Bound states of two bosons in an optical lattice near an association resonance

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We model two bosons in an optical lattice near a Feshbach or photoassociation resonance, focusing on the Bose-Hubbard model in one dimension. Whereas the usual atoms-only theory with a tunable scattering length yields one bound state for a molecular dimer for either an attractive or repulsive atom-atom interaction, for a sufficiently small direct background interaction between the atoms a two-channel atom-molecule theory may give two bound states that represent attractively and repulsively bound dimers occurring simultaneously. Such unusual molecular physics may be observable for an atom-molecule coupling strength comparable to the width of the dissociation continuum of the lattice dimer, which is the case, for instance, with narrow Feshbach resonances in Na, $^{87}\text{Rb}$, and $^{133}\text{Cs}$ or low-intensity photoassociation in $^{174}\text{Yb}$.

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An optical lattice [1] modifies the motion of atoms profoundly compared to free space. Moreover, the site-to-site hopping of the atoms can be controlled by varying the intensity of the lattice laser, which enables phenomena ranging from Mott insulators [2] to atomtronics [3]. The interactions between the atoms can also be tuned by utilizing Feshbach [4, 5] and photoassociation [6, 7] resonances. In effect, both the mass of the atoms and the atom-atom interactions can be controlled experimentally, possibly leading to custom-tailored molecules and unprecedented experimental control of molecular physics.

As the prime example to date, dimers bound by repulsive atom-atom interactions have been demonstrated experimentally [8] and confirmed theoretically [8–12].

In the conventional single-channel description of the lattice dimers [8, 10–16] the atoms have an interaction between them characterized by a scattering length that diverges at the resonance. The more nuanced two-channel theory [9, 17, 18] asserts that there are also molecules present as an independent degree of freedom. In this view atom pairs may be converted into molecules, and a resonance occurs when the atom pairs and the molecules have the same energy.

In the present communication we formulate and solve the time-independent Schrödinger equation for a lattice dimer within the two-channel model. We find a peculiar qualitative change in the molecular physics compared to the single-channel model: while the latter always presents one bound state for the dimer, in the case of sufficiently weak direct interactions between the atoms the two-channel model may exhibit two bound states, one below and one above the band of dissociated dimer states. In particular, while the single-channel description provides for a bound state below the continuum band for attractive atom-atom interactions or a bound state above the dissociation continuum for repulsive interactions, the two bound states for the two-channel dimer may be viewed under certain conditions as the analogs of attractively and repulsively bound pairs occurring simultaneously for the same system parameters.

We begin with the Bose-Hubbard Hamiltonian for a one-dimensional lattice in the single-channel picture [11],

$$\frac{H}{\hbar} = -\frac{J}{2} \sum_k \left( a_{k+1}^\dagger a_k + a_k a_{k-1}^\dagger \right) + \frac{U}{2} \sum_k a_k^\dagger a_k a_k a_k^\dagger. \quad (1)$$

The index $k$ runs over the lattice sites, $L$ of them. We use periodic boundary conditions, so that the site $k = L$ is the same as the site $k = 0$. The parameter $J$ characterizes tunneling from site to site, $U$ quantifies the atom-atom interactions, and $a_k$ is the annihilation operator for bosonic atoms at the site $k$.

The corresponding two-channel model describes an association resonance where a bound molecular state and a state of two asymptotically free atoms become degenerate. The Hamiltonian is

$$\frac{H}{\hbar} = -\frac{J}{2} \sum_k \left( a_{k+1}^\dagger a_k + a_k a_{k-1}^\dagger \right) + \delta \sum_k b_k^\dagger b_k \nonumber$$

$$-\xi \sum_k \left( b_k^\dagger a_k a_k + a_k^\dagger a_k b_k \right), \quad (2)$$

where $b_k$ is the annihilation operator for a molecule at the site $k$, and the detuning $\delta$ quantifies the difference in energy between a molecule and an atom pair; $\delta = 0$ denotes the resonance. The entities annihilated by $a_k$ and $b_k$ are bare atoms and molecules that would exist without the atom-molecule conversion $\propto \xi$. Diagonalization of the Hamiltonian (2) gives a description of the physically observable dressed molecules.

