Scattering tightly bound dimers off a scattering potential

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(Dated: October 7, 2009)

The motion of two attractively interacting atoms in an optical lattice is investigated in the presence of a scattering potential. The initial wavefunction can be prepared by using tightly bound exact two-particle eigenfunction for vanishing scattering potential. This allows to numerically simulate the dynamics in the generation of two-particle Schrödinger cat states using a scheme recently proposed for scattering of quantum matter wave solitons.

PACS numbers: 03.65.Nk,03.67.Bg,34.50.-s
Keywords: optical lattice, quantum superpositions, ultra-cold atoms

I. INTRODUCTION

For ultra-cold atoms in an optical lattice [1,2,3] dynamical aspects include transverse resonances [4] density waves [5], the evolution of quantum fluctuations [6], the speed of sound [7,8] and time-resolved observation and control of superexchange interactions [9]. The aim of the present manuscript is to perform exact two-particle dynamics in an optical lattice similar to what has been suggested in Ref. [10], a bright soliton in a one-dimensional waveguide. As the dispersion relation for the bound two-particle states in the lattice approach case without lattice for suitable parameters, this can be used to quantitatively test the N-particle predictions of Ref. [10] via exact numerics on the two-particle level for which a soliton is simply a dimer.

Besides the analytical N-particle quantum mechanical calculations [10], the scattering of the soliton has also been investigated via numerical methods on the N-particle level [11]. Different approaches to obtain such Schrödinger cat states or related fragmentations have been investigated in Refs. [12,13]. Contrary to Schrödinger cat states of a single atom [14], cat-like states of radiation [15] or mesoscopic spin-squeezed states (which have already been realized experimentally [16]), the experimental realisation of Schrödinger cat states of say, 100 atoms, is still a challenge of fundamental research. Suggestions how interesting quantum superpositions might be obtained can be found, e.g., in Refs. [17,18,19,20,21,22,23,24,25] and references therein.

For bright quantum wave solitons [26,27,28], the mean-field (Gross-Pitaevskii) limit has been shown to be achievable already for particle numbers as low as $N \approx 3$ [29]. Many of the papers published after the groundbreaking experiments [30,31] solve the Gross-Pitaevskii equation for solitons. However, any mesoscopic entangled state which involves superpositions of wavefunctions cannot be described by a non-linear equation and therefore the reasoning of Ref. [29] is not valid in the situation considered here. Thus, instead of applying the Gross-Pitaevskii equation, the N-particle Schrödinger equation has to be used to reveal true quantum behaviour of a soliton created from a Bose-Einstein condensate. Under experimentally realistic conditions, the Schrödinger equation is given by the analytically solvable Lieb-Liniger(-McGuire) model.

The challenge of the generation of mesoscopic superpositions via scattering of solitons is that to add a scattering potential removes the separability of the centre-of-mass motion and the relative motion; in order to avoid that the scattering potential acts like a beam splitter on each single atom (rather than the entire soliton), the initial state has to be prepared carefully. Mesoscopic entangled states with the soliton being in a quantum superposition with $\approx 50\%$ probability of moving to the right/left should thus be obtainable. The probability to find – in a single measurement – (at least) one particle moving to the right and at (at least) one particle moving in the other direction will be negligible. However, this will not be enough to prove that the two parts of the wavefunction really are in a quantum superposition – if someone claims that a coin is in a quantum superposition of heads and tails, an experiment showing only the classical outcomes would hardly convince anyone. The experimental verification could be delivered via interference experiments [10].

Rather than dealing with bright N-particle quantum solitons, this paper treats a simpler but nevertheless instructive case: dimers in an optical lattice. The paper is organised as follows: after a short summary of how to describe the scattering of bright solitons analytically [10] (Sec. II), the two-particle bound states used to describe the scattering of the dimer are introduced in Sec. III. Section IV shows the numeric results in the limit where the motion in the optical lattice mimics the motion without lattice.

