Durham Research Online

Deposited in DRO:
15 October 2014

Version of attached file:
Other

Peer-review status of attached file:
Peer-reviewed

Citation for published item:

Further information on publisher’s website:
http://dx.doi.org/10.1088/0953-4075/45/16/165301

Publisher’s copyright statement:
© 2012 IOP Publishing Ltd. This is an author-created, un-copyedited version of an article accepted for publication in Journal of physics B: atomic, molecular and optical physics. IOP Publishing Ltd is not responsible for any errors or omissions in this version of the manuscript or any version derived from it. The Version of Record is available online at 10.1088/0953-4075/45/16/165301.

Additional information:

Use policy

The full-text may be used and/or reproduced, and given to third parties in any format or medium, without prior permission or charge, for personal research or study, educational, or not-for-profit purposes provided that:

- a full bibliographic reference is made to the original source
- a link is made to the metadata record in DRO
- the full-text is not changed in any way

The full-text must not be sold in any format or medium without the formal permission of the copyright holders.

Please consult the full DRO policy for further details.
Nonlocal quantum superpositions of bright matter-wave solitons and dimers

Bettina Gertjenken and Christoph Weiss

1 Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany
2 Department of Physics, Durham University, Durham DH1 3LE, United Kingdom

(Dated: 24 August 2012)

The scattering of bright quantum solitons at barrier potentials in one-dimensional geometries is investigated. Such protocols have been predicted to lead to the creation of nonlocal quantum superpositions. The centre-of-mass motion of these bright matter-wave solitons generated from attractive Bose-Einstein condensates can be analysed with the effective potential approach. An application to the case of two particles being scattered at a delta potential allows analytical calculations not possible for higher particle numbers as well as a comparison with numerical results. Both for the dimer and a soliton with particle numbers on the order of \( N = 100 \), we investigate the signatures of the coherent superposition states in an interferometric setup and argue that experimentally an interference pattern would be particularly well observable in the centre-of-mass density. Quantum superposition states of ultra-cold atoms are interesting as input states for matter-wave interferometry as they could improve signal-to-noise ratios.

I. INTRODUCTION

The experimental realisation of macroscopic quantum superpositions is a challenge of current research. Besides opening up a new realm for the study of fundamental quantum effects there would be possible applications in interferometry and quantum information science. As quantum superposition states are very sensitive to decoherence the creation of these fragile objects is a difficult task. So far experimental achievements include the realisation of mesoscopic superposition states on the single-atom level \(^1\), a six-atom Schrödinger-cat state \(^2\) and superposition states in radiation fields \(^3\). Further systems of interest for the creation of many-particle entanglement are cavity quantum optomechanical systems \(^4\) and mesoscopic superpositions of internal degrees of freedom. In the field of ultra-cold atoms mesoscopic superposition states are important for matter-wave interferometry as they allow improved signal-to-noise ratios \(^5\). Many-particle entanglement in macroscopic systems enables investigations of the quantum-classical boundary and decoherence mechanisms \(^6\). Therefore larger interferometric objects are required. While interferences have been observed with fullerences \(^7\) \(^8\) and large organic molecules \(^9\) the creation of a macroscopic nonlocal Schrödinger-cat state of ultra-cold atoms still is a challenge. Recent proposals have been the creation of a nonlocal state of a Bose-Einstein condensate suspended between the two wells of a two-site optical lattice \(^10\) or via scattering of bright matter-wave solitons (BMWS) \(^11\) \(^12\). Single BMWS \(^13\) and soliton trains \(^14\) \(^15\) have already been realised experimentally in low-dimensional attractive Bose gases. Theoretical investigations of one-dimensional attractive Bose-gases \(^16\) \(^17\) comprise the investigation of BMWS collisions \(^18\) and collision-induced entanglement \(^19\).

In one-dimensional geometries the scattering of a BMWS or a tightly bound dimer off a barrier potential like a laser focus has been predicted to lead to the creation of a nonlocal quantum superposition of all the atoms being located to the left and to the right of the scattering potential. In a Fock space representation with states \( | n_L, n_R \rangle \), where \( n_L \) (\( n_R \)) denotes the particles left (right) of the barrier, this would correspond to the NOON-state \(^20\)

\[
| \Psi_{\text{NOON}} \rangle = \frac{1}{\sqrt{2}} \left( | N, 0 \rangle + e^{i\phi} | 0, N \rangle \right)
\]

where \( \phi \) is the relative phase between the two parts of the superposition. Experimental parameters for this proposed realization of the ideal of a nonlocal quantum superposition have been estimated in \(^11\): for a BMWS consisting of \( N \approx 100 \) \(^7\)Li atoms with a typical size of about 1 \( \mu \)m a spatial separation of about 100 \( \mu \)m is found to be reachable. The initial wave-function should be prepared carefully such that the beam-splitter acts on the soliton as a whole and not on each single atom. Using the effective potential approach from \(^11\) it is possible to investigate the dynamics of the centre of mass (CoM). While in Ref \(^11\) the effective potential approach has been applied to broader potentials, here it will be applied for smaller potentials which is more interesting from the point of view of a theoretical physicist: for low particle numbers, it allows to perform Rayleigh-Schrödinger perturbation theory beyond the leading order of the effective potential investigated in Ref. \(^11\). This thus renders a detailed test of the effective-potential approach possible.