In our simplest possible model we do not include site-to-site tunneling of the molecules. This is reasonable since the molecules are twice as heavy as the atoms and the tunneling amplitude $J$ is exponentially small in mass. There could also be atom-atom interactions as in the
the c.m. momentum. The problems with the notation \( \frac{1}{2} P \pm q \) are irrelevant in our final limit when the momentum becomes a continuous variable. Defining a characteristic frequency \( \Omega_P \) and scaling all dimensional quantities to it,

\[
\Omega_P = 2J \cos(\frac{1}{2} P); \quad \Xi = \frac{\sqrt{2} \xi}{\Omega_P}, \quad \Delta = \frac{\delta}{\Omega_P}, \quad \omega = \frac{E}{\hbar \Omega_P},
\]
we find the time independent Schrödinger equation for the energy \( E \leftrightarrow \omega \) in the form

\[
(\omega + \cos q) A(q) + \frac{\Xi \beta}{\sqrt{2L}} = 0, \quad (\Delta - \omega) \beta - \frac{\sqrt{2} \Xi}{\sqrt{L}} \sum_q A(q) = 0 .
\]

From the Schrödinger equations (8) and (9) one may deduce the condition for the (scaled) eigenstate energy \( \omega \),

\[
f(\omega, L) \equiv \frac{1}{L} \sum_q \frac{\omega - \Delta}{\Xi^2} = \frac{\omega - \Delta}{\Xi^2} .
\]

For comparison, the single-channel result is

\[
f(\omega, L) = \frac{1}{K},
\]
with \( K = U/\Omega_P \). Once the eigenenergy \( \omega \) has been solved from Eq. (10), the unit-normalized solution to the Schrödinger equation is

\[
\beta = - \left[ 1 + \frac{\Xi^2}{L} \sum_q \frac{1}{(\omega + \cos q)^2} \right]^{-1/2}, \quad A(q) = \frac{-\Xi \beta}{\sqrt{2L} (\omega + \cos q)} .
\]

We plot the function \( f(\omega, L) \) for \( L = 16 \) as a function of the variable \( \omega \) in Fig. 1. The right-hand sides of Eqs. (10) and (11) for the parameters \( K = \Delta = 1/2 \) and \( \Xi = 1/\sqrt{2} \) are also represented as straight lines in Fig. 1. The solutions occur where the straight lines and the graph of \( f(\omega, L) \) intersect. Equations (10) and (11) both have one solution \( \omega \) between each value of \( -\cos q \) for the successive discrete values of the quasimomentum \( q \). This is the finite-lattice analog of the dissociation continuum of the dimer. The single-channel eigenvalue equation (11) also has one solution \( \omega \) outside of the range \((-1, 1)\). For a positive atom-atom interaction coefficient \( U \) this is the celebrated repulsively bound dimer [8]. On the other hand, the two-channel model as in Eq. (10) always has \textit{two} bound states; one above and one below the dissociation continuum.

With the addition of the explicit molecular degree of freedom, for each fixed c.m. momentum \( P \) the dimer system has one more degree of freedom in the two-channel
The technical rule is that any sum over the lattice momenta is continuous variable in the interval $[-\pi, \pi]$. The dashed vertical lines are the asymptotes of $f(\omega, L)$ at the values of $\omega = -\cos q$ such that $f(\omega, L) = \pm \infty$.

