Quantum many-body dynamics of bright matter-wave solitons

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Abstract

The interplay of particle and resonant wave scattering including nonlinear effects creates systems of diverse and interesting quantum many-body physics. A better understanding of the physics in these systems could lead to new and exiting application exploiting their quantum nature.

As an example, in this thesis we investigate the scattering of bright matter-wave solitons in ultracold gases on a square well in one spatial dimension. For this, solutions of the mean-field Gross-Pitaevskii approximation and a full quantum many-body method, the so-called multiconfigurational time-dependent Hartree approach (MCTDH), are compared.

The MCTDH method is based on a finite basis set expansion, which naturally leads to errors in system properties, such as energies and densities, when compared to exact results. In this thesis, we propose an efficient solution to this problem by rescaling the interaction strength between the particles. Even for very large interactions in the Tonks-Girardeau limit, the rescaling leads to significant improvements. This is validated by successfully applying the rescaling to problems in ring systems as well as external confinements, such as a harmonic well and a double-well.

The MCTDH method is then applied to the soliton scattering problem and compared to results from mean-field calculations. The latter verify that solitons, when scattered on a well, show quantum effects, such as reflection. For the first time, we show that a soliton can be additionally permanently trapped by the well due to resonances with bound states.

For this thesis, to extend these results to a full many-body approach, we developed QiwiB. It is a program package implementing the MCTDHB method, which is a derivative of the MCTDH method, but optimised for bosonic systems. Limits for the validity of the MCTDHB approach are addressed by convergence studies on the soliton scattering problem. Furthermore, we demonstrate that the scattering on the well enables the creation of macroscopic binary quantum superposition states, i.e. *NOON* states. Novel *NOON* states corresponding to a superposition of a reflected soliton and a trapped soliton are observed. These states are shown to exist for a large range of initial conditions, and a possible experimental realisation is discussed.

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General abbreviations

BEC	Bose-Einstein condensate
GP	Gross-Pitaevskii
GPE	Gross-Pitaevskii equation
1D	one dimension or one-dimensional
NOON	NOON state: superposition of N particles occupying the first natural orbital and N particles occupying the second one, i.e. $\alpha\|N,0\rangle + \beta\|0,N\rangle$ with α and β being complex numbers.
MCTDH	Multiconfigurational time-dependent Hartree
MCTDHB	Multiconfigurational time-dependent Hartree explicitly optimised for bosonic symmetry
MCTDH(B)	MCTDH and/or MCTDHB
QiwiB	Quantum integrator with interacting bosons, a program package developed for this thesis, which solves the MCTDHB equations
TG	Tonks-Girardeau
LL	Lieb-Liniger
RK	Runge-Kutta

Physical observables and operators

T	Transmission, i.e. in this thesis the relative number of particles that passed the well
R	Reflection, i.e. in this thesis the relative number of particles that got reflected from the well
L	Trapping, i.e. in this thesis the relative number of particles that got trapped inside the well
TRL	TRL window: range of potential depths around the resonance with a bound state of the well and where the reflection is less than one.

RT	RT window: range of potential depths between a regime of full reflection and full transmission
N	number of particles
M	number of single-particle functions, equivalent to the number of natural orbitals
N_g	number of grid points for the discretised spatial coordinate in the numerical calculations
$\psi(x,t)$	Gross-Pitaevskii wave-function in one dimension
$\Psi(x_1,\ldots,x_N,t)$	Total wave function for N particles in one dimension
$\lvert\Psi(t)\rangle$	Total wave function for N particles in second quantised form
g	dimensionless effective interaction strength in one dimension
μ	chemical potential
$\rho(x,y,t)$	Reduced one-body density matrix given as $\rho(x,y,t) = N\int dx_2\ldots dx_N \Psi^\star(x,x_2\ldots,x_N)\Psi(y,x_2\ldots,x_N)$
ϕ_i	ith single particle function
ϕ_i^{NO}	ith natural orbital defined by $\rho(x,y,t) = \sum_{i=1}^M \rho_i \left[\phi_i^{NO}(y)\right]^\star \phi_i^{NO}(x)$
ρ_{kq}	Density matrix in single-particle representation defined by $\rho(x,y,t) = \sum_{k,q=1}^M \rho_{kq}\phi_k^\star(y)\phi_q(x)$
ρ_i	Density matrix in natural-orbital representation defined by $\rho(x,y,t) = \sum_{i=1}^M \rho_i \left[\phi_i^{NO}(y)\right]^\star \phi_i^{NO}(x)$
$\lvert\vec{n}\rangle$	many-body state in second quantisation: $\lvert\vec{n}\rangle = \prod_{k=1}^M \frac{1}{\sqrt{n_k!}}[b_k^\dagger(t)]^{n_k}\lvert\mathrm{vac}\rangle$ with $\vec{n} = (n_1,\ldots,n_M)$ and $\sum_{i=1}^M n_i = N$
$C_{\vec{n}}$	Configuration amplitude defined by $\lvert\Psi(t)\rangle = \sum_{\vec{n}} C_{\vec{n}}\lvert\vec{n}\rangle$ in the single-particle representation
$C_{\vec{n}}^{NO}$	Configuration amplitude defined by $\lvert\Psi(t)\rangle = \sum_{\vec{n}} C_{\vec{n}}\lvert\vec{n}\rangle$ in the natural-orbital representation

Physical constants

$\hbar$	Planck's constant $\hbar = 1.054571726(47)\times 10^{-34} Js$
k_b	Boltzmann constant $k_b = 1.3806488(13)\times 10^{-23} J/K$