Quantum dynamics of one and two bosonic atoms in a combined tight-binding periodic and weak parabolic potential

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received 7 March 2008; accepted in final form 9 June 2008
published online 18 July 2008

PACS 03.75.Lm – Tunneling, Josephson effect, Bose-Einstein condensates in periodic potentials, solitons, vortices, and topological excitations
PACS 37.10.Jk – Atoms in optical lattices
PACS 03.65.Ge – Solutions of wave equations: bound states

Abstract – Strongly interacting bosonic particles in a tight-binding periodic potential superimposed by a weak parabolic trap is a paradigm for many cold atom experiments. Here, after revisiting the single-particle problem, we study interaction-bound dimers of bosonic atoms in the combined lattice and parabolic potential. We consider both repulsively and attractively bound dimers and find pronounced differences in their behaviour. We identify conditions under which attractive and repulsive dimers exhibit analogous dynamics. Our studies reveal that coherent transport and periodic oscillations of appropriately prepared one- and two-atom wave packets can be achieved, which may facilitate information transfer in optical-lattice–based quantum computation schemes.

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Introduction. – Quantum transport in periodic structures is one of the central topics of condensed matter physics [1]. Recent interest towards spatially periodic systems has been largely motivated by the remarkable progress in cooling and trapping bosonic and fermionic atoms in optical lattices [2]. The relevant parameters of these systems can be controlled with very high precision and can be tuned to implement some of the fundamental models of condensed matter physics. In a tight-binding regime, the Hubbard model accurately describes static and dynamic properties of these systems [2,3]. Importantly, in actual experiments with cold atoms, the lattice is finite and often it is superimposed by a weak harmonic trap. This breaks the translational invariance of the lattice and thereby strongly modifies the properties of the system even in the limit of non-interacting particles [4–6]. In particular, the low-energy states of the single-particle spectrum behave like harmonic oscillator states, while the higher-energy states are localized at the sides of the parabolic trap, which can lead to inhibition of quantum transport and dipole oscillations in a degenerate atomic gas [6–9].

Atom-atom interactions profoundly enrich the optical lattice realizations of Hubbard model [2,3]. A wealth of non-linear phenomena with atomic matter-waves, including discrete solitons and breathers [10], can be observed in optical lattices [2]. Strongly interacting bosons in periodic potentials can form tightly bound “dimers” [11–13] realized in a recent experiment [14] with repulsively interacting atoms in a lattice. Here we first discuss static and dynamic properties of a single atom in a combined periodic and weak parabolic potential [4–6]. We show that coherent transport and periodic oscillations of properly prepared atomic wave packets can be achieved, which may be employed for information transfer in optical-lattice–based quantum computation schemes. We then study strongly interacting atom pairs —dimers, examining both regimes of attractive and repulsive interactions, and find that low-energy dimers behave as single composite particles with appropriately rescaled parameters of the system. There are, however, important differences between the attractively bound and repulsively bound dimers, stemming from the properties of their respective ground states [12]. Our studies reveal that many aspects of interaction-bound atom pairs can be understood in terms of a simple effective model [11] modified by the presence of a parabolic trap, which can mediate non-dispersive transport of two-particle wave packets. This is reminiscent to, but should be contrasted with, the behaviour of lattice solitons [2,10] where dispersion compensation is due to the internal non-linearity and not an external trap.

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The model. – We consider cold bosonic atoms in a combined tight-binding periodic and weak parabolic potential. In 1D, the system is described by the Bose-Hubbard Hamiltonian

$$H = \sum_{j} \left[ \Omega_j^2 \hat{n}_j + \frac{U}{2} \hat{n}_j (\hat{n}_j - 1) - J (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j) \right],$$

(1)

where $b_j^\dagger (b_j)$ is the creation (annihilation) operator and $\hat{n}_j = b_j^\dagger b_j$ the number operator for site $j$. $J$ is the tunnel coupling between adjacent sites, $U$ is the on-site interaction, and $\Omega > 0$ quantifies the strength of the superimposed parabolic potential due to which site $j = \pm 1, \pm 2, \ldots$ acquires energy offset $\Omega_j^2$ with respect to site $j = 0$ corresponding to the minimum of the potential. A natural basis for Hamiltonian (1) is that of the eigenstates $|n_j\rangle \equiv \frac{1}{\sqrt{\Omega_j^2}} (b_j^n |0\rangle$ of operator $\hat{n}_j$ whose eigenvalues $n = 0, 1, 2, \ldots$ denote the number of particles at site $j$, and $|0\rangle \equiv |\{0_j\}\rangle$ is the vacuum state.