Two-particle bound states are interesting both experimentally \(^21\) and theoretically \(^22\) \(^25\). An application of the effective potential approach \(^11\) to the case of a tightly-bound dimer being scattered off a delta potential is particularly interesting: contrary to higher particle numbers \( N \geq 3 \) analytical calculations of the effective potential, even in higher orders, still are possible with reasonable effort and can be compared with numerical results. These can be obtained via discretisation of the
Schrödinger equation. The scattering of bright solitons of 

\[ x \]

delta function like potentials has also been investigated on the mean-field level and has been found to successfully describe many aspects of the dynamics [26–28]. The nonlinear Gross-Pitaevskii equation is not investigated here as it does not allow superposition states which are in the focus of this work.

Considering the nonlocal quantum superposition [1] in an experiment, one should always find all particles on the same side of the scattering potential. As by itself this is not yet a convincing signature of a quantum superposition rather than a statistical mixture, we will investigate the subsequent recombination and interference of the two coherent parts of the quantum superposition. The combined measurement of both signatures would be a demonstration for the existence of a Schrödinger-cat state. Interference experiments with matter waves can be of two very different kinds [6]: while the first one involves the interference of two independent condensates [29], the other one is based on the splitting of a single system into two components. In the interference of two independent condensates [29] an interference pattern is visible in a single run of the experiment but will eventually wash out by averaging over many realisations due to the random phase between the condensates. Here we investigate a complementary kind of interference where the random phase between the condensates. Here we investigate the subsequent recombination and interference in a sequence of runs:

\[ \rho_{\text{CoM}}(x) = \langle \delta(x - X) \rangle, \]

where \( x \) denotes the spatial coordinate, whereas the single-particle density reads

\[ \rho_{\text{one}}(x) = \frac{1}{N} \sum_j \langle \delta(x - x_j) \rangle \]

with the position \( x_j \) of the particles. While there are set-ups for which a single experiment yields an interference pattern [29], in general quantum mechanical expectation values like equations (2) and (3) only make statements about an average of many runs of the experiment. For the CoM density (2), a single experiment will only give a point (the CoM of all atoms measured). As for the double-slit experiment with single photons [30], the interference pattern only builds up after repeating the experiment many times. The same experiments can also be used to determine the single-particle density (3): here the positions of all atoms from all experiments are added. Here we assume adequate experimental stability to guarantee that the shift of the interference pattern from run to run is smaller than the distance of neighboring interference maxima to avoid washing out of the pattern: an experiment will have to combine the low temperatures of Ref. [31] (to prepare the initial state, cf. [11]) with the vacuum of Ref. [32] (to suppress decoherence introduced by free atoms) and the particle-number control available in Experiments like [33].

The paper is organized as follows: In the next section we will introduce the Lieb-Liniger model [34, 35] for the description of a one-dimensional attractive Bose gas and review the effective potential approach from [11]. The third section covers numerical investigations of the scattering of a tightly bound dimer at a delta potential and the resulting interference patterns as well as the application of the effective potential to this two-particle case. In the fourth section the considerations about interference patterns in the CoM and single-particle density are extended to the experimentally relevant \( N \)-particle case.

II. MODELS

A. Lieb-Liniger model of a one-dimensional attractive Bose gas

One-dimensional Bose gases can be described in the exactly solvable Lieb-Liniger model [34, 35] where the many-body Hamiltonian for \( N \) bosons of mass \( m \) interacting via contact interaction with coupling constant \( g_{1d} \) is given by

\[ \hat{H}_0 = \sum_{j=1}^N \frac{p_j^2}{2m} + g_{1d} \sum_{j < \ell} \delta(x_j - x_\ell). \] (4)

The resulting Schrödinger equation is separable in CoM and relative coordinates and can be diagonalised with the Bethe ansatz. For attractive interaction with \( g_{1d} < 0 \) bound states with negative energies are expected. The ground state of the system is the quantum soliton

\[ \psi_0(x) = C_N \exp \left( -\beta \sum_{1 \leq j < \ell \leq N} \frac{|x_j - x_\ell|}{\beta} \right), \] (5)

where \( \beta = -mg_{1d}/2\hbar^2 > 0 \) and \( C_N = \left[ \frac{(N - 1)!}{N^{1/2}} \right]^{1/2} \) [17]. For \( N \gg 1 \) the single-particle density (3) for the CoM being localised around \( x = 0 \) is well approximated by the mean-field density profile [36]

\[ \rho_N(x) = \int dx_1 \ldots dx_N |\psi_0(x)|^2 \delta(x_1 + \ldots + x_N) \delta(x_1 - x) = \frac{m \alpha^2}{4 \pi} N^2 \left[ \cosh \left( \frac{mg_{1d}}{2\hbar^2} N x \right) \right]^{-2}. \] (6)

Thus, \( x \) represents the distance from the CoM of the soliton. Note that the wave-function (4) already is symmetric with respect to any permutation of particles. The ground state (5) of the Hamiltonian (4) has energy

\[ E_0(N) = \frac{1}{24} \frac{mg_{1d}^2}{\hbar^2} N (N^2 - 1) \] (7)

and is separated by an energy gap

\[ |\mu| = E_0(N - 1) - E_0(N) = \frac{mg_{1d}^2N(N - 1)}{8\hbar^2}. \] (8)
from a continuum of solitonic fragments. The corresponding \( N \)-particle solutions with CoM wave vector \( K = N k \), total mass \( M = N m \) and energies
\[
E_K(N) = E_0(N) + \frac{\hbar^2 K^2}{2M}.
\]
read
\[
\psi_{N,k}(x) = \psi_0(x) \exp\left( i k \sum_{j=1}^N x_j \right).
\]