II. EFFECTIVE POTENTIAL APPROACH

The Hamiltonian of the Lieb-Liniger-McGuire [32,33] model with attractive interaction and an additional
where the scattering-potential \( V \) is given by

\[
\hat{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + g \sum_{i<j} \delta(x_i - x_j) + V, \quad g < 0 .
\]  

(1)

Bright solitons are well described by this model. For \( V = 0 \), exact eigenfunctions of this Hamiltonian are known. Solutions corresponding to \( N \)-particle solitons with momentum \( k \) read:

\[
\psi_{N,k}(x) = \exp \left\{ -\beta \sum_{1 \leq \nu < \mu \leq N} |x_{\nu} - x_{\mu}| + i k \sum_{\nu=1}^{N} x_{\nu} \right\} ,
\]

where

\[
\beta = -mg_{1d}/(2\hbar^2) > 0 .
\]  

(3)

The corresponding energies are given by

\[
E_k = E_0 + \frac{N\hbar^2k^2}{2m}
\]

(4)

where

\[
E_0 = -\frac{mg^2}{24\hbar^2}N(N^2 - 1)
\]  

(5)

is the ground state energy of the system. As long as the kinetic energy is not too large, these states are separated from the first excited internal state (which corresponds to one particle having left the soliton) by a finite energy barrier \( \propto g^2N^2 \) (see, e.g., Ref. [27]).

Had the scattering potential been a function of the centre of mass of all \( N \) particles \( V = V(\frac{1}{N} \sum_{\nu} x_{\nu}) \), the situation would have been easy as the centre of mass and relative coordinates then still separate. However, the potential in the Hamiltonian (1) is given by

\[
V = \sum_{\nu} \tilde{V}(x_{\nu})
\]

(6)

It would nevertheless be tempting to argue that, given the fact that the particles are tightly bound, they behave essentially as a single particle and one could thus approximate \( \tilde{V}(x_{\nu}) \) by \( \tilde{V}(X) \) and thus

\[
V \approx N \tilde{V}(X)
\]  

(7)

where

\[
X = \frac{1}{N} \sum_{\nu=1}^{N} x_{\nu}
\]

(8)

is the centre-of-mass coordinate. However, this approximation can give wrong results (as will be shown towards the end of this paper) and the mathematically justified [10] effective potential approach:

\[
\hat{H}_{\text{eff}} = -\frac{\hbar^2}{2M} \partial^2_X + V_{\text{eff}}(X)
\]

(9)

has to be used. The effective potential is given by the convolution [10]

\[
V_{\text{eff}}(X) = \int \! d^N x \; \delta \left( X - \frac{1}{N} \sum_{\nu=1}^{N} x_{\nu} \right) \times |C\psi_{N,k}(x)|^2 \sum_{\nu=1}^{N} \tilde{V}(x_{\nu}) .
\]

This approach is valid for sufficiently well behaved potentials (like a laser focus) and for solitons which cannot break apart for energetic reasons (see the paragraph below Eq. (3)).

### III. TWO-PARTICLE BOUND STATES

Two-particle bound states in optical lattices are interesting both experimentally [34] and theoretically [34, 35, 36, 37, 38, 39]; recently even three-particle bound states [40] have been investigated. Within a Bose-Hubbard Hamiltonian,

\[
\hat{H}_{\text{lattice}} = -J \sum_{j} \left( \hat{c}_{j}^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_{j} \right) + \frac{U}{2} \sum_{j} \hat{n}_{j} \left( \hat{n}_{j} - 1 \right), \quad U < 0
\]

(11)

one can use exact eigen-states to do the numerics (the restriction to negative pair interactions \( U \) is not necessary, however the idea is to discuss a case close to the bright solitons created from attractive Bose-Einstein condensates; the creation/annihilation operators of particles at lattice cite \( j \) are denoted by \( \hat{c}_{j}^\dagger / \hat{c}_{j} \). Rather than using the approach via Green’s functions of Ref. [34], we proceed in Ref. [38] along the lines of Ref. [41] to show in a straight-forward but somewhat lengthy calculation that the dimer wavefunctions in a tight-binding lattice with band-width \( W \) and lattice spacing \( b \) are given by

\[
c_{\nu \mu} = \begin{cases} x_{|\nu - \mu|} \exp[ikb(\nu + \mu)] & : \; \mu \neq \nu \\ \exp[ikb(\nu + \mu)]/\sqrt{2} & : \; \mu = \nu \end{cases}
\]