Single-particle spectrum. We first discuss the single-particle case with the on-site interaction $U$ playing no role. Recall that in the absence of parabolic potential, $\Omega = 0$, the eigenstates of the Hubbard Hamiltonian (1) form a Bloch band of width $4J$ centered around zero. More quantitatively, given a finite flat lattice of $N$ sites, the Bloch eigenenergies and corresponding eigenstates are given by

$$E_k = -2J \cos \left[ \frac{\pi (k + 1)}{N + 1} \right],$$

(2a)

$$|\chi_k\rangle = N \sum_{i=1}^{N} \sin \left[ \frac{\pi (k + 1)}{N + 1} \right] |l_i\rangle,$$

(2b)

with $0 \leq k < N$ a normalization constant. In the limit of $N \to \infty$, eq. (2a) yields the well-known dispersion relation $|E_k| = -2J \cos (q)$, with quasi-momentum $0 \leq q \leq \pi$ and lattice constant $d = 1$. Remarkably, however, even a very weak parabolic potential $\Omega \ll J$ drastically modifies the spectrum of Hamiltonian (1) [4,5], as shown in fig. 1. Note that the spectrum, bound from below by $-2J$, is composed of discrete energy levels $E_k$. Two distinct groups of levels can be identified: i) the low-energy levels $E_k \leq 2J$ forming a modified Bloch band, and ii) the high-energy ones $E_k > 2J$.

i) The parabolic potential effectively restricts the number of sites accessible to a particle with energy within the Bloch band $-2J \leq E_k \leq 2J$. Roughly, only sites $j = 0, \pm 1, \ldots$, for which $\Omega_j^2 < 2J$, can participate in the formation of the low-energy part of the spectrum [5]. More precisely, using second-order perturbative corrections, we find that the modified Bloch band is restricted to sites $j$ satisfying

$$|j| \leq j_{\text{max}} \equiv \sqrt{\left( 1 + \frac{1}{\sqrt{2}} \right) \frac{J}{\Omega}} \simeq 1.3 \sqrt{\frac{J}{\Omega}}.$$

(3)

The low-energy part of the spectrum therefore contains $N = 2j_{\text{max}} + 1$ energy levels $E_0, E_1, \ldots, E_{2j_{\text{max}} - 1}$, which is illustrated in fig. 1, and we have verified this conclusion for a wide range of values of $J/\Omega$. Note that the weak parabolic potential modifies the Bloch band in such a way that its lowest energy part is approximately linear in $k$, similar to the spectrum of harmonic oscillator. Indeed, using the properties of the Mathieu functions [15], it can be shown [5] that in the limit of $J/\Omega \gg 1$, the low-energy eigenvalues $E_k$ and eigenstates $|\chi_k\rangle$ of Hamiltonian (1) are well approximated by

$$E_k \approx -2J + 2\sqrt{J\Omega} (k + \frac{1}{2}),$$

(4a)

$$|\chi_k\rangle \approx N \sum_{j} (2^k k!)^{-1/2} e^{-\zeta_j^2/2} H_k(|\chi_j\rangle |l_j\rangle),$$

(4b)

where $N$ is a normalization constant, $\zeta_j = j \sqrt{\Omega/J}$ is the discretized coordinate, and $H_k(\zeta)$ is the $k$-th Hermite polynomial. Thus, the lowest-energy eigenvalues $E_k$ and eigenstates $|\chi_k\rangle$ correspond to those of an energy-shifted harmonic oscillator with an effective frequency $\omega = 2\sqrt{J\Omega}$ and an effective mass given by the usual expression $m = \hbar^2/(2Jd^2) [1]$ which is valid near the bottom of the lowest Bloch band of a periodic potential. In particular, the ground state with $E_0 = -2J + \sqrt{J\Omega}$ is given by $|\chi_0\rangle = \sqrt{\Omega/(\pi^2 J)} \sum_j e^{-\zeta_j^2/2} |l_j\rangle$. The spectrum at the top of the modified Bloch band approaches that of a uniform $(\Omega = 0)$ finite $(N = N)$ lattice given by eq. (2a).

ii) On the other hand, the high-energy eigenvalues $E_k > 2J$ with $k \geq N$ are two-fold degenerate, as seen in fig. 1. The pairs of degenerate states with indices $k = 2|j| + 1$ and $k' = 2|j| + 2$ are localized around sites $j = \pm |j| (|j| > j_{\text{max}})$ equidistant from the center of the parabolic potential, the corresponding energies being $E_{k,k'} = \Omega_j^2 [4,5]$. For such states, the localization occurs because, for large enough $|j|$, the transitions $|l_j\rangle \to |l_{j+1}\rangle$ effected by the last term of Hamiltonian (1) become non-resonant and the particle tunneling between neighboring lattice sites is suppressed.
corresponds to the ground state as a single-particle wave packet \( \rho \) showing the density distribution shifted by 7 sites from the trap center. (b) Initial state from the transport of a single-particle wave packet from one side to the lowest part of the energy spectrum, we can expect ourselves to the harmonic-oscillator-like states belonging to the same site.