Hence, for low CoM kinetic energies \( E_K(N) - E_0(N) < |\mu| \) the scattering of the BMWS at an additional scattering potential
\[
V(x) = \sum_{j=1}^N \tilde{V}(x_j),
\]
leading to the total Hamiltonian \( H = H_0 + V(x) \), will be elastic. In this work we assume the scattering potentials to be delta distributions \( \tilde{V}(x_j) \propto \delta(x_j) \) which will be motivated in section III. As the soliton cannot break up into parts nonzero probability amplitudes of the scattered wave-function on both sides of the scattering potential imply the generation of a Schrödinger-cat state. For higher energies particle excitations are possible and the soliton can break up into several 'lumps' of bound particles. Those excited states can be found in a generalised Bethe ansatz \[17\]. For \( N = 2 \) they read
\[
|\Psi\rangle \propto \left[ \cos(kx_1) - \frac{\beta}{k} \sin(k|x_1|) \right] e^{iKX} \]
with CoM and relative coordinates
\[
X = \frac{x_1 + x_2}{2}, \quad K = k_1 + k_2,
\]
\[
x_r = x_2 - x_1, \quad k = \frac{k_1 - k_2}{2}.
\]

**B. Effective potential approach**

Adding the additional scattering potential \[11\] to the Hamiltonian \[1\] renders the Schrödinger equation nonintegrable via the Bethe ansatz. Nonetheless, for suitably smooth scattering potentials and low kinetic energies the CoM motion can again be solved independently of the relative motion in the mathematically justified effective potential approach \[11\]. It is essentially based on the existence of the energy gap \[8\]. To solve the CoM simply replacing the exact potential \[11\] by \( NV(X)\) is not sufficient, see section III B. Instead the Schrödinger equation for the CoM motion is given by
\[
H_{\text{eff}} = \frac{\hbar^2}{2M} \frac{\partial^2}{\partial X^2} + V_{\text{eff}}(X)
\]
where \( X = \frac{1}{N} \sum_{j=1}^N x_j \) is the CoM of the particles and the effective potential is the convolution of the internal density profile of the ground state soliton with the barrier potential:
\[
V_{\text{eff}}(X) = \int d^N x \delta\left( X - \sum_{j=1}^N x_j \right) \left| \psi_{N,k}(x) \right|^2 \sum_{j=1}^N \tilde{V}(x_j).
\]

**III. SCATTERING OF A DIMER OFF A DELTA POTENTIAL**

In an experiment single atoms could serve as scattering potentials, in the following mathematically simplified as delta distributions. We therefore investigate the scattering of a dimer off such a delta potential in a one-dimensional geometry and discuss signatures of the resulting Schrödinger-cat states. Moreover the effective potential approach of section III B will be applied to this situation which is mathematically more challenging than the case of broader potentials. Contrary to higher particle numbers, for two particles analytical calculations nonetheless still are possible and can furthermore be compared with numerical results obtained via discretising the Schrödinger equation.

Within a Bose-Hubbard Hamiltonian \[37, 38\]
\[
\hat{H}_{\text{lattice}} = -J \sum_j \left( \hat{a}_j^\dagger \hat{a}_{j+1} + \hat{a}_{j+1}^\dagger \hat{a}_j \right) + \frac{U}{2} \sum_j \hat{n}_j \left( \hat{n}_j - 1 \right), \quad U < 0, \quad J > 0,
\]
describing the dynamics of \( N \) bosonic particles on a lattice, it is possible to use exact eigenstates. Here, \( J \) is the tunnelling strength, \( U \) denotes the pair interaction, \( \hat{a}_j^\dagger \) and \( \hat{a}_j \) are the usual boson creation and annihilation operators and \( \hat{n}_j = \hat{a}_j^\dagger \hat{a}_j \) is the number operator for site \( j \). For a single particle on a lattice the dispersion relation is given by
\[
E_{\text{one}} = -2J \cos(kb).
\]

Comparing equation \[17\] with the dispersion relation for suitably small lattice step sizes \( b \) under consideration of the lower band edge \(-2J\) and choosing \( Jb^2 = \frac{\hbar^2}{2m} \) then renders a numerical investigation of the free particle motion possible. In the case of a dimer the two-particle bound states \[21, 24, 39, 40\] are given by
\[
|\Psi\rangle = \sum_{j, \ell} c_{j\ell} |j\rangle |\ell\rangle
\]
with
\[
c_{j\ell} = \begin{cases} x_{j-\ell} \exp[ikb(j + \ell)] & , j \neq \ell \\ \frac{1}{\sqrt{2}} \exp[ikb(j + \ell)] & , j = \ell \end{cases}
\]
and
\[
x_+ = \sqrt{\frac{U^2}{16J^2 \cos^2(kb)} + 1 - \frac{|U|}{4J \cos(kb)}}
\]

\[20\]
This leads to a dispersion relation

$$E_{\text{two}} \simeq -4J \left( \frac{U^2}{16J^2} + 1 \right)^{1/2} + \frac{8J^2 \hbar^2}{(16J^2 + U^2)^{3/2}} k^2.$$  \hspace{1cm} (21)

Analogue to the one-particle case for small values of \( b \) and under consideration of the offset \(-4J\) a comparison with the energy

$$E_{N=2, \text{soliton}} = -\frac{\hbar^2 \beta^2}{m} + \frac{h^2 k^2}{m}$$ \hspace{1cm} (22)

of a two-particle soliton according to equation \([9]\) then enables the numerics for a tightly bound dimer moving in a one-dimensional geometry using the dimer wavefunctions in a tight-binding lattice.

