Breakdown of time-dependent mean-field theory for a one-dimensional condensate of impenetrable bosons

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We show that the time-dependent nonlinear Schrödinger equation of mean-field theory has limited utility for a one-dimensional condensate of impenetrable bosons. Mean-field theory with its associated order parameter predicts interference between split condensates that are recombined, whereas an exact many-body treatment shows minimal interference.

Mean-field theory (MFT) has proven remarkably successful at predicting both the static and dynamic behavior of Bose-Einstein condensates (BECs) in weakly-interacting atomic vapors \cite{1}, including the ground state properties \cite{2}, the spectrum of collective excitations \cite{3}, four-wave mixing \cite{4}, matter-wave solitons \cite{5}, and interference between BECs \cite{6,7}. The basic notion underlying MFT is of a macroscopic wave function \cite{8,9}, or order parameter, which defines the spatial mode into which a significant fraction of the atoms condense below the critical temperature. The macroscopic wave function typically obeys a nonlinear Schrödinger equation (NLSE), the Gross-Pitaevskii equation, and is most suitable for dilute Bose gases. But the success of MFT is not assured in all cases. For example, in one-dimension (1D) a spatially homogeneous ideal gas in its many-body ground state exhibits complete BEC into the lowest single-particle state, but no BEC at any nonzero temperature. Furthermore, previous exact analysis \cite{10,11} of a gas of impenetrable or hard core bosons in 1D by one of us (MG) and its extension by Lenard \cite{12} and Vaidya and Tracey \cite{13} have shown that in the many-body ground state the occupation of the lowest single-particle state is of order $\sqrt{N}$ where $N$ is the total number of atoms, in contrast to $N$ for usual BEC. Nevertheless, since $N \gg 1$ and the momentum distribution has a sharp peak in the neighborhood of zero momentum \cite{10,14}, this system shows some coherence effects. Moreover, Olshanii \cite{15} has shown theoretically that such a 1D gas of impenetrable bosons can be realized at sufficiently low temperatures and densities in thin atom waveguides, and there is also considerable experimental effort towards realizing atom waveguides for producing 1D atom clouds \cite{16,17}, a new and fertile system for studying the physics of condensed systems.

Our goal in this Letter is to show that mean-field theory breaks down in the analysis of the dynamics of 1D atom clouds, in that it predicts interference effects that are absent in the exact theory. In particular, we have recently analyzed many-body solitons in a 1D gas of bosons using the time-dependent generalization of the Fermi-Bose mapping \cite{18}, which maps a 1D gas of hard core bosons to a gas of free fermions \cite{19,20}, and Kolomeisky et al. \cite{21} have proposed a corresponding NLSE with a quartic nonlinearity to extend the usual mean-field theory for 1D atom clouds. For a harmonic trap the ground-state density profiles from their theory show excellent agreement with the exact many-body results (see Fig. 1 of their paper). The key question, then, is whether this extended NLSE can be used in all circumstances. To address this issue we examine the problem of a 1D atomic cloud in the ground state of a harmonic trap that is split by a blue-detuned laser and recombined, both using an exact many-body treatment based on the Fermi-Bose mapping and the approximate NLSE: the NLSE predicts interference whereas the exact analysis does not.

The fundamental model we consider is a 1D gas of $N$ hard core bosons at zero temperature described by the Schrödinger Hamiltonian

\begin{equation}
\hat{H} = \sum_{j=1}^{N} \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + V(x_1, \ldots, x_N; t),
\end{equation}

where $x_j$ is the one-dimensional position of the $j$th particle and the many-body potential $V$ is symmetric (invariant) under permutations of the particles. The two-particle interaction potential is assumed to contain a hard core of 1D diameter $a$. This is conveniently treated as a constraint on allowed wave functions $\psi(x_1, \ldots, x_N; t)$:

\begin{equation}
\psi = 0 \text{ if } |x_j - x_k| < a, \quad 1 \leq j < k \leq N,
\end{equation}

rather than as an infinite contribution to $V$, which then consists of all other (finite) interactions and external potentials. To construct time-dependent many-boson solutions of Eq. (1) we employ the Fermi-Bose mapping \cite{14,15,20} and start from fermionic solutions $\psi_F(x_1, \ldots, x_N; t)$ of the time-dependent many-body Schrödinger equation (TDMBSE) $\hat{H}\psi = i\hbar \partial \psi / \partial t$ which are antisymmetric under all particle pair exchanges $x_j \leftrightarrow x_k$, hence all permutations. Next introduce a “unit antisymmetric function”

\begin{equation}
\psi(x_1, \ldots, x_N) = \prod_{1 \leq j < k \leq N} \text{sgn}(x_k - x_j),
\end{equation}

