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Photon-assisted tunneling in optical lattices: Ballistic transport of interacting boson pairs

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In a recent experiment [PRL 100, 040404 (2008)] an analog of photon-assisted tunneling has been observed for a Bose-Einstein condensate in an optical lattice subject to a constant force plus a sinusoidal shaking. Contrary to previous theoretical predictions, the width of the condensate was measured to be proportional to the square of the effective tunneling matrix element, rather than a linear dependence. For a simple model of two *interacting* bosons in a one-dimensional optical lattice, both analytical and numerical calculations indicate that such a transition from a linear to a quadratic dependence can be interpreted through the ballistic transport and the corresponding exact dispersion relation of bound boson pairs.

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I. INTRODUCTION

Bose-Einstein condensates (BECs) in optical lattices provide an excellent tool to study solid state systems [1]. One of the methods which are currently established experimentally [2, 3, 4] for BECs in an optical lattice is tunneling control via time-periodic potential differences [5, 6, 7, 8]. Effects investigated theoretically in periodically shaken systems include multi-particle entanglement [9, 10] and nonlinear Landau-Zener processes [11].

The experimental realization [2, 12, 13] of destruction of tunneling via time-periodic potential differences [5] was the breakthrough for tunneling control via time-periodic potential differences. The systems used so far in experiments are as divers as BECs in an optical lattice [2], single particles in a double well [12] and light in a double-well system [13].

Reference [8] suggested to use time-periodic shaking for a tilted double-well potential to measure an analog of photon-assisted tunneling – the "photon"-frequencies corresponding to shaking-frequencies in the kilo-Hertz regime. Recently, photon-assisted tunneling was observed for a BEC in a periodically shaken optical lattice [3]. When the BEC was allowed to expand for some time, the width of the condensate was measured to be roughly proportional to the tunneling matrix element for small BECs whereas it was proportional to the square of the tunneling matrix element for larger condensates.

While this might be an indication of a transition from ballistic to diffusive transport [3], the verification of such a transition requires the precise measurement of the time-dependence of the width of the wave function in order to distinguish both regimes of transport (see, e.g., Ref. [14] and references therein). Without such measurements, other explanations for the observed dependence of the width of the BEC cannot be excluded.

Here we develop an alternative interpretation of the experimental results: Using two interacting bosons in a simple tight-binding one-band model we show that the transition from a linear to a quadratic dependence on the tunneling amplitude might be an interaction-induced effect within the ballistic regime. We demonstrate, both with the help of analytical arguments and numerical simulations, that the wave function of an interacting boson pair indeed behaves qualitatively very similar to the BEC in the experiment: On the one hand, weakly interacting particles can reproduce the linear scaling with the tunneling matrix element observed for small condensates. On the other hand, more strongly interacting particles reproduce the quadratic scaling for larger condensates (which have a larger total interaction energy).

The paper is organized as follows. In Sec. II we introduce the one-dimensional Bose-Hubbard Hamiltonian with a constant force and time-periodic driving used to model the experimental situation. In the case of high driving frequencies, the time-dependent Hamiltonian can be replaced by an effective, time-independent Hamiltonian. For this Hamiltonian, exact two-particle energy eigenstates describing bound boson pairs can be derived [15, 16] as is explained in Sec. III. In Sec. IV we investigate the dynamical behavior of two-particle wave packets. Employing the obtained exact dispersion relation for interacting boson pairs, we derive the dependence of the width of the wave packet after some time of free ex-

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pansion on the ratio of interaction and tunneling matrix element. These theoretical considerations are supported by numerical simulations of the two-particle Schrödinger equation for the full driven Bose-Hubbard Hamiltonian. Some conclusions are drawn in Sec. V.

II. THE MODEL

Using the notation of Ref. [3], the one-dimensional Bose-Hubbard Hamiltonian with time-periodic shaking describing the experiment can be written as:

$$\begin{aligned}\hat{H}_0 &= -J\sum_j\left(\hat{c}_j^\dagger\hat{c}_{j+1}+\hat{c}_{j+1}^\dagger\hat{c}_j\right)+\frac{U}{2}\sum_j\hat{n}_j\left(\hat{n}_j-1\right)\\ &\quad+\Delta E\sum_j j\hat{n}_j+K\cos(\omega t)\sum_j j\hat{n}_j,\end{aligned}\tag{1}$$

where the operators $\hat{c}_j^{(\dagger)}$ annihilate (create) bosons at the lattice site j and $\hat{n}_j\equiv\hat{c}_j^\dagger\hat{c}_j$ are number operators; J is the hopping matrix element, $\Delta E\equiv Fd_L$ is the potential difference of two adjacent wells with lattice spacing $d_{\rm L}$, $\omega/(2\pi)$ the frequency with which the system is shaken and K the amplitude of the shaking. Thus, the Hamiltonian (1) describes a system of interacting bosons in a tilted and driven optical lattice. For an untilted and undriven lattice we have $\Delta E=0$ and $K=0$.