We discuss the limit when the lattice is infinitely long, $L \to \infty$, whereupon the quasimomentum becomes a continuous variable in the interval $[-\pi, \pi]$. The main technical rule is that any sum over the lattice momenta is replaced with an integral, $\sum_q \to \frac{1}{2\pi} \int_{-\pi}^{\pi} dq$. Here we only look into the two bound states with $|\omega| > 1$. The eigenvalue equation and the amplitude of the molecules in the bound state are

$$\frac{\omega - \Delta}{\Xi^2} = \frac{\text{sgn}(\omega)}{\sqrt{\omega^2 - 1}}, \quad \beta = -\left[\frac{(\omega^2 - 1)^{3/2}}{(\omega^2 - 1)^{3/2} + |\Xi|^2}\right]^{1/2}. \quad (14)$$

An expansion of the other bound state energy $\omega_T \approx -1$ that approaches the continuum threshold in the limit $\Delta \to \infty$ is found similarly. Analytical expansions are also available in the neighborhood of the association resonance $\Delta \sim 0$. In this case the energies $\omega_{\pm}$ are found in the form $\omega_{\pm} = \pm \text{sgn}(\omega) b_0 + b_1 \Delta + \ldots$.

The extra bound state can be characterized starting from the asymptotic expansions of the bound-state energies. For large detuning the expansions (17) and its counterpart for the energy $\omega_T$ give the molecular fractions $f = |\beta|^2$

$$f_{\Delta} \simeq 1 - \frac{\Xi^2}{\Delta^2}, \quad f_T \simeq \frac{\Xi^4}{|\Delta|^4}, \quad (18)$$

whereas for $\Delta \sim 0$ the molecular fractions for both bound states are

$$f_{\pm} \simeq \frac{2\Xi^4}{1 + 4\Xi^4 + \sqrt{1 + 4\Xi^2}}. \quad (19)$$

According to Eq. (3), the single-channel model is recaptured from the two-channel model in the limit when the parameters $\Delta$ and $\Xi$ both tend to infinity in such a way that $\mathcal{K} = -\Xi^2/\Delta$ remains constant. $\mathcal{K}$ is then nothing but the two-channel counterpart of the dimensionless atom-atom interaction constant that we also denoted by $\mathcal{K}$ in our single-channel theory [11]. In fact, in this particular limit the energy of the bound state $\omega_T$ converges to the single-channel result $\omega = \text{sgn}(\mathcal{K})\sqrt{1 + K^2}$. Moreover, the molecular fraction $f_T$ of this bound state vanishes.
The $|\Delta| \to \infty$ bound state that we have denoted by the subscript $T$ is the counterpart in the two-channel model of the bound state in the single-channel model. The character of the other $|\Delta| \to \infty$ bound state that we have denoted by the subscript $A$ is equally obvious. The energy tends to $\omega_\Delta \to \Delta$, the energy of the bare molecule, and the molecular fraction behaves as $f_\Delta \to 1$. This bound state simply represents a bare molecule that has decoupled from the atoms.

The bound states at resonance $\Delta \sim 0$ make a more interesting tale. First, the structure of the state space and of the coupling between bare atoms and molecules, the kinematics of the problem, forces the existence of two bound states for the dressed molecule. Second, from Eq. (20) we see that the fraction of bare molecules $f_\Xi$ in both bound states tends to zero when the atom-molecule coupling $\propto \Xi$ vanishes, and to 1/2 when the atom-molecule coupling is strong. In dimensional quantities the borderline between the two cases is approximately at $\xi \sim \Omega_R$ when the strength of the atom-molecule coupling is comparable to the width of the continuum band of the dissociated states of the molecule.

In the limit of strong atom-molecule coupling, $|\Xi| \to \infty$, the width of the continuum band is negligible. Formally, $\cos q \equiv 0$ in Eq. (8) and an effective two-level system for the amplitude $\beta$ and the collective amplitude $\sum_q A_q$ emerges. The association resonance then splits these two states apart. All told, the corresponding bound states represent association in a system that behaves as if there were no kinetic energy for the atoms. On the other hand, for weak atom-molecule coupling, $\Xi \to 0$, the bound states are already far-detuned from the association resonance as a result of the width of the continuum band, and are effectively described by the single-channel theory. The two coexisting bound states we have denoted by $\pm$ then mean that the usual bound state for an attractive atom-atom interaction and the repulsively bound state are present simultaneously.