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where \( \text{sgn}(x) \) is the algebraic sign of the coordinate difference \( x = x_k - x_j \), i.e., it is \(+1(−1)\) if \( x > 0(x < 0) \). For given antisymmetric \( \psi_F \), define a bosonic wave function \( \psi_B \) by

\[
\psi_B(x_1, \ldots, x_N; t) = A(x_1, \ldots, x_N)\psi_F(x_1, \ldots, x_N; t)
\]

which defines the Fermi-Bose mapping. Then \( \psi_B \) satisfies the hard core constraint (2) if \( \psi_F \) does, is totally symmetric (bosonic) under permutations, and obeys the same boundary conditions \([16,17]\). In the Olshanii limit \([24]\) (low density, very thin atom waveguide, large scattering length) the dynamics reduces to that of the impenetrable point Bose gas, the \( a \to 0 \) limit of Eq. (3). Then under the assumption that the many-body potential \( V \) of Eq. (1) is a sum of one-body external potentials \( V(x_j, t) \), the solution of the fermion TDMBSE can be written as a determinantal wavefunction \([14,15]\)

\[
\psi_F(x_1, \cdots, x_N; t) = C \det_{i,j=1}^N \phi_i(x_j, t),
\]

where

\[
i\hbar \frac{\partial \phi_i(x,t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t) \right] \phi_i(x,t).
\]

It then follows that \( \psi_F \) satisfies the TDMBSE, and it satisfies the impenetrability constraint (vanishing when any \( x_j = x_i \)) trivially due to antisymmetry. Then by the mapping theorem \( \psi_B \) of Eq. (4) satisfies the same TDMBSE. For each \( i = 1, \ldots, N \) the initial normalized wave functions \( \phi_i(x,0) \) represent different orbitals of the potential at \( t = 0 \). For example, for a harmonic trapping potential \( \phi_i(x,0) \) are given by the well-known Hermite-Gaussian orbitals, with one particle occupying each of the \( N \) lowest levels for the \( N \)-particle ground state \([25]\).

We have performed numerical simulations based on Eqs. (6), using the split-step beam propagation method \([20]\), for an initial harmonic trap containing \( N \) particles in their ground state which is subjected to a centered Gaussian repulsive potential, \( \phi_i(x,0) \) are given by the well-known Hermite-Gaussian orbitals, with one particle occupying each of the \( N \) lowest levels for the \( N \)-particle ground state \([25]\). In contrast, the density \( |\phi_i(x,t)|^2 \) for each individual orbital \( i = 1, \ldots, N \) can show large interference fringes, but with a different period in each case. Thus, the minimal interference seen in Fig. 1 is a result of washing out of the individual interferences by averaging over \( N \) orbitals. Thus, the remnant of any interference fringes decreases with increasing \( N \) and vanishes in the thermodynamic limit.

Physically, it makes sense that the interference fringes are all but absent since the Fermi-Bose mapping shows that in this 1D limit the system of bosons acts effectively like a system of free fermions insofar as effects expressible only in terms of \( |\psi_B|^2 \) are concerned, so interference is not expected \([27]\). The lack of interference is therefore a signature of the Fermi-Bose duality that occurs in 1D systems of impenetrable particles \([16]\).

We next turn to the mean-field description proposed by Kolomeisky et al. \([24]\) for low-dimensional systems. In particular, they introduce an order parameter \( \Phi(x,t) \), of \( \omega t \) (horizontal axis) and position \( x/x_0 \) (vertical axis), with white being the highest density.

FIG. 1. Exact many-body theory simulation of the cool, cut, interfere scenario. The figure shows a gray-scale plot of the particle density \( \rho_N(x,t) \) as a function of \( \omega t \) (horizontal axis) and position \( x/x_0 \) (vertical axis), with white being the highest density.
normalized to the number of particles \( N \), for such systems, though they do not discuss what this represents physically. Using energy functional arguments they deduce the following NLSE with quartic nonlinearity for a 1D system of impenetrable bosons:

\[
i\hbar \frac{\partial \Phi}{\partial t} = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t) + \frac{\hbar^2}{2m} |\Phi|^4 \right] \Phi.
\]  

with \( V(x,t) \) the same as in Eq. (1). Our goal now is to compare the predictions of this NLSE for the same cool, cut, interfere simulation in Figure 1 with the initial condition \( \Phi(x,0) = \sqrt{\rho(x,0)} \) corresponding to the exact many-body solution, all other parameters being equal. Figure 2 shows the corresponding gray-scale plot of the density \( \rho(x,t) = |\Phi(x,t)|^2 \), and two features are apparent: First, during the splitting phase when the repulsive potential is on there is very good overall agreement between the exact many-body theory and the NLSE prediction. Second, when the split components are released and recombine they produce pronounced interference fringes, in contrast to the exact theory. Indeed, this interference in the MFT is to be expected on the basis of previous theoretical work [12], even though a quartic (rather than quadratic) nonlinearity is employed here. Thus the MFT cannot accurately capture the time-dependent dynamics in all situations.