In the following, like in figure 1 (a), the initial wave function with mean momentum \( k_0 \) and width \( a \) is built up of the two-particle eigenfunctions \([19]\) where \( k \) should be restricted to \( 0 < k < \beta \) so that the dimer cannot break apart for energetic reasons. We choose the upper integral boundary \( k_{\text{max}} \) to be about twice the mean momentum:

$$\Psi_0(x_1, x_2; t = 0) \propto \int_0^{k_{\text{max}}} dk \exp \left( -\frac{a^2 (k - k_0)^2}{2} \right) \times \Psi_{2, k}(x_1 - x_0, x_2 - x_0).$$ \hspace{1cm} (23)

A. Interference patterns

In the low energy-regime the scattering of a dimer at a delta potential

$$V(x_1, x_2) = v_0 [\delta(x_1) + \delta(x_2)],$$ \hspace{1cm} (24)

located in the middle of the lattice, can lead to the creation of nonlocal mesoscopic superposition states where both particles always should be found on the same side of the scattering potential. To probe the existence of such a Schrödinger-cat state we thus use the criterion \([11]\)

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

and ensure that it takes on sufficiently low values on the order of \(10^{-8}\). To investigate the interference patterns the contrast

$$C = \frac{I_{\text{max}} - I_{\text{min}}}{I_{\text{max}} + I_{\text{min}}}$$ \hspace{1cm} (26)

will be calculated on a suitable interval in the middle of the pattern.

Figure 1 shows numerical results for the CoM density distribution \([2]\): The initial wave function in figure 1 (a) is implemented according to \([23]\). Scattering at the delta potential then leads to the creation of a nonlocal superposition, displayed in figure 1 (b). To allow for a subsequent recombination of the wave packets reflection potentials are added at the edges of the lattice. After being reflected, cf. figure 1 (c), an interference pattern with maximal contrast \( C = 1 \) arises in the CoM density which can be seen in figure 1 (d). The contrast has been calculated on the interval \( x\beta \in [-10, 10] \).

The results for the single-particle density \([3]\) which are displayed in figure 2 differ clearly from this. The contrast of the interference pattern is reduced to about 0.75, again calculated for \( x\beta \in [-10, 10] \).

Summarising, the scattering of a dimer off a delta potential can lead to the creation of a Schrödinger-cat state. While the subsequent recombination of the two coherent parts of the wave-function leads to an interference pattern with maximum contrast in the CoM density the visibility of the pattern in the single-particle density is reduced. These numerical results will in section IV be compared with analytical considerations which can be extended to the \( N \)-particle case.

B. Effective potential approach for the scattering of a dimer at a delta potential

The existence of the energy gap \([8]\) allowed the creation of the mesoscopic superposition state in III A and

FIG. 1. CoM density (thin line) for the scattering of a dimer at a delta potential \( V(x_1, x_2) = v_0 [\delta(x_1) + \delta(x_2)] \). The delta potential situated in the middle of the lattice as well as the reflection potentials at the edges are displayed schematically (thick lines). Lattice size: 801x801 lattice points. (a) Initial wave function with width \( a\beta = 18 \) and mean wave vector \( k_0/\beta = 0.75 \) centred around \( x_0\beta = -40 \). (b) Schrödinger-cat state with \( p_{\text{miaou}} = 0.25 \cdot 10^{-4} \) and 50%-50% splitting, shown at \( th\beta^2/m = 136 \). (c) Reflection of the two parts of the quantum superposition at reflection potentials on the edges. Scattering potential is switched off. (d) Recombination of the two parts of the wave function leading to an interference pattern in the CoM coordinate with maximal contrast \( C = 1 \) at \( th\beta^2/m = 255 \). The contrast is calculated using equation \([20]\) on the interval \( x\beta \in [-10, 10] \).
renders the effective potential approach from section IIIB possible. For the scattering of a dimer off a delta potential it is possible to compare the effective potential approach even in higher order perturbation theory with numerical results using again the tight-binding wavefunctions of section IIIA. The exact potential \([24]\) can be expressed as

\[ V(x_1, x_2) = V_X(x) + \Delta V(x_1, x_2) \tag{27} \]

where \(V_X(x) = 2v_0\delta(x)\) and

\[ \Delta V(x_1, x_2) = v_0 [ -2\delta(x) + \delta(x_1) + \delta(x_2)]. \tag{28} \]

This perturbation \(\Delta V(x_1, x_2)\) to the CoM contribution \(V_X(x)\) induces an energy shift \(\Delta E\) on the CoM motion. The Schrödinger equation for the CoM wave-function \(\Psi(X)\) then is given by

\[ i\hbar \partial_t |\Psi(X)\rangle = \left[-\frac{\hbar^2}{2M} \partial_X^2 + V_X(X) + \Delta E(X) \right] |\Psi(X)\rangle. \tag{29} \]