Floquet-theory [17] can be applied to understand the physics of such a driven system. For not too low driving frequencies ($\hbar\omega\gg J$), the resonance condition

$$n\hbar\omega=\Delta E\tag{2}$$

with integer n leads to photon-assisted tunneling ([3, 8]). In the high-frequency limit ($\hbar\omega\gg J$ and $\hbar\omega\gg U$ [18]) many aspects of the physics behind the system can be understood by replacing the time-dependent Hamiltonian with constant force by a time-independent Hamiltonian without any additional force:

$$\hat{H}_{\rm eff}=-J_{\rm eff}\sum_j\left(\hat{c}_j^\dagger\hat{c}_{j+1}+\hat{c}_{j+1}^\dagger\hat{c}_j\right)+\frac{U}{2}\sum_j\hat{n}_j\left(\hat{n}_j-1\right),\tag{3}$$

where the effective tunneling matrix element is given by

$$J_{\rm eff}=J\mathcal{J}_n(K_0),\quad K_0\equiv\frac{K}{\hbar\omega},\tag{4}$$

with the nth order Bessel function $\mathcal{J}_n$. Thus, in this time-periodic system photon assisted tunneling can lead to an increase of the tunneling amplitude (as the energy difference between neighboring wells is removed in the effective Hamiltonian). Moreover, within an n-photon resonance, tunneling can also be suppressed by tuning the driving amplitude K such that the ratio K_0 of driving amplitude and $\hbar\omega$ corresponds to a zero of the Bessel function $\mathcal{J}_n(K_0)$.

Without interactions ($U=0$), the effective Hamiltonian reduces to a well-known single-particle Hamiltonian with extended Bloch-waves as eigenfunctions

$$|\psi_k\rangle=\sum_{j=-\infty}^{\infty}e^{ikjd_{\rm L}}|j\rangle,\tag{5}$$

where $|j\rangle$ is the Wannier-function at lattice-site j, with the corresponding energy eigenvalues

$$E(k)=-2J_{\rm eff}\cos(kd_{\rm L}).\tag{6}$$

Within a parameter regime for which the cos-dispersion relation can be replaced by a quadratic dispersion relation, $E(k)\simeq-2J_{\rm eff}+J_{\rm eff}k^2d_{\rm L}^2$, the single particle in a tight-binding lattice behaves like a free particle. In fact, such model Hamiltonians can be used to do numerics for a free particle by setting

$$J_{\rm eff}d_{\rm L}^2=\frac{\hbar^2}{2m},\tag{7}$$

where m is the mass of the free particle with dispersion relation $E_f(k)=\hbar^2k^2/(2m)$.

Without interaction, a BEC of N bosons would simply be the product of N single-particle wave functions. If one measures the width of a condensate after a certain time of free expansion [3], this thus corresponds to the popular text-book exercise [19] of calculating the width $\Delta x(t)$ for a single free particle. Starting from a Gaussian wave packet at time zero,

$$\psi(x,t=0)=\frac{1}{(2\pi a^2)^{1/4}}\exp\left(-\frac{x^2}{4a^2}\right),\tag{8}$$

one finds

$$\Delta x(t)=a\sqrt{1+\left(\frac{\hbar t}{2ma^2}\right)^2},\tag{9}$$

where $\Delta x(t)^2\equiv\langle\psi(t)|x^2|\psi(t)\rangle-\langle\psi(t)|x|\psi(t)\rangle^2$.

For a non-interacting BEC in an optical lattice one can thus expect to find for not too small free expansion times t:

$$\Delta x(t)\propto|E''(0)|\,t,\tag{10}$$

where the dashes denote derivatives with respect to the argument (k). This equation was used in Ref. [3] to measure the effective tunneling matrix element $J_{\rm eff}$ as using Eqs. (6) and (10) one has:

$$\Delta x(t)\propto 2|J_{\rm eff}|d_{\rm L}^2t.\tag{11}$$

In order to see if this relation always survives interaction, two interacting bosons are investigated in the following sections, starting with the construction of corresponding energy eigenstates. Two-particle effects in optical lattices are interesting both experimentally and theoretically [15]. Recent investigations include superexchange interactions for mixtures of different spins [20]. Motivated by the experiment [3], this manuscript concentrates on pairs of indistinguishable particles.

