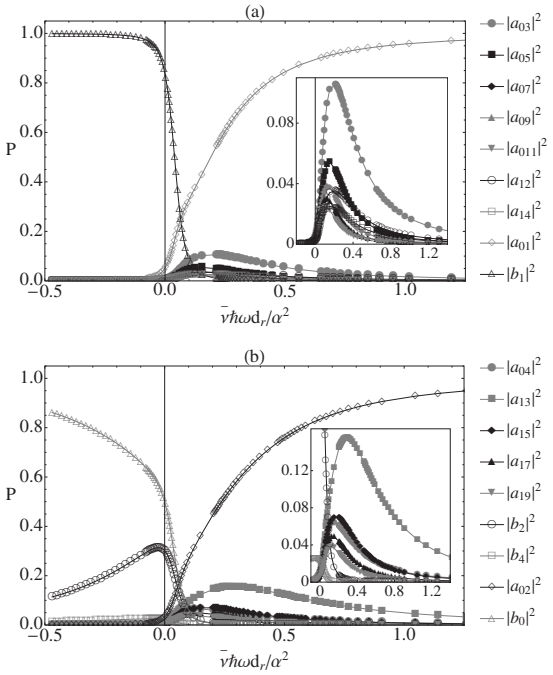

FIG. 4. Ground and first-excited pseudospin $S=1/2$ state composition as a function of detuning $\bar{\nu}(\tilde{\alpha}=100)$. The probabilities $|a_{kl}|^2$ and $|b_n|^2$ correspond to open-channel and atom-dimer probabilities, respectively, (see, the Eq. (11) for definition of a_{kl} and b_n). (a) Lowest-energy state with odd inversion symmetry (lowest gray data in Fig. 2). (b) Lowest-energy state with even inversion symmetry (lowest black data in Fig. 2).

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 in the figure. Figure 4(b) gives an example with even inversion symmetry. The state is asymptotically the $|\chi_0\rangle$ atom-dimer state at large negative detunings. Closer to the resonance at negative $\bar{\nu}$ there is also a significant $|\chi_2\rangle$ 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 $|\chi_1\rangle$ dominates in the lowest-energy state with odd inversion symmetry, both $|\chi_0\rangle$ and $|\chi_2\rangle$ 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 α_{kln}. As discussed in Sec. III, the wavefunctions involved should have similar symmetries to ensure a finite value for α_{kln}. 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 α_{kln} that contribute to the lowest-energy states are α_{011} and α_{013} for the odd-parity state and α_{020} and α_{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 $|\alpha_{020}|\sim|\alpha_{022}|$. In terms of Eq. (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 $|\chi_0\rangle$ and $|\chi_2\rangle$ 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 Eq. (16). We see that the admixture of high-energy levels is small. This allows us to ignore the contribution of $|\chi_n\rangle$ 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: $V(\vec{r}) = g\delta(\vec{r})$, with a potential strength g that depends on the detuning [7,12]. 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.

Let us review the results for two atoms in three dimensions. We have been discussing the branch of bound states induced by Feshbach interaction. The effective interaction between the atoms close to the resonance can be described by an effective contact potential with $g_{3D} = 2\pi\hbar^2 a_{3D}/\mu$ which diverges as one sweeps the system across the resonance at $\bar{\nu} = 0$. Without a harmonic trap, the bound states are weakly bound with a binding energy that vanishes as we approach the resonance ($\bar{\nu} = 0$) from negative detuning. In other words, these eigenstates have only small amplitude in the closed-channel dimer state. Therefore, the matching to a one-channel model is best *near* the resonance in 3D without confinement. The range of validity of the one-channel model will be wide if the Feshbach coupling is strong. (There are also narrow resonances where a one-channel model does not apply [29] due to the significant admixture of the closed-channel component.)

These arguments for the wide resonance remain valid in the presence of a harmonic trap. The admixture of the dimer component to the low-energy states is very small [8] and the effective interaction between the atoms close to the resonance can be described by an effective contact potential [7,12,27,28] which diverges across the resonance at $\bar{\nu} = \hbar\omega/2$.