The energy shift \(\Delta E\) on the CoM motion due to the relative motion can be computed in Rayleigh-Schrödinger perturbation theory. In first order it is given by

\[ \Delta E^{(1)}(X) = \langle \Psi^{(0)}_{0, N = 2} | \Delta V(x_1, x_2) | \Psi^{(0)}_{0, N = 2} \rangle, \tag{30} \]

with the ground state soliton \([9]\) for two particles,

\[ \Psi^{(0)}_{0, N = 2}(x_1) = \sqrt{2\beta} \exp(-\beta|x_1|), \tag{31} \]

using CoM and relative coordinates \([13]\). As shown in \([4]\) the energy correction adopts the form

\[ \Delta E^{(1)}(X) = -2v_0\delta(X) + 4\beta v_0 \exp(-4\beta|X|) \tag{32} \]

such that up to first order perturbation theory the effective potential in the Schrödinger equation \([14]\) for the CoM can be identified as the convolution

\[ V^{(0)}(X) + V^{(1)}(X) = V_X(X) + \Delta E^{(1)}(X) = 4\beta v_0 \exp(-4\beta|X|) \tag{33} \]

of the scattering potential \([24]\) with the density profile \([31]\) of the dimer. Taking into account excited states \([17]\) gives the higher order corrections

\[ V^{(2)}(X) = -\frac{2\beta^2 m}{\hbar^2} \exp(-4\beta|X|) \left[ 1 - 8\beta|X| \exp(-4\beta|X|) \right] \tag{34} \]

and

\[ V^{(3)}(X) = \frac{16\beta^3 m^2}{\hbar^4} \exp(-4\beta|X|) \times \left[ C_1(X) + C_2(X) \exp(-4\beta|X|) \right] + C_3(X) \exp(-8\beta|X|) \tag{35} \]

to the effective potential (cf. \([4]\)), where \(C_1(X) = \frac{1}{16\beta} + \frac{1}{8\beta^2} \delta(X), C_2(X) = -\left( |X| + \frac{1}{4\beta} + \frac{1}{16\beta^2} \delta(X) \right)\) and \(C_3(X) = \left( 8|X|^2 \beta + |X| + \frac{1}{8\beta} \right)\).

In the following the scattering of a dimer at a delta potential will be investigated numerically for suitable parameters, on the one hand using the exact potential \([24]\) and on the other hand the results for effective potential. The scattering potential is again located in the middle of a lattice with spatial size \(L\) where \(-L/2 < X < L/2\) and the initial wave-function is chosen according to (23) to ensure the dimer not to break apart. Figure 3 shows the reflection coefficient

\[ R(v_0) = \int_{-L/2}^{0} dX |\Psi(X)|^2, \tag{36} \]

which is increasing with the strength of the scattering potential \(v_0\). Neglecting the correction \(\Delta E(X)\) leads to full transmission over the whole range of values for the height of the scattering potential and thus in zeroth order the dynamics is not described correctly at all. As can be seen in figure 3 the reflection coefficient \(R_0(v_0)\) for the exact potential is well-approximated in third order perturbation theory. In the inset it is shown that already in first order the dynamics are qualitatively well-described. Especially in the experimentally interesting regime with \(R \approx 0.5\) a convergence towards \(R_3(v_0)\) can be observed: the second order leads to a clear improvement while the additional contribution in third order is small. For larger potential heights with \(R > 0.8\) taking into account only up to 2nd rather than 3rd order contributions leads to better results.
and mean momentum $k_0 / \beta = 0.375$ was located at $x_0 \beta = -80$. Numerics for exact potential (solid line) and effective potential up to 3rd order perturbation theory (dash-dotted line). Taking only the zeroth order corrections into account leads to full transmission over the whole range of parameters and hence does not describe the dynamics correctly at all. Inset: Deviation $\Delta R = R_{\text{eff}}(v_0) - R_{\text{eff}}(v_0)$ including up to 1st order corrections (dotted line), 2nd order corrections (dashed line) and 3rd order corrections (dashed-dotted line).

IV. INTERFERENCE PATTERNS AS SIGNATURES OF QUANTUM SUPERPOSITION STATES

In section III A the interference of the two coherent parts of the quantum superposition has been investigated. In the following we will analytically explain the different values of the contrast in the CoM and the single-particle density and extend the two-particle results to considerations for $N$ particles. We will omit the envelopes of the wavepackets and restrict to the interference of two plane waves with opposed CoM wave vector $K$. If already in this case no interference is observed neither with wave-packets built up of plane waves this would be the case.

For the description of a dimer we use again the relative and CoM coordinates (13). The wave function (10) then reads

$$\Psi_\pm = \sqrt{2\beta} e^{-\beta|x|} e^{\pm i K X}. \quad (37)$$

The interference of the two parts $\Psi_+$ and $\Psi_-$ of the superposition

$$\Psi_+ + \Psi_- = 2 \sqrt{2\beta} e^{-\beta|x|} \cos(KX) \quad (38)$$

results in the following interference pattern in the CoM-density distribution (2)

$$\langle \delta(x-X) \rangle_{\text{gr}} = \int_0^\infty dx_r \int_{-\infty}^{\infty} dX |\Psi_+ + \Psi_-|^2 \delta(x-X) \propto \cos^2(KX). \quad (39)$$

Hence, in the CoM-coordinate an interference pattern with fringe spacing $\pi/K$ can always be observed and the contrast (26) takes on its maximal value $C_{\text{gr,CoM}} = 1$.