III. EXACT ANALYTIC TWO-PARTICLE EIGENFUNCTIONS

The aim is to find exact analytical expressions for the eigenfunctions of the Hamiltonian (3) for two bosons and non-zero interaction $U \neq 0$. Rather than using the approach via Green's functions of Ref. [15], one can proceed along the lines of Ref. [21] to show in a straightforward calculation (see the appendix for details) that a large class of two-particle wave functions is given by

$$|\phi_k\rangle = \sum_{\nu \leq \mu} a_{\nu,\mu}(k)|\nu\rangle|\mu\rangle, \tag{12}$$

where $\nu \leq \mu$ is required because the bosons are indistinguishable, and $|\nu\rangle|\nu\rangle$ corresponds to the Fock state with two particles at lattice site ν. The coefficients $a_{\nu,\mu}$ are given by

$$a_{\nu,\mu}(k) = \begin{cases} b_{\nu,\mu}(k) & : \ \mu \neq \nu, \\ b_{\nu,\mu}(k)/\sqrt{2} & : \ \mu = \nu, \end{cases} \tag{13}$$

where

$$b_{\nu,\mu}(k) = (\eta x_-)^{|\mu-\nu|} \exp\left[ikd_{\mathrm{L}}(\nu+\mu)\right] \ , \tag{14}$$

$$\eta = \begin{cases} -1 & : \ U/J_{\mathrm{eff}} > 0, \\ +1 & : \ U/J_{\mathrm{eff}} < 0, \end{cases} \tag{15}$$

and

$$x_- = \sqrt{\frac{U^2}{16J_{\mathrm{eff}}^2\cos^2(kd_{\mathrm{L}})} + 1} - \frac{|U|}{|4J_{\mathrm{eff}}|\cos(kd_{\mathrm{L}})} \ . \tag{16}$$

As for the Bloch-waves (5) and for plane waves for free particles, these wave functions cannot be normalized in the usual sense. Nevertheless, to avoid divergence for $|\mu-\nu| \to \infty$, one needs $|x_-| \leq 1$ and thus $\cos(kd_{\mathrm{L}}) > 0$.

The energy eigenvalue of the state $|\phi_k\rangle$ can be written as (see Eq. (A9) and Ref. [15]):

$$E_2(k) = -4\eta J_{\mathrm{eff}}\sqrt{\frac{U^2}{16J_{\mathrm{eff}}^2} + \cos^2(kd_{\mathrm{L}})}, \tag{17}$$

and one thus obtains

$$|E_2''(0)| = \frac{16J_{\mathrm{eff}}^2 d_{\mathrm{L}}^2}{\sqrt{16J_{\mathrm{eff}}^2 + U^2}}. \tag{18}$$

The solutions calculated above represent the bound states of a boson pair. In addition to these solutions one has a continuum of scattering eigenstates [22, 23] which will play, however, only a minor role in the description of the physical situation considered here: The initial wave function is given by a narrow Gaussian centered around a lattice site. Thus, both particles are likely to be sitting at the same lattice site and, therefore, the initial state lies nearly entirely in the subspace of bound states of the two-boson system.

IV. BALLISTIC EXPANSION OF TWO-PARTICLE WAVE PACKETS

The value that is relevant for the spreading of two-particle wave packets is not the energy $E_2(k)$ of a pair but the energy per particle. Hence, for the effective Hamiltonian (3) we have

$$|E''(0)| = \frac{8J_{\mathrm{eff}}^2 d_{\mathrm{L}}^2}{\sqrt{16J_{\mathrm{eff}}^2 + U^2}}. \tag{19}$$