From the above analysis, it is clear that if we restrict ourselves to the harmonic-oscillator-like states belonging to the lowest part of the energy spectrum, we can expect quasi-periodic dynamics in the system. Non-dispersive transport of a single-particle wave packet from one side of the shallow parabolic potential to the other can then be achieved. In fig. 2(a) we show the dynamics of a single-particle wave packet \( |\psi\rangle \), represented by the ground state of the system, \( |\chi_0\rangle \), initially shifted by 7 sites from the trap center. Numerical solution of the Schrödinger equation using Hamiltonian (1) reveals almost perfect periodic oscillations of the discrete Gaussian wave packet between the two sides of the parabolic potential with period \( \tau \simeq 2\pi/\omega = (\hbar/\Omega)\sqrt{J/\Omega} \).

From the set of harmonic-oscillator-like states \( |\chi_k\rangle \) of eq. (4b), we can construct a well-localized wave packet \( |\psi(j')\rangle \) centered at a prescribed site \( j' (|j'| < j_{\text{max}}) \). If we write the initial state as

\[
|\psi(0)\rangle = \sum_k A_k |\chi_k\rangle, \tag{5}
\]

the probability amplitude \( a_j \) for a particle to be at site \( j \) is given by

\[
a_j = (\langle j|\psi(0)\rangle \propto \sum_k A_k (2^k k!)^{-1/2} e^{-\zeta_j^2/2} H_k(\zeta_j). \tag{6}
\]

To obtain a localized around site \( j' \) state \( |\psi(j')\rangle \), we maximize \( |a_j|^2 \), which determines the set of coefficients \( \{A_k\} \) in eq. (5). In fig. 2(b) we show the time evolution of density \( \rho_j \equiv \langle \hat{n}_j \rangle \) for such a localized state, which exhibits periodic collapses and partial revivals at sites \( -j' \) and \( j' \) with time steps \( \tau/2 \). The revivals are not complete since, as noticed above, the energy spectrum \( E_k \) for small \( k \) is only approximately linear in \( k \). Nevertheless, our results suggest that coherent non-dispersive transport of carefully engineered atomic wave packets can be achieved in optical lattices in the presence of a shallow parabolic potential.

Two-particle dynamics. – We now consider two bosonic particles in the combined periodic and weak parabolic potential. Clearly, in the simplest case of feeble interaction \( |U| \ll J \), we have two independent particles for which the results of the previous section apply. But even for strong on-site interaction \( U \), the combined dynamics of two low-energy particles can be inferred from the independent-particle picture modified by short-range collisions. This applies when the initial state \( |\Psi(0)\rangle = |\psi\rangle \otimes |\psi^{(')}\rangle \) is composed of two non-overlapping single-particle wave packets, \( |\langle \psi|\psi^{(')}\rangle|^2 \ll 1 \), which upon collision with each other only acquire a unitary scattering phase shift \( \delta(U) \) [12]. Example of such a situation is shown in fig. 3(a); analogous dynamics is observed for any value of on-site interaction \( U \), since density \( \rho_j \equiv \langle \Psi | \hat{n}_j | \Psi \rangle \) is invariant under phase shift of \( |\Psi\rangle \).

More intriguing is the case of the initial state \( |\Psi(0)\rangle = |\psi\rangle \otimes |\psi^{(')}\rangle \) consisting of overlapping single-particle wave packets shown in fig. 3(b). This state has a significant population of two-particle states \( |2\rangle \) given by

\[
\sum_j |\langle 2|j|\Psi\rangle|^2 \gg \sum_j |a_j|^4,
\]

where \( a_j \) are the single-particle probability amplitudes. Clearly, the population of two-particle states is largest in the central part of the initial density distribution. As seen in fig. 3(b), this part exhibits slow dynamics, characterized by the effective tunnelling constant \( J^{(2)} = -2J^2/U \) (see below), and separates from the wings of the initial density profile. The wings, formed by single-particle states \( |1\rangle \), oscillate between the two sides of the parabolic potential with the usual period \( \tau \).