For the single-particle density (3) the corresponding expectation value is

$$\rho_{\text{gr,one}} = \frac{1}{2} \sum_{j=1,2} \langle \delta(x-x_j) \rangle \propto \frac{1}{(\beta^2 + K^2)} \left[4\beta^2 \cos(2Kx) + 4\beta^2 + K^2 \right] \quad (40)$$

and as the ratio $\beta/|K|$ is related to the ratio of binding to CoM kinetic energy via $2\beta/|K| = \sqrt{\frac{\mu}{E_{\text{kin}}}}$ the contrast now is given by

$$C_{\text{gr,one}} = \frac{1}{1 + \frac{E_{\text{kin}}}{|\mu|}}. \quad (41)$$

For low CoM kinetic energies the contrast is maximal while for high values of $E_{\text{kin}}$ the interference vanishes:

$$\lim_{E_{\text{kin}}/|\mu| \to 0} C_{\text{gr,one}} = 1, \quad (42)$$

$$\lim_{E_{\text{kin}}/|\mu| \to \infty} C_{\text{gr,one}} = 0. \quad (43)$$

This agrees qualitatively with our numerical observations, cf. figure 2. The dependence of the contrast on $E_{\text{kin}}/|\mu|$ is shown in figure 3 (a).

For CoM kinetic energies larger than the binding energy in an experiment excitations could occur. What would be the influence on the visibility of the interference pattern in the CoM density? Repeating the same considerations as for the ground state for the excited states (12) leads again to an interference pattern

$$\lim_{L \to \infty} \langle \delta(x-X) \rangle_{\text{exc}} \propto \cos^2(Kx) \quad (44)$$

with maximal contrast $C_{\text{exc,CoM}} = 1$, cf. 3. For the ground state we discovered the same result and looking separately at ground or excited wave functions additional phase factors are irrelevant for the contrast. However, in an experiment involving excitations phase factors could become important. Hence a superposition of the patterns $\cos^2(Kz)$ and $\cos^2(Kz + \phi)$ could lead to extinction.

In the following we will investigate the experimentally relevant $N$-particle case. In the low-energy regime the scattering of a soliton off a scattering potential has been predicted to lead to the creation of a nonlocal quantum superposition of the form (1). Again the superposition of wave-functions (10) with opposing $K$ leads to an interference pattern

$$\langle \delta \left( x - \frac{x_1 + \cdots + x_N}{N} \right) \rangle_{N,\text{CoM}} \propto \cos^2(Kx) \quad (45)$$
with contrast $C_{N,\text{CoM}} = 1$ in the CoM density distribution while the contrast of the single-particle density is given by \[C_{N,\text{one}} = \frac{\pi \sqrt{N - 1} \sqrt{E_{\text{kin}}/|\mu|}}{\text{sinh} \left( \frac{\pi \sqrt{N - 1} \sqrt{E_{\text{kin}}/|\mu|}}{2} \right)}.\] (46)

As shown in figure 4(b) the contrast only takes on values $C_{N,\text{one}} \approx 1$ for extremely small ratios $E_{\text{kin}}/|\mu|$ and vanishes otherwise. A comparison of CoM and single-particle density interference patterns is shown for experimentally realistic parameters \[11\] in figure 4(c). Though the calculations have been performed for plane waves of the CoM rather than wave-packets it can be deduced that also with wave-packets no interference in the single-particle density could be observed.

Within the effective potential approach \[11\] it is possible to numerically investigate the time evolution of the CoM density for the scattering of a soliton consisting of $N = 100$ atoms at a delta potential which is shown in figure 5. The effective potential \[11\] being the convolution of the scattering potential with the mean-field soliton density \[6\] is again of the form $V_{\text{eff}} \sim 1/\cosh^2 (X/2\xi)$ where $\xi = h^2/g_{\text{sd}}/N$ is the soliton size. Clearly the splitting of the wave packet due to scattering at the barrier potential can be observed. After switching off the barrier potential the coherent parts of the wave packet recombine and display an interference pattern with high contrast.

Summarising these results we have shown that the interference pattern of the CoM density distribution for the ground state soliton always has maximum contrast both for the dimer and the $N$-particle BMWS. For the dimer the contrast in the single-particle density interference pattern is, depending on the ratio of kinetic to binding energy for the dimer, (b) Contrast \[26\] for a soliton with $N = 50$ (solid line), $N = 100$ (dashed line) and $N = 200$ (dash-dotted line) particles.

To summarise, for sufficiently low kinetic energies the scattering of tightly bound dimers or BMWS can lead to the creation of nonlocal mesoscopic quantum superposition states \[1\]. For the scattering of a dimer off a delta potential the effective potential approach from \[11\] could be tested numerically. The approach has been found to describe qualitatively correct the dynamics though the consideration of higher order terms in the perturbation theory leads to clearly improved results. While so far only first order corrections to the effective potential have been investigated \[11\], here we have presented a case where higher-order corrections become necessary.