Equations (10) and (19) therefore show that the width of the BEC in the driven and tilted lattice is given by

$$\Delta x_{J_{\mathrm{eff}}}(t) \propto \frac{8J_{\mathrm{eff}}^2 d_{\mathrm{L}} t}{\sqrt{16J_{\mathrm{eff}}^2 + U^2}}, \tag{20}$$

from which we find the following limiting behavior,

$$\Delta x_{J_{\mathrm{eff}}}(t) \propto \begin{cases} 2\,|J_{\mathrm{eff}}|\, d_{\mathrm{L}}^2 t & : \ |U/J_{\mathrm{eff}}| \ll 1, \\ 8J_{\mathrm{eff}}^2/|U| d_{\mathrm{L}}^2 t & : \ |U/J_{\mathrm{eff}}| \gg 1, \end{cases} \tag{21}$$

where $J_{\mathrm{eff}} = J\mathcal{J}_n(K_0)$ was introduced in Eq. (4). The corresponding expression for the width in the undriven and untilted lattice, which we denote by $\Delta x_J(t)$, is obtained by replacing J_{eff} by J,

$$\Delta x_J(t) \propto \frac{8J^2 d_{\mathrm{L}} t}{\sqrt{16J^2 + U^2}}. \tag{22}$$

Thus we see that the transition from a linear to a quadratic dependence on the Bessel function observed in Ref. [3] can, within this simple two-particle model, be explained as being a continuous transition based on the dispersion relation (17) for two interacting particles.

It is important to note that one does not have to wait until the dependence of $\Delta x(t)$ on t becomes linear in order to see the scaling when comparing, e.g., an undriven system without tilt with a periodically shaken, tilted system with n-photon-assisted tunneling. In the high-frequency limit, the main difference is that the modulus of J_{eff} will be lower than J by a factor of $|\mathcal{J}_n(K_0)|$. If one plots the width of an initially localized wave packet (cf. Ref. [3]) as a function of $\tau \equiv Jt/\hbar$, the undriven system will thus spread faster. Only by rescaling the time scale for the undriven system one can hope to make both functions agree. For weak interactions, the following equation relates the width of the undriven system at time $|\mathcal{J}_n(K_0)|\tau$ to that of the driven system at time τ:

$$\Delta x_J\left(|\mathcal{J}_n(K_0)|\tau\right) \simeq \Delta x_{J_{\mathrm{eff}}}(\tau) \ , \quad \left|\frac{U}{J_{\mathrm{eff}}}\right| \ll 1. \tag{23}$$

For stronger interactions another factor of $|\mathcal{J}_n(K_0)|$ is necessary:

$$\Delta x_J\left(|\mathcal{J}_n(K_0)|^2\tau\right) \simeq \Delta x_{J_{\mathrm{eff}}}(\tau) \ , \quad \left|\frac{U}{J_{\mathrm{eff}}}\right| \gg 1. \tag{24}$$

The above reasoning explains why the width of the BEC can be proportional to $\mathcal{J}_n^2(K_0)$ even within the

ballistic regime. However, the experimental results of Ref. [3] show even more, namely that $\Delta x_{J_{\rm eff}}(t)$ is not only proportional to $\mathcal{J}_n^2(K_0)$, but also that the ratio of the width in the tilted and driven lattice to the width in the untilted and undriven lattice is approximately equal to $\mathcal{J}_n^2(K_0)$, i. e.

$$\frac{\Delta x_{J_{\rm eff}}(t)}{\Delta x_J(t)} \simeq \mathcal{J}_n^2(K_0). \tag{25}$$

We demonstrate in Figs. 1 and 2 that it is indeed possible to find parameters which reproduce the experimentally observed behavior within the framework of the theory presented here. In Fig. 1 we compare the driven interacting system ($U \neq 0$) with the undriven system for non-interacting particles ($U = 0$). We see that for $U/J = 3.6$ (dotted curves) the left-hand side of Eq. (25) nearly lies on top of the curves representing the right-hand side of this equation (dashed curves). For lower interactions (dash-dotted curves), the scaling is again $\propto |\mathcal{J}_n(K_0)|$ as in the single-particle case.

In Fig. 1 the width of the wave function was compared to the width for non-interacting particles. However, the observed scaling even occurs (for larger interactions than those chosen in Fig. 1) when comparing the untilted, undriven interacting system with the periodically driven interacting system: Figure 2 shows that again a very similar scaling of the width of the condensate is found.