Interaction-bound dimers. At this point, let us recall [11–14] that two bosonic particles occupying the same site \( j \) can form an effective “dimer” bound by the on-site interaction \( U \). Thus, when \( |U| \gg J \), the first-order transitions \( |2\rangle \rightarrow |1\rangle |1\rangle \) effected by the last term of Hamiltonian (1) are non-resonant and the particles cannot separate. However, the second order
two particles in a combined periodic and parabolic potential with $J/J\Omega = 1.40$ and $U = -10J$. (a) Initially both particles in the ground state $|\psi_0\rangle$ are shifted from the trap center by 7 sites in opposite directions. (b) Initial state $|\Psi(0)|$ corresponds to both particles in state $|\psi_0\rangle$ shifted from the trap center by 7 sites in the same direction. Inset in (b) shows the projection $\sum_j |(2_j)|^2$.

in $J$ transitions $|2_j\rangle \rightarrow |2_{j+1}\rangle$ via virtual intermediate states $|1_j\rangle, |1_{j+1}\rangle$ are resonant. Consequently, the dimer can tunnel as a whole with the effective rate $J^{(2)} = -2J^2/U \ll J [11]$. This explains the dynamics seen in fig. 3(b) where the initial density distribution splits into slow- and fast-propagating components, the former composed of the dimer states $|2_j\rangle$ while the latter containing the monomer states $|1_j\rangle$.

If the initial state is prepared in such a way that only two-particle (dimer) states are populated, as implemented in, e.g., [14], for $|U| > J$ the system can, to a good approximation, be described by an effective dimer Hamiltonian derived in the second order in $J/U$ [11]. In terms of the dimer creation $c_j^\dagger = (b_j^\dagger)^2/[1/\sqrt{2}(\hat{n}_j + 1)]$ and annihilation $c_j = [1/\sqrt{2}(\hat{n}_j + 1)](b_j^\dagger)^2$ operators, and number operator $\hat{m}_j = c_j^\dagger c_j = \hat{n}_j/2$, the effective Hamiltonian for a single dimer reads

$$H_{\text{eff}} = \sum_j \left[ \sqrt{\Omega^{(2)}} J^{(2)} \hat{m}_j + (U - 2J^{(2)}) \hat{m}_j - J^{(2)} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) \right],$$

where $\Omega^{(2)} = 2\Omega$ is the strength of the parabolic potential seen by the dimer, while $(U - 2J^{(2)})$ represents the "internal" energy of a dimer.

Before proceeding, we note that, differently from the flat lattice situation considered in [11], here the effective Hamiltonian $H_{\text{eff}}$ is not applicable in the vicinity of sites $|j| \approx |U|/(2\Omega)$ where near-resonant dissociation of a dimer can occur via transitions $|2_j\rangle \rightarrow |1_j\rangle |1_{j\pm1}\rangle$. But since we are interested in the dynamics of low-energy dimers with $|U| > J \gg \Omega$, such high-$j$ states cannot be reached.

Consider first the case of strong attractive interaction $U < 0$ leading to a positive tunnelling constant $J^{(2)} > 0$. Then the effective Hamiltonian (7) has the same form as the Hubbard Hamiltonian (1) for a single particle in a combined periodic and parabolic potential. We can therefore immediately write the lowest-energy eigenvalues and eigenstates for an effective dimer as

$$E_k^D \approx -2J^{(2)} + 2\sqrt{J^{(2)} \Omega^{(2)}}(k + \frac{1}{2}),$$

$$|\chi_k^D\rangle \approx N \sum_j (2^k k!)^{-1/2} e^{-\xi_j^2/2} H_k(\xi_j) |1_j^D\rangle,$$

where energies $E_k^D$ are relative to the dimer internal energy $(U - 2J^{(2)})$, $\xi_j = j \sqrt{\Omega^{(2)}}/J^{(2)} = j \sqrt{\Omega U}/J^2$ is the discrete coordinate, and $|1_j^D\rangle \equiv c_j^\dagger |0\rangle$ denotes a state with a single dimer at site $j$; obviously $|1^D_j\rangle = |2_j\rangle$. The modified Bloch band $-2J^{(2)} \leq E_k^D \leq 2J^{(2)}$ for the dimer is restricted to the sites with

$$|j| \leq j^{\text{max}} \equiv \sqrt{\frac{1}{\sqrt{2}} \frac{J^{(2)}}{\Omega^{(2)}} \approx 1.3 \frac{J}{\Omega} \frac{J}{|U|}}$$