We will now turn to the case of one dimension, starting with two atoms without a trap. We have already studied in Sec. IV 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. As in our discussion for the 3D case, we expect the one-channel and two-channel models to converge for weakly bound states. We noted that the most weakly bound states are found at large *positive* detuning *away* from the resonance, unlike the 3D case where these states are found at negative $\bar{\nu}$ near the resonance. More quantitatively, the weak-binding condition is that $|E| \sim \hbar^2/2\mu a_{1D}^2 \ll \bar{\nu}$. This can be expressed in terms of the dimensionless Feshbach and detuning parameters used in our study Eq. (25)

$$\frac{\bar{\nu}\hbar\omega d_r}{\alpha^2} \simeq \frac{a_{1D}}{d_r} \gg \frac{1}{\tilde{\alpha}^{2/3}}. \tag{28}$$

Note that the regime of validity improves at strong coupling ($\tilde{\alpha} \gg \infty$) so that such a theory may be applicable for realistic ^{40}K systems except very close to the resonance. In terms of an effective contact potential strength, we have $g_{1D} = -\hbar^2/\mu a_{1D}$ [7] 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.

We also note that, near the resonance, the one-channel model [7] gives a negative energy which diverges as $a_{1D} \to 0^+$ while the two-channel model (23) does not show a divergence as $\bar{\nu} \to 0^+$. Indeed, the bound-state energy is finite as a_{1D} (and detuning $\bar{\nu}$) changes sign, approaching the dimer energy $\bar{\nu}$ for large negative a_{1D}. This fundamental difference between the one-channel and two-channel models remains even if we refine our treatment of the closed channel.

We will now turn to our three-atom results. The conclusions above about the regime of validity of the one-channel approximation for the two-body problem remain true for our three-body results. 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 Fig. 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 Fig. 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 ($\tilde{\alpha} \gg 1$). Therefore, we conclude that the system cannot be modeled 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 modeled in an effective theory for the open-channel states.

Furthermore, we have performed a one-channel calculation for three atoms in a well for our system using an effective g_{1D} [30], 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.

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 $\tilde{\alpha} = 100$.

VII. SUMMARY AND DISCUSSION

We have considered two species of fermionic ^{40}K atoms at ultracold temperatures trapped in a 1D optical lattice and

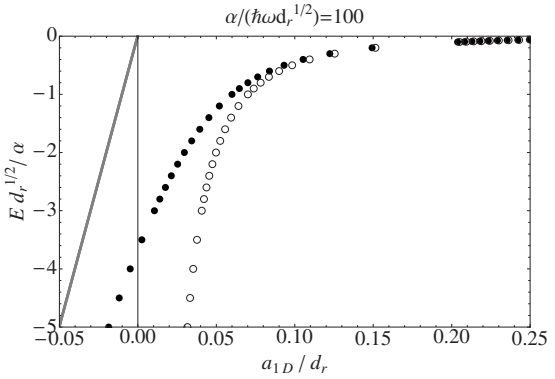

FIG. 5. The lowest-energy state with odd inversion symmetry for three atoms calculated using the two-channel models (solid circles) and one-channel model (open circles). The one-channel calculation has been performed with an analogous cutoff in basis states as in the two-channel calculation. The horizontal axis is plotted using the correspondence in Eq. (28). Grey line represents the closed-channel state in the two-channel model in the absence of Feshbach coupling ($E=\bar{\nu}+3\hbar\omega/2$).

close to an interspecies Feshbach resonance. We have concentrated on the zero-tunneling 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 $|\chi_n\rangle$ 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 $(r_1-r_2)/d_r^{1/2}$. So, the probability for the spectator to be in the vicinity of a dimer of size d_m is proportional to $\int^{d_m}(r/d_r)^2 dr/d_r \sim (d_m/d_r)^3$. We estimate the residual attraction ϵ_{ad} between the atom and the dimer would be of the order of $\bar{V}(d_m/d_r)^3$ where $\bar{V}$ 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 $\bar{V}$ 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 renormalized scattering strength α, but our results are not sensitive to the value of α in this regime of large $\tilde{\alpha}$.) In fact, the even-symmetry state has a similar but larger correction of $\bar{V}d_m/d_r$ 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 $|\uparrow\circ\rangle$. 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 ratio of 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 tunneling between a set of wells. Consider the case with three atoms per site on average. From the level crossing we found in Fig. 3, 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 intersite tunnelling would couple the states of different inversion symmetries. We need to investigate collective quantum fluctuations to study this possibility.

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