Although several papers have shown the validity of the effective Hamiltonian approach used so far (see, e.g., Ref. [18] and references therein), one should demonstrate that it also is valid for the present situation. To do this, we numerically solve the time-dependent Schrödinger equation corresponding to the full Hamiltonian (1) (Fig. 3). As the initial wave function we choose a Gaussian function for the center-of-mass wave function (corresponding to an initial confinement via a harmonic trapping potential),

$$|\psi(t=0)\rangle \equiv \sum_k \exp\left(-a^2(k-k_0)^2/2\right)|\psi_k\rangle, \tag{26}$$

where the sum over all possible k values (rather than an integral) is necessary as numeric calculations cannot be done in infinite lattices. The initial wave function is sitting in the middle of the lattice (for an odd number $N_{\rm L}$ of lattice-sites, the sites can be labelled as $j = -(N_{\rm L}-1)/2 \ldots (N_{\rm L}-1)/2$). In the finite, shaken lattice relevant for the numerics in this paper, vanishing boundary conditions are a suitable choice [24]. For the center-of-mass part of the wave function (cf. Eq. (13)), $\mu_{\rm c.o.m.} = (\mu+\nu)/2$, the wave-vector is $2k$, possible values for k are thus $n\pi/[(N_{\rm L}-1)d_{\rm L}], n = 1, 2, 3, \ldots$. The initial wave function was calculated without any initial momentum ($k_0 = 0$) and with $a = 10d_{\rm L}$. For the undriven system, $U/J = 10.0$ was chosen in the initial wave function, for the driven system with $K_0 = 2.0$, we chose $U/J = 10.0/\mathcal{J}_1(2.0)$ to mimic an experimental situation where the initial wave function is prepared in a harmonic-oscillator potential and the periodic shaking is switched on before switching off this potential. The quadratic scaling as predicted in Eq. (24) can thus indeed be observed numerically (Fig. 3).

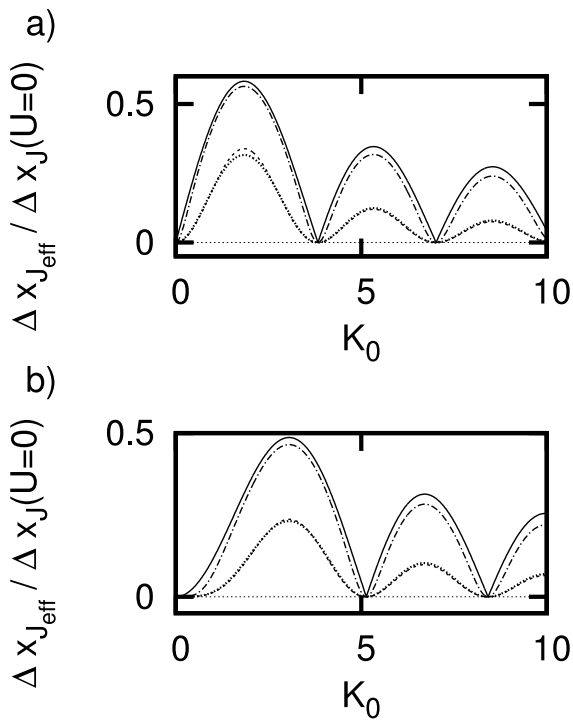

FIG. 1: The width of the two-particle wave function as a function of the ratio of driving amplitude and driving frequency $K_0 = K/(\hbar\omega)$. The width is normalized to the value for *non*-interacting particles ($U = 0$) in an undriven, untilted lattice. The curves are based on the analytic Eqs. (4), (20) and (22). For the one-photon resonance (upper panel) one has $J_{\rm eff} = J\mathcal{J}_1(K_0)$ and for the two-photon resonance (lower panel) $J_{\rm eff} = J\mathcal{J}_2(K_0)$. Solid curves: $|\mathcal{J}_n(K_0)|$, dashed curves: $\mathcal{J}_n^2(K_0)$, dash-dotted curves: $U/J = 0.6$, dotted curves: $U/J = 3.6$.

V. CONCLUSION

Photon-assisted tunneling in a periodically shaken optical lattice was investigated for two interacting bosons. Both numerical and analytical calculations were done for a periodically driven one-band Bose-Hubbard model. Figures 1-3 demonstrate that the experimentally observed [3] dependence of the width of the BEC on the square of the tunneling matrix element can be explained – at least qualitatively within the simple two-particle model investigated here – as being an interaction-induced effect which is based on the dispersion relation for bound boson pairs.