thus containing $N^D = 2[j^{\text{max}}] + 1$ energy levels $E_k^D$ with $0 \leq k < N^D$. The effective harmonic oscillator frequency at the bottom of the modified Bloch band is $\hbar \omega^D = 2\sqrt{J^{(2)} \Omega^{(2)}}$ and the dimer effective mass $\mu^D = \hbar^2/(2J^{(2)}d^2)$ is large ($J^{(2)} \ll J$) and positive. We have verified these conclusions by numerically solving the Schrödinger equation using the exact Hamiltonian (1) with the initial conditions corresponding to eigenstates (8b) of the effective Hamiltonian (7). As an example, in fig. 4(a1) we show the time evolution, or nearly complete absence thereof, of the system in the ground state of (7),

$$|\chi_0^D\rangle \approx \sqrt{s} \frac{\Omega^{(2)}}{\pi^{1/2} J^{(2)}} \sum_j e^{-\xi_j^2/2} |1_j^D\rangle$$

with energy $E_0^D = -2J^{(2)} + \sqrt{J^{(2)} \Omega^{(2)}}$ and quasi-momentum $Q = 0$.

We next turn to the case of strong repulsive interaction $U > 0$. The dimer tunneling constant is negative, $J^{(2)} < 0,$

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corresponding to a negative effective mass $\mu_D$ \cite{11}. As a result, $|\chi^D_0\rangle$ in eq. (10) is no longer the ground state of Hamiltonian (7), as attested in fig. 4(b1). Rather, it is a highly excited state. To see this, consider for a moment a single particle in a flat lattice of $\bar{N}$ sites with $J<0$. It follows from eqs. (2a), (2b) that the lowest energy state with $\bar{E}_{\bar{N}-1} = -2J \cos[\pi \bar{N}/(\bar{N}+1)] = -2 |J| \cos[\pi/(\bar{N}+1)] \approx (11)$

Thus, in the limit of infinite lattice $\bar{N} \to \infty$, the ground state corresponds to the Bloch wave with quasi-momentum $q = \pi$. Returning back to the repulsively bound dimer in the combined periodic and parabolic potential, we find that the low-energy eigenvalues are those of eq. (8a) with the replacement $J^{(2)} \to |J^{(2)}|$, while the corresponding eigenstates are given by

$$|\hat{\chi}^D_{N-1}\rangle = -\mathcal{N} \sum_{l=1}^{\bar{N}} \sin \left[ \frac{l \pi}{\bar{N}+1} \right] e^{i\pi l} |1_l\rangle, \quad (11)$$

The ground state with $E^D_0 = -2|J^{(2)}| + \sqrt{|J^{(2)}|^2 + \Omega^2}$ and quasi-momentum $Q = \pi$ is then

$$|\hat{\chi}^D_0\rangle \approx \sqrt{\frac{\Omega^2}{\pi^2 |J^{(2)}|^2}} \sum_j e^{-\xi_j^2/2} e^{i\pi j} |1_j^D\rangle = \sqrt{\frac{\Omega |U|}{\pi |J|^2}} \sum_j e^{-\xi_j^2/2} (-1)^j |2_j\rangle, \quad (13)$$

which is confirmed by our numerical simulations illustrated in fig. 4(b2). Remarkably, the ground state of the repulsive dimer appears to be tighter bound than that of the attractive one (compare insets in figs. 4(a1) and (b2)). The explanation of this phenomenon lies in the fact that for dimer quasi-momentum $Q = \pi$ and any $U \neq 0$, the pair of particles comprising the dimer are perfectly co-localized at the same lattice site, $\sum_j |\langle 2_j | \Psi \rangle|^2 = 1$ \cite{12,13}. For other values of quasi-momentum $Q$ the dimer “internal state” has sizable admixture of single-particle states, $\sum_j |\langle 1_j | \Psi \rangle|^2 \sim 8J^2 \cos^2 (Q/2)/U^2 \approx 1$ \cite{12}. Since the ground state $|\hat{\chi}^D_0\rangle$ of the repulsive dimer has $Q = \pi$, it is composed only of two-particle states $|2_j\rangle$, while the ground state $|\chi^D_0\rangle$ of the attractive dimer has
weak magnetic (or optical) traps [2]. After revisiting the single-particle problem, we considered effective interaction-bound dimers recently realized in the experiment [14] with strong repulsive atom-atom interactions. We examined both cases of repulsively bound and attractively bound dimers and identified similarities and differences in their static and dynamic properties. We have shown that non-dispersive transport of carefully prepared atomic wave packets can be achieved. As an extension of the present work, we plan to study dimer-monomer resonant collisions and resulting entanglement. Our results may be pertinent to quantum information schemes with cold atoms in optical lattices.

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This work was supported by the EC Marie-Curie Research Training Network EMALI.

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