In conclusion, the numerical simulations presented show that MFT seriously overestimates the magnitude of interference phenomena in a 1D gas of impenetrable bosons. However, Kolomeisky et al. have demonstrated that their NLSE produces excellent results for the ground state density profile of 1D atomic clouds, and our simulations show that during the splitting process there is excellent agreement between the exact theory and the MFT. During the splitting the density profile is found to closely follow the ground state of the local applied potential, harmonic trap plus repulsive potential, meaning that the phase of the order parameter is not a key element during this time interval. In this case the order parameter for the NLSE is physically \( \Phi(x,t) = \sqrt{\rho(x,t)} \), to within an arbitrary overall phase factor. In contrast, during the recombination phase the relative phase of the order parameter between the two split components is the key element allowing for the appearance of the interference fringes in the MFT. Since the exact many-body theory does not show such fringes this means that the MFT approach endows the order parameter with phase information that is beyond the real degree of coherence present in the system. Thus, as long as this coherence does not manifest itself in the form of interference, the MFT is of some utility, but not if the predictions are sensitive the the order parameter phase. This view is consistent with the lack of off-diagonal-long-range-order in the 1D gas of impenetrable bosons [8][19], which is normally required for the introduction of an order parameter [4][15].

In future work we hope to investigate the transition of impenetrable bosons from the 1D regime, with no interference effects, to the 3D regime, which is well described by MFT and shows interference [10]. In particular, at 1D atom waveguide junctions such as atom beam splitters or recombiners, the system will be sensitive to the fact that the 1D waveguides are actually embedded in a higher-dimensional space, in which case atom interferometers employing 1D atom waveguides may still be capable of producing interference fringes. Another very interesting question is whether or not the usual GP NLSE or its 2D modification proposed by Kolomeisky et al. [2] gives reliable predictions of interference between BECs in the 2D regime. This has potentially important experimental consequences in view of progress in construction of 2D atom waveguides and their potential applicability to atom interferometry [28].

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[1] For a recent review see F. Dalfovo et al., Rev. Mod. Phys. 71, 463 (1999).
[2] G. Baym and C. J. Pethick, Phys. Rev. Lett. 76, 6 (1996).
[3] Y. Kagan, G. V. Shlapnikov, and J. T. M. Walraven, Phys. Rev. Lett. 76, 2670 (1996).
[4] M. Edwards et al., Phys. Rev. Lett. 77, 1671 (1996).
[5] S. Stringari, Phys. Rev. Lett. 77, 2360 (1996).
[6] E. V. Goldstein, K. Plüttner, and P. Meystre, Quantum Semiclass. Opt. 7, 743 (1995).
[7] L. Deng et al., Science 308, 218 (1999).
[8] S. A. Morgan, R. J. Ballagh, and K. Burnett, Phys. Rev. A 55, 4338 (1997).
[9] W.P. Reinhardt and C.W. Clark, J. Phys. B 30, L785 (1997).
[10] M. Naraschewski et al., Phys. Rev. A 54, 2185 (1996).
[11] J. Javanainen and M. Wilkens, Phys. Rev. Lett. 78, 4675 (1997); ibid. 81, 1345 (1998).
[12] A. J. Legget and F. Sols, Phys. Rev. Lett. 81, 1344 (1998).
[13] E. M. Wright et al., Phys. Rev. A 56, 591 (1997).
[14] O. Penrose and L. Onsager, Phys. Rev. 104, 576 (1956).
[15] C. N. Yang, Rev. Mod. Phys. 34, 694 (1962).
[16] M. Girardeau, J. Math. Phys. 1, 516 (1960).
[17] M.D. Girardeau, Phys. Rev. 139, B500 (1965). See particularly Secs. 2, 3, and 6.
[18] A. Lenard, J. Math. Phys. 7, 1268 (1966).
[19] H.G. Vaidya and C.A. Tracey, Phys. Rev. Lett. 42, 3 (1979).
[20] M. Olshanii, Phys. Rev. Lett. 81, 938 (1998).
[21] E. A. Hinds et al., Phys. Rev. Lett. 80, 645 (1998); J. Schmiedmayer, Eur. Phys. J. D 4, 57 (1998); M. Key et al., Phys. Rev. Lett. 84, 1371 (2000); D. Müller et al., physics/9908031.
[22] J. H. Thywissen et al., Eur. Phys. J. D 4, 57 (1998); Phys. Rev. Lett. 83, 3762 (1999); Eur. Phys. J. D 7, 261 (1999).
[23] M. D. Girardeau and E. M. Wright, “Many-body solitons in a one-dimensional condensate of hard core bosons,” cond-mat/0002062.
[24] A. G. Rojo, G. L. Cohen, and P. R. Berman, Phys. Rev. A 60, 1482 (1999).
[25] E. B. Kolomeisky, T. J. Newman, J. P. Straley, and Xiaoya Qi, “Low-dimensional Bose liquids: Beyond the Gross-Pitaevskii equation,” cond-mat/0002282. Note that the expression for the condensate width given following Eq. (8) therein is in error; the factor $m\omega$ should be in the denominator of the square root instead of the numerator.
[26] J. A. Fleck, J. R. Morris, and M. D. Feit, Appl. Opt. 10, 129 (1976).
[27] K. E. Cahill and R. J. Glauber, Phys. Rev. A 59, 1538 (1999).
[28] Atom Interferometry, ed. P. R. Berman (Academic Press, Boston, 1997).