While our simplified approach thus explains some aspects of the experiment [3], calculations for larger particle numbers (which are not straightforward to generalize

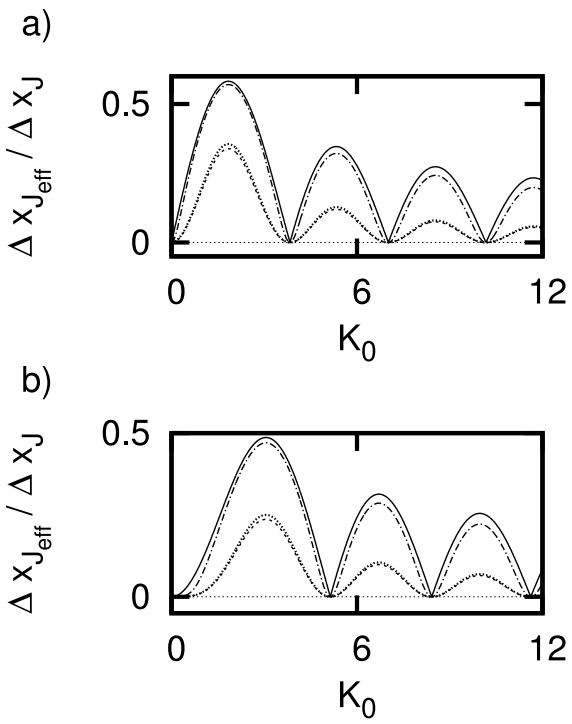

FIG. 2: The width of the two-particle wave function as a function of the ratio of driving amplitude and driving frequency $K_0 = K/(\hbar\omega)$ normalized to the value for *interacting* particles in an undriven, untilted lattice. Labels can be found in Fig. 1 but for the dotted curves which are calculated for an interaction of $U/J = 10.0$. As in Fig. 1, the transition from linear to quadratic dependence on $\mathcal{J}_n(K_0)$, $n = 1, 2$, can be observed.

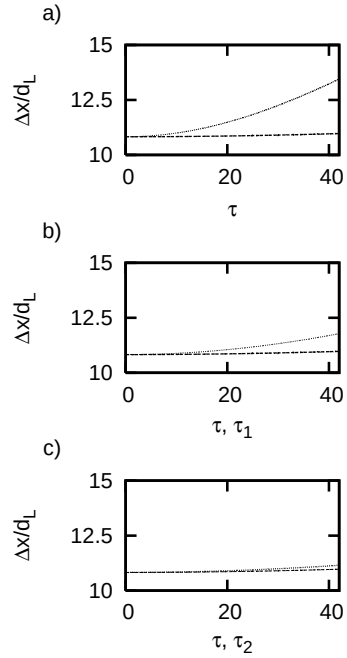

FIG. 3: Numeric simulation of a two-atom wave function in an optical lattice with $N_{\rm L} = 201$ lattice sites in the high-frequency limit ($\hbar\omega = 40J$) with large interactions $U/J = 10.0$ (cf. Fig. 2) and initial wave functions given by Eq. (26). a) The width is plotted as a function of dimensionless time $\tau \equiv Jt/\hbar$. Dotted curves: the undriven, untilted lattice. Dashed curves: the same lattice but with periodic driving for parameters corresponding to a one-photon resonance [3, 8] ($K_0 = 2$, cf. Eq. (4)). The wave packet in the undriven system spreads faster than in the driven system. b) Without the knowledge of Figs. 1 and 2, one might expect both curves to agree if one plots $\Delta x(\tau_1)$, $\tau_1 \equiv |\mathcal{J}_1(2)|\tau$ for the undriven system. However, one needs another factor of $\mathcal{J}_1(2)$: for $\tau_2 \equiv [\mathcal{J}_1(2)]^2\tau$, the data of the undriven system plotted as $\Delta x(\tau_2)$ coincides with $\Delta x(\tau)$ for the driven system (c).

from the method presented here) are likely to lead to further insights into the experiment for which additional effects like decoherence by particle losses might also play an important role. An experimental measurement of the time-dependence of the width of the wave function would be of great interest for the theoretical analysis and the modelling of the transport properties of quantum condensates. In particular, it would be interesting to see if indeed a transition from ballistic to diffusive transport takes place, or if the simple two-particle model presented in this paper can explain the relevant features of the experiment.