(12)

where

\[
x_{-} = \sqrt{\frac{U^2}{16J^2 \cos^2(kb)} + 1 - \frac{|U|}{4J \cos(kb)}} ;
\]

(13)

the coordinates \( \nu \) and \( \mu \) label the lattice points on which the particles “sit” and as a basis the Fock basis is used (i.e., \( \nu = \mu \) refers to the Fock state with two particles at the lattice-site \( \nu \)). The interaction energy of two particles sitting at the same lattice site is \( \hbar k < 0 \); for the wavefunction to be normalisable for fixed centre of mass, \( kb < \pi/2 \) (which implies \( |x_{-}| < 1 \). To avoid a breaking of the dimer, the energy

\[
E_{\text{two}} = -4J \sqrt{\frac{U^2}{16J^2} + \cos^2(kb)}
\]

(14)
should be lower than two times the minimal possible energy of two particles:

$$E_{\text{two}} < -4J$$  \hspace{1cm} (15)

As for the single particle energy band,

$$E_{\text{one}} = -2J \cos(kb),$$  \hspace{1cm} (16)

the dispersion relation for two particles approaches the free-particle behaviour in the limit $bk \rightarrow 0$ which can thus be used to model particles not restricted by optical potentials:

$$E_{\text{two}} \simeq -4J \left( \frac{U^2}{16J^2 + 1} \right)^{1/2} + \frac{8J^2b^2}{16J^2 + U^2} k^2.$$  \hspace{1cm} (17)

By choosing the parameters to approximate the dispersion relation for a two-particle “soliton” (cf. Eq. (2))

$$E_{N=2 \text{ soliton}} = -\frac{\hbar^2 \tilde{\beta}^2}{m} + \frac{\hbar^2 k^2}{m},$$  \hspace{1cm} (18)

the effective potential approach of Ref. [10] (cf. Eq. (10)) will thus be valid for small enough $b$.

\section*{IV. NUMERIC RESULTS}

The initial centre-of-mass wavefunction in Ref. [10] is suggested to be a Gaussian (obtained by preparing the system in a swallow harmonic oscillator potential). If the system can be described within a centre-of-mass approximation, the expected result will always look similar to Fig. 1. For the initial Gaussian to be realisable experimentally, the length scale on which the wavefunctions of the relative coordinates decays has to be smaller than the width of the initial wavefunction. Given the fact that the dimer cannot break into two free particles, this implies that in the final wavefunction measuring one particle on one side of the barrier would also lead to measuring the other particle on the same side - thus the final state indeed is a Schrödinger cat state.

Figure 2 shows the result for a two-particle soliton scattered off a step potential.

$$V_{\text{step}} = \begin{cases} V_0 : |x| \leq \ell \\ 0 : \text{else} \end{cases}.$$  \hspace{1cm} (19)

The initial wavefunction is constructed as a superposition of the eigen-solutions (12) with $0 < k < \bar{\beta}$ which ensures the validity of Eq. (15) (cf. Eq. (18)):

$$\Psi(x_1, x_2; t = 0) \propto \int_0^{\bar{\beta}} dk \exp \left( -a^2(k - k_0)^2 / 2 \right)$$  \hspace{1cm} (20)

$$\times \psi_{2,k}(x_1 - x_0, x_2 - x_0).$$

If $a$ is not too small this leads to a Gaussian centre-of-mass wavefunction initially centred at $x_0$. Surprisingly, for the parameters chosen in Fig. 2 the wavefunction splits into three rather than the expected two parts. If one of the particles was measured, the second would be much closer to the location of the first than the width of the three moving wave-packets. The strange behaviour of Fig. 2 clearly demonstrates that the centre-of-mass approximation is not valid here: the effective potential (10) as displayed in the inset of Fig. 2 at least qualitatively explains why resonances can occur which makes parts the dimer wave-function stay at the potential.