Furthermore, for the two-particle case we have numerically shown that the subsequent interference of the two coherent parts of the wave-function leads to a perfect contrast in the CoM coordinate while the visibility of the interference pattern in the single-particle density is reduced. Our analytical calculations confirm this be-
haviour. For a tightly bound dimer the contrast will only be reduced whereas for experimentally realistic atom numbers on the order of \( N = 100 \) the contrast in the single-particle density vanishes in all but experimentally unrealistic regimes. Nevertheless, in the CoM density an interference pattern still is clearly displayed.

Concluding, we have shown the occurrence of an interference pattern with high contrast both for the dimer and a soliton consisting of about 100 atoms in the CoM density distribution. Additionally, after the scattering all the particles should be clustered in a single lump, in repeated measurements randomly distributed on either side of the scattering potential. Combining these two characteristics can serve as a signature of nonlocal quantum superposition states.

Note added in proof: The effective potential method [11] was also independently developed in [44].

ACKNOWLEDGMENTS

We acknowledge discussions with S. Arlinghaus, Y. Castin, S. A. Gardiner, T. Gasenzer, M. Holthaus, R. Hulet and M. Oberthaler. BG thanks C. S. Adams and S. A. Gardiner for hospitality at the University of Durham and acknowledges funding by the ‘Studienstiftung des deutschen Volkes’ and the ‘Heinz Neumüller Stiftung’. CW acknowledges funding from UK EPSRC (Grant No. EP/G056781/1).

Appendix A: Effective potential approach for the scattering of a dimer at a delta potential

The energy change (30) in first order perturbation theory is

\[
\Delta E^{(1)}(X) = \int_0^\infty dx |\Psi^{(0)}_{0,N=2}(x)|^2 V_X = -2\nu_0 \delta(X) + 4\beta \nu_0 \exp(-4\beta |X|), \quad (A1)
\]

leading to the effective potential (33). For compactness we omit the argument in \( V_X(X) \).

For higher order corrections the excited states (13) for a dimer are required. Their relative part reads

\[
\Psi_{k,\text{rel}}^{(0)}(x_2) = 2\sqrt{\mathcal{N}_k} \left[ \cos(kx_2) - \frac{\beta}{k} \sin(k|x_2|) \right]. \quad (A2)
\]

Here the particles have been enclosed in a fictitious box of size \( L \), later assumed to be infinitely large. Using periodic boundary conditions this leads to the norm

\[
\mathcal{N}_k = \frac{1}{2L(1 + \frac{\beta^2}{k^2})}. \quad (A3)
\]

In Rayleigh-Schrödinger perturbation theory with continuous eigenstates (A2) the energy correction in second order is given by

\[
\Delta E^{(2)}(X) = \int_0^\infty dk g(k) \left| \int_0^L dx \Psi_{0,N=2}^{(1)}(x) \Psi_{k,\text{rel}}^{(0)} \right|^2 \frac{E_k^{(0)}(2) - E_k^{(0)}(2)}{E_k^{(0)}(2)} \quad (A4)
\]

where \( g(k) = \frac{L}{\pi k} \) and the argument \( x_2 \) in (A2) is again omitted. The integral is restricted to the interval \( 0 < k < \infty \) as the relative part of the wave-function (A2) is symmetric with respect to \( k \). With \( E_k^{(0)}(N = 2) = -\frac{\hbar^2}{2m}, E_k^{(0)}(N = 2) = \frac{\hbar^2}{m} \),

\[
\left| \int_0^L dx \Psi_{0,N=2}^{(1)}(x) \Psi_{k,\text{rel}}^{(0)} \right|^2 = 32\beta \nu_0^2 \mathcal{N} \exp(-4\beta |X|) \times \left[ \cos(2k|x|) - \frac{\beta}{k} \sin(2k|x|) \right]^2 \quad (A5)
\]

and using the Gradsteyn integrals (3.264), (3.773) and (3.264) we get

\[
\Delta E^{(2)}(X) = -2\nu_0^2 m \frac{\hbar^2}{k^2} \exp(-4\beta |X|) \left( 1 - 8\beta |X| \exp(-4\beta |X|) \right). \quad (A6)
\]

corresponding to the contribution \( V_{\text{eff}}^{(2)} \) to the effective potential in second order, given by equation (34). The energy correction in third order is given by
\[ E_0^{(3)}(X) = \frac{L^2}{4\pi^2} \int_0^\infty dk_1 \int_0^\infty dk_2 \frac{\langle \Psi_{0,N=2}^{(0)} \rvert \Psi_{1,rel}^{(0)} \rangle \langle \Psi_{1,rel}^{(0)} \rvert \Psi_{2,rel}^{(0)} \rangle \langle \Psi_{2,rel}^{(0)} \rvert \Psi_{0,N=2}^{(0)} \rangle}{E_0(2) - E_{k_1}(2)} \left[ E_0(2) - E_{k_2}(2) \right] \]

\[ - \frac{L}{2\pi} \int_0^\infty dk_1 \frac{\langle \Psi_{0,N=2}^{(0)} \rvert \Psi_{1,rel}^{(0)} \rangle \langle \Psi_{1,rel}^{(0)} \rvert \Psi_{0,N=2}^{(0)} \rangle}{E_0(2) - E_{k_1}(2)} \]