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APPENDIX A: EIGENFUNCTIONS

In order to show that exact two-particle eigenfunctions [23] of the effective Hamiltonian (3) are indeed given by Eqs. (12) and (13), one can start with

$$\begin{aligned}
\sum_j \hat{c}_j^\dagger \hat{c}_{j+1} |\mu\rangle|\mu\rangle &= \sqrt{2}|\mu-1\rangle|\mu\rangle \,, \qquad \text{(A1)}\\
\sum_j \hat{c}_{j+1}^\dagger \hat{c}_j |\mu\rangle|\mu\rangle &= \sqrt{2}|\mu\rangle|\mu+1\rangle \,,\\
\sum_j \hat{c}_j^\dagger \hat{c}_{j+1} |\mu-1\rangle|\mu\rangle &= |\mu-2\rangle|\mu\rangle + \sqrt{2}|\mu-1\rangle|\mu-1\rangle \,,\\
\sum_j \hat{c}_{j+1}^\dagger \hat{c}_j |\mu-1\rangle|\mu\rangle &= |\mu-1\rangle|\mu+1\rangle + \sqrt{2}|\mu\rangle|\mu\rangle \,,
\end{aligned}$$

and for $\nu < \mu - 1$

$$\sum_j \hat{c}_j^\dagger \hat{c}_{j+1} |\nu\rangle|\mu\rangle = |\nu-1\rangle|\mu\rangle + |\nu\rangle|\mu-1\rangle \ , \tag{A2}$$
$$\sum_j \hat{c}_{j+1}^\dagger \hat{c}_j |\nu\rangle|\mu\rangle = |\nu+1\rangle|\mu\rangle + |\nu\rangle|\mu+1\rangle \ .$$

Using the notation of Eq. (12) one thus has

$$\begin{aligned}\hat{H}_{\rm eff}|\phi_k\rangle &= U\sum_\mu a_{\mu,\mu}(k)|\mu\rangle|\mu\rangle \\ &-J_{\rm eff}\sum_\mu \sqrt{2}a_{\mu,\mu}(k)\left(|\mu-1\rangle|\mu\rangle + |\mu\rangle|\mu+1\rangle\right) \\ &-J_{\rm eff}\sum_\mu a_{\mu-1,\mu}(k)\left(|\mu-2\rangle|\mu\rangle + \sqrt{2}|\mu-1\rangle|\mu-1\rangle\right) \\ &-J_{\rm eff}\sum_\mu a_{\mu-1,\mu}(k)\left(|\mu-1\rangle|\mu+1\rangle + \sqrt{2}|\mu\rangle|\mu\rangle\right) \\ &-J_{\rm eff}\sum_{\nu<\mu-1} a_{\nu,\mu}(k)\left(|\nu-1\rangle|\mu\rangle + |\nu\rangle|\mu-1\rangle\right) \\ &-J_{\rm eff}\sum_{\nu<\mu-1} a_{\nu,\mu}(k)\left(|\nu+1\rangle|\mu\rangle + |\nu\rangle|\mu+1\rangle\right).\end{aligned} \tag{A3}$$

In oder to show that this indeed leads to an eigenfunction of the effective Hamiltonian (3), we use Eq. (13) and start with the last two lines of Eq. (A3). Performing appropriate shifts of the summation indices these lines can be written as

$$\begin{aligned}&- J_{\rm eff}\sum_{\nu<\mu}\left(b_{\nu,\mu+1}(k) + b_{\nu-1,\mu}(k)\right)|\nu\rangle|\mu\rangle \\ &- J_{\rm eff}\sum_{\nu<\mu-2}\left(b_{\nu+1,\mu}(k) + b_{\nu,\mu-1}(k)\right)|\nu\rangle|\mu\rangle.\end{aligned} \tag{A4}$$

The second, third and fourth line of Eq. (A3) can be combined to yield

$$\begin{aligned}&- J_{\rm eff}\sum_{\nu}\sqrt{2}\left(b_{\nu-1,\nu}(k) + b_{\nu,\nu+1}(k)\right)|\nu\rangle|\nu\rangle \\ &- J_{\rm eff}\sum_{\nu=\mu-1}\left(b_{\nu+1,\mu}(k) + b_{\nu,\mu-1}(k)\right)|\nu\rangle|\mu\rangle \\ &- J_{\rm eff}\sum_{\nu=\mu-2}\left(b_{\nu+1,\mu}(k) + b_{\nu,\mu-1}(k)\right)|\nu\rangle|\mu\rangle.\end{aligned} \tag{A5}$$

Adding (A4) and (A5) and including the first line of Eq. (A3) we find

$$\begin{aligned}\hat{H}_{\rm eff}|\phi_k\rangle &= \frac{U}{\sqrt{2}}\sum_\nu b_{\nu,\nu}(k)|\nu\rangle|\nu\rangle \\ &- J_{\rm eff}\sum_\nu \sqrt{2}\left(b_{\nu-1,\nu}(k) + b_{\nu,\nu+1}(k)\right)|\nu\rangle|\nu\rangle \\ &- J_{\rm eff}\sum_{\nu<\mu}\left(b_{\nu,\mu+1}(k) + b_{\nu-1,\mu}(k)\right)|\nu\rangle|\mu\rangle \\ &- J_{\rm eff}\sum_{\nu<\mu}\left(b_{\nu+1,\mu}(k) + b_{\nu,\mu-1}(k)\right)|\nu\rangle|\mu\rangle.\end{aligned} \tag{A6}$$