However, rather than being able to qualitatively understand the scattering behaviour, the effective potential approach can also be tested quantitatively for realistic
scattering potentials. If the scattering potential is realised via the focus of a laser beam, the potential can be approximated by a Gaussian or even the potential

$$V_c(x) = \frac{V_0}{\cosh(x/\ell)^2}$$  \hspace{1cm} (21)

which is analytically solvable on the single particle level. Figure 3 a compares the wave-function after scattering for the exact potential

$$V(x_1, x_2) = V_c(x_1) + V_c(x_2),$$  \hspace{1cm} (22)

the center of mass approximation

$$V(x_1, x_2) \approx 2V_c((x_1 + x_2)/2)$$  \hspace{1cm} (23)

and the effective potential [10]

$$V(x_1, x_2) \approx 2V_c((x_1 + x_2)/2) + \frac{V''((x_1 + x_2)/2)}{8\beta^2},$$  \hspace{1cm} (24)

where \(\tilde{\beta}\) is given by Eq. (3). The effective potential clearly is a huge improvement over the center-of-mass approximation. It still remains to be shown that the final state indeed is entangled in the sense that whenever one measures one particle on the right (left) side, the other particle will be on the same side. To do this, a Measure If An Outgoing Wave is Unentangled,

$$p_{\text{miaou}}(t) \equiv \int_{-\infty}^{0} dx_1 \int_{0}^{\infty} dx_2 |\Psi(x_1, x_2; t)|^2,$$  \hspace{1cm} (25)

where the wavefunction is taken to be normalised to one. Figure 3 b demonstrates that for the wave-function to be entangled, the initial velocity cannot be too large. Experimental verifications that such states are indeed quantum superpositions could be done via interference experiments [10].

V. CONCLUSION

To summarise, scattering of bright quantum matter wave solitons [10, 11] has been investigated for two attractive atoms in an optical lattice via exact numerics. It has been demonstrated that the beyond centre-of-mass approximation approach of Ref. [10] is indeed necessary to describe the physical situation at least qualitatively: the effective potential derived in Ref. [10] can explain the break-down of the centre-of-mass approximation observed for specific parameters in the numerics (Fig. 2).

For a scattering potential given by a laser focus (the potential would then be approximately Gaussian) such an effect does not occur. The wavefunction then splits into two parts as shown for a single particle in Fig. 1 and the effective potential even gives excellent quantitative agreement (Fig. 3) with exact numerics.

FIG. 3: a) Modulus squared of the scalar product after scattering of the solution of the approximate Schrödinger equation corresponding to Eq. (23) with the unapproximated solution (both calculated on a 801 x 801 lattice). The potential is given by Eq. (22). From top to bottom: \(\ell\beta = 2.5, 1.5, 1\). Inset: with the approximation expressed by Eq. (24), the agreement is much better. The lines are a guide to the eye. b) If the soliton splits into two parts, \(p_{\text{miaou}} \approx 0\) (Eq. (25); plotted as a function of the centre of the momentum distribution) indicates entanglement (for \(\ell\beta = 2.5\)). The wave-packet was defined to be \(\propto \int 0^{(k^*/k_0)^\beta} dk \exp(-a^2(k-k^*)^2/2) \psi_{2,k}(x_1 - x_0, x_2 - x_0); V_0\) was chosen such that Eq. (23) predicts 50 : 50 splitting; \(k_0/\tilde{\beta} = 0.75\).

Acknowledgments

I acknowledge insightful discussions with Y. Castin, A. Sinatra and C. Salomon at the Laboratoire Kastler Brossel at the ENS in Paris where this research was started (funded by the European Union via contract MEIF-CT-2006-038407). Furthermore, I would like to thank M. Holthaus for his continuous support.
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