With equations (A1), (A5) and

\[ \langle \Psi_{k_1,rel}^{(0)} \rvert V_X \rvert \Psi_{k_2,rel}^{(0)} \rangle = \frac{4v_0}{L} \left( \frac{1 + \beta^2}{1 + \frac{1}{2} \beta^2} \right)^{1/2} \times \left[ \cos(2k_1 \rvert X \lvert) - \frac{\beta}{k_1} \sin(2k_1 \rvert X \lvert) \right] \]
\[ \times \left[ \cos(2k_2 \rvert X \lvert) - \frac{\beta}{k_2} \sin(2k_2 \rvert X \lvert) \right] \]

as well as the Gradsteyn integrals (3.773) and (3.251) this gives

\[ E_0^{(3)}(X) = 16v_0^2 \frac{m^2}{\hbar^2} \exp(-4\beta \rvert X \lvert) \]
\[ \times \left[ \frac{1}{16\beta^2} \left( \rvert X \lvert + \frac{1}{4\beta} \right) \exp(-4\beta \rvert X \lvert) \right] \]
\[ + \left[ 8 \rvert X \lvert^2 \beta + \rvert X \lvert + \frac{1}{8\beta} \right] \exp(-8\beta \rvert X \lvert) \]
\[ + \left[ \frac{1}{8\beta^2} - \frac{1}{16\beta^2} \exp(-4\beta \rvert X \lvert) \right] \delta(\rvert X \lvert) \]

This corresponds to the third order correction \( V_{\text{eff}}^{(3)} \) to the effective potential, cf. [33].

**Appendix B: Interference patterns**

1. **Calculation of the interference pattern for the excited states** [12] **in the two-particle case**

For the wave function \( \Psi_+ \) with \( K \) and \( k \) the corresponding wave function \( \Psi_- \) has been obtained by the replacements \( K \to -K \) and \( k \to -k \). With the superposition state

\[ \lvert \Psi_+ \rangle + \lvert \Psi_- \rangle = 4\sqrt{N_k} \left[ \cos(kx) - \frac{\beta}{k} \sin(kx) \right] \cos(Kx) \]

(B1)

this leads to a CoM density distribution

\[ \lim_{L \to \infty} \langle \delta (x - X) \rangle_{\text{exc}} = \lim_{L \to \infty} \int_0^L dx_r \int_{-L/2}^{L/2} dX 16N_k \]
\[ \times \left[ \cos(kx) - \frac{\beta}{k} \sin(kx) \right]^2 \cos^2(Kx) \]

(B2)

2. **N-particle case**

The interference pattern in the CoM density under consideration of equation (6) is

\[ \langle \delta (x - \frac{x_1 + \cdots + x_N}{N}) \rangle_{N,\text{CoM}} = 4 \int dx_1 \cdots dx_N \lvert \Psi_{0,rel} \rvert^2 \cos^2(Kx + \frac{x_1 + \cdots + x_N}{N}) \]
\[ \times \delta \left( x - \frac{x_1 + \cdots + x_N}{N} \right) \]

\[ = 4 \int_{-\infty}^{\infty} dy \cos^2(Kx) \int dx_1 \cdots dx_N \lvert \Psi_{0,rel} \rvert^2 \]
\[ \times \delta \left( x - \frac{x_1 + \cdots + x_N}{N} \right) \delta (x_1 - y) \]
\[ = \frac{m^2}{\hbar^2} N^2 \cos^2(Kx) \int_{-\infty}^{\infty} dy \left[ \cosh \left( \frac{m^2}{\hbar^2} N (y - x) \right) \right]^-2 \]
\[ = 4N \cos^2(Kx) \]

(B3)

The interference pattern in the single-particle density [3] is, again using equation (6) and Gradsteyn (3.982), given by

\[ \langle \delta (x - x_1) \rangle_{N,\text{one}} = \int_{-\infty}^{\infty} dX \cos^2(Kx) \int dx_1 \cdots dx_N \lvert \Psi_{0,rel} \rvert^2 \]
\[ \times \delta \left( X - \frac{x_1 + \cdots + x_N}{N} \right) \delta (x - x_1) \]
\[ = 2\beta N^2 \int_{-\infty}^{\infty} dX \frac{\cosh(Kx)}{\cosh^2(\beta N(x - x_1))} \]
\[ = \beta N^2 \int_{-\infty}^{\infty} dX \frac{1 + \cosh(2Kx)}{\cosh^2(\beta N(x - x_1))} \]
\[ = 2N + \frac{2Kx}{\beta} \frac{1}{\sinh(\frac{Kx}{\beta})} \cos(2Kx) \]

(B4)

Thus, the intensity can take on the following maximal and minimal values

\[ I_{\text{max}} = \langle \delta (0 - x_1) \rangle = 2N + \frac{2Kx}{\beta} \frac{1}{\sinh(\frac{Kx}{\beta})}, \] (B5)
\[ I_{\text{min}} = \langle \delta (x - x_1) \rangle = 2N - \frac{2Kx}{\beta} \frac{1}{\sinh(\frac{Kx}{\beta})}. \] (B6)

This leads to the contrast

\[ C_{N,\text{one}} = \frac{Kx}{\beta N} \frac{1}{\sinh \left( \frac{Kx}{\beta N} \right)}. \] (B7)

Using equation (8) and (9) gives expression (46) for the contrast in dependence of

\[ E_{\text{kin}} \]

[\mu] = \frac{K^2}{\beta^2 N^2 (N - 1)}. \] (B8)