In order to simplify the last two lines of Eq. (A6) we use the notation of Eqs. (14)-(16) to obtain

$$\begin{aligned}&b_{\nu+1,\mu}(k) + b_{\nu-1,\mu}(k) + b_{\nu,\mu+1}(k) + b_{\nu,\mu-1}(k) \\ &= b_{\nu,\mu}(k)\eta\Big[x_-^{-1}e^{ikd_{\rm L}} + x_- e^{-ikd_{\rm L}} \\ &\qquad + x_- e^{ikd_{\rm L}} + x_-^{-1}e^{-ikd_{\rm L}}\Big] \\ &= b_{\nu,\mu}(k)2\eta\cos\left(kd_{\rm L}\right)\left[x_- + x_-^{-1}\right]\end{aligned}$$

with

$$x_- + x_-^{-1} = 2\left(\frac{U^2}{16J_{\rm eff}^2\cos^2(kd_{\rm L})} + 1\right)^{1/2}.$$

Thus, for $\nu < \mu$ we have

$$\begin{aligned}&\langle\mu|\langle\nu|\hat{H}_{\rm eff}|\phi_k\rangle \\ &= -4\eta J_{\rm eff}\cos(kd_{\rm L})\left(\tfrac{U^2}{16J_{\rm eff}^2\cos^2(kd_{\rm L})} + 1\right)^{1/2} a_{\nu,\mu}(k).\end{aligned} \tag{A7}$$

The terms with $\nu = \mu$ in Eq. (A6) yield:

$$\begin{aligned}&(U/\sqrt{2})b_{\nu,\nu}(k) - J_{\rm eff}\sqrt{2}\left[b_{\nu,\nu+1}(k) + b_{\nu-1,\nu}(k)\right] \\ &= \left[U/\sqrt{2} - J_{\rm eff}\sqrt{2}x_- 2\eta\cos(kd_{\rm L})\right]b_{\nu,\nu}(k) \\ &= \left[U - J_{\rm eff}4x_-\eta\cos(kd_{\rm L})\right]a_{\nu,\nu}(k),\end{aligned}$$

and thus (cf. Eq. (16)):

$$\begin{aligned}&\langle\nu|\langle\nu|\hat{H}_{\rm eff}|\phi_k\rangle \\ &= -4\eta J_{\rm eff}\cos(kd_{\rm L})\left(\tfrac{U^2}{16J_{\rm eff}^2\cos^2(kd_{\rm L})} + 1\right)^{1/2} a_{\nu,\nu}(k) \\ &\quad + \left[U + \eta J_{\rm eff}\frac{|U|}{|J_{\rm eff}|}\right]a_{\nu,\nu}(k),\end{aligned} \tag{A8}$$

where $U + \eta J_{\rm eff}|U|/|J_{\rm eff}| = 0$ [Eq. (15)]. This shows that $|\phi_k\rangle$ indeed is a 2-particle eigenfunction of the effective Hamiltonian,

$$\hat{H}_{\rm eff}|\phi_k\rangle = E_2(k)|\phi_k\rangle,$$

with the energy eigenvalue

$$E_2(k) = -4\eta J_{\rm eff}\sqrt{\frac{U^2}{16J_{\rm eff}^2} + \cos^2(kd_{\rm L})}. \tag{A9}$$

Note that $\cos(kd_{\rm L})$ was required to be positive for x_- to have a modulus lower than or equal to one, because otherwise the wavefunction would diverge.

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[23] For repulsive interactions, the bound states (Eqs. (12) and (13)) lie above the band formed by scattering states (cf. Refs. [15, 22]; the two-particle energy band emerges from the single particle energy band in Eq. (6)), for attractive atoms, they lie below the scattering states.

[24] Instead of $\exp\left[ikd_{\mathrm{L}}(\nu+\mu)\right]$, the center of mass wavefunctions in Eqs. (26) and (13) alternately are given by $\cos\left[ikd_{\mathrm{L}}(\nu+\mu)\right]$ and $i\sin\left[ikd_{\mathrm{L}}(\nu+\mu)\right]$.