The two bound states also provide unexpected insights into modeling of Feshbach resonances. In molecular physics it is customary to think of Feshbach resonances in terms of multiple channels, whereas single-channel pictures are the norm in condensed-matter physics. Oddly enough, there seems to be little difference [19] between the predictions from single- and two-channel theories in common experimental situations with quantum degenerate gases. In contrast, one bound state in the single-channel description and two bound states in the two-channel description is a stark qualitative difference.

The characteristic frequency scale of the lattice physics [1] is the recoil frequency set by the atomic mass $m$ and the lattice spacing $d$ as $\epsilon_R = \pi^2 \hbar / 2md^2$, roughly $10 \times 2 \pi $ kHz; the tunneling amplitude $J$ is typically a fraction thereof. The two bound states are similar in character and therefore presumably easiest to detect simultaneously on resonance, $\Delta \sim 0$. To have the bound states well separated from the dissociation continuum we would like to have $\xi \gtrsim \Omega_R \sim J$. On the other hand, the resonance will overwhelm the lattice physics if $\xi \gg \epsilon_R$, and the Bose-Hubbard model itself may need to be amended [20, 21]. Overall, it appears that the best experimental parameters are in the neighborhood of $\xi \sim \epsilon_R$. Our question is, are atom-molecule couplings of this order available in practice?

We proceed along the lines of Refs. [22] and [23]. We write the atom-molecule coupling as $\xi = \bar{\omega}^{1/4} \Omega^{3/4}$, where $\bar{\omega}$ characterizes the free-space molecular physics and $\Omega$ the lattice physics. Assuming that the Wannier functions for atoms and molecules at each lattice site are ground states of a three-dimensional harmonic oscillator with frequencies $\omega_i$, we have $\Omega = (\omega_1 \omega_2 \omega_3)^{1/3} / 2 \pi$. The characteristic order of magnitude of the lattice contribution is then of the order of the recoil frequency and, in turn, so should be the free-space contribution, which calls for a weak association resonance.

For the Feshbach resonance, the free-space coupling for a given resonance is fixed once and for all. The remaining molecular frequency is $\tilde{\omega} = 4 \pi^2 m a^2 \bar{\omega}^2 \Delta^2 / \hbar^3$, where the background scattering length is $a_0$, and the magnetic field width of the resonance is $\Delta_B$, while the difference between the magnetic moments of a bare molecule and two bare atoms is $\Delta \mu$. To achieve $\tilde{\omega} \sim \epsilon_R$ requires a narrow Feshbach resonance. Potential candidates include the 853 G resonance in Na [24] ($\tilde{\omega} \sim 1.6 \times 2 \pi $ kHz), the 191 G resonance in $^{87}$Rb [25] $(31 \times 2 \pi $ Hz), and the 20 G resonance in $^{133}$Cs [26] $(75 \times 2 \pi $ Hz).

In photoassociation the atom-molecule coupling $\xi$ is adjustable according to the laser intensity. Borrowing from Ref. [23], we have $\tilde{\omega} = 4 \pi^2 m L_{PA}^2 / \hbar$, where $L_{PA} = m K/(4 \pi)$ is determined from the low-intensity rate constant $K \propto I$, and the natural linewidth of the molecular state is $\Gamma$. The broad natural linewidths complicate photoassociation in alkali metals [6], but the alkali-earth metals have narrow linewidths and, in particular, the 192 MHz line in $^{174}$Yb [7] is a ready candidate for a laser intensity of the order of 1 mW/cm$^2$, so that $\tilde{\omega} \approx 63 \times 2 \pi $ Hz.

We have discussed the stationary states of two bosons in a one-dimensional optical lattice within the two-channel Bose-Hubbard model. The particular result that there are two bound states, one of them effectively a dimer bound by attractive interactions and the other by repulsive interactions, provides a dramatic example of molecular physics in a lattice with no counterpart in free space. We have identified several Feshbach and photoassociation systems for which this unusual situation might be observable.

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