Many-body ground-state properties of an attractive Bose-Einstein condensate in a one-dimensional ring

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We study a Bose-Einstein condensate with attractive interactions in a one-dimensional ring and show that the ground state is well described by the superposition of bright solitons. A position measurement of some atoms gives rise to the state reduction of the soliton position, which increases the condensate fraction. The bunched many-body ground state is well approximated by a simple variational wave function.

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I. INTRODUCTION

Recently, one-dimensional Bose-Einstein condensates (BEC) have been obtained in a cylindrical harmonic potential with a tight trapping in the radial direction [1–3]. At finite temperature, the Bose-Einstein condensation does not occur in infinite one-dimensional systems with repulsive interaction, since long-wavelength fluctuations of the phase [4] destroy the long-range order. At large distances there is an exponential decay of the one-particle density matrix [5]. Even at $T=0$, the long-range order is destroyed by the repulsive atomic interaction and the density matrix has a power-law decay [6]. Also, in attractive infinite one-dimensional systems, BEC is absent even at $T=0$, however, this is due to long-wavelength density fluctuations and not phase fluctuations, as in the repulsive case. The long-wavelength fluctuations are cut off in the presence of spatial confinement and, for sufficiently low interactions, the atomic distribution is flat. The system can be described by a uniform macroscopic wave function. Attractive bosons confined in a finite length with periodic boundary conditions have been studied within the mean field approximation [7] or for three bosons [8] or using few modes of the quantum field [9]. It has been shown that the system undergoes a symmetry breaking increasing the strength of the interatomic interaction and the uniform macroscopic wave function becomes a bright soliton in the mean-field approximation. In Ref. [9] it has been shown that the quantum fluctuations modify qualitatively the results of the mean-field approximation near the critical point. Above the critical point, the macroscopic population of the condensate begins to decrease when the strength of the interaction increases, and it becomes negligible for a sufficiently high strength. In this case the one-particle density matrix does not have an eigenvalue much larger than the other ones [9] and the system cannot be described by a macroscopic wave function. The limit of high interactions corresponds to the case of an infinite system. Thus, as in the repulsive case, the long-range order is absent at $T=0$ in infinite systems.

In this work, we show that a condensate can be present, even if there is no macroscopically populated state. The loss of coherence is easily understandable from the mean-field point of view. Let ψ be the normalized macroscopic wave function with minimal energy evaluated in the mean-field approximation. It should be the common state of almost all the atoms. The attractive interaction clusters the particles in the same region, thus ψ has a localized peak. There are infinite minimal energy states, which are obtained by a spatial translation of ψ. The many-body ground state is better described by a coherent superposition of the infinite soliton states, hence the one-particle distribution probability is spatially uniform. It is clear that this state has no long-range coherence, since there is entanglement between the position of each particle and the remaining ones. This entanglement can be used to select a single soliton of the superposition. If we measure the position of $\tilde{N}$ particles, we filter only a few solitons. The selection becomes more precise when $\tilde{N}$ is increased. It is reasonable to suppose that the coherence is recovered with a conditional measurement of the barycenter of some particles, i.e., that the lack of coherence is mainly due to the spreading of the barycenter position. In this sense, the condensate is always present, although the one-particle density matrix has not an eigenvalue much larger than the other ones. Experimentally, when a one-dimensional boson gas with attractive interaction is cooled at sufficiently low temperatures and the interaction strength is above the critical point, a bright soliton is created with macroscopic coherence. If the experiment is repeated many times, many solitons with different positions are created, but each one has a macroscopic coherence. Similar results have been reported in Ref. [10] for a one-dimensional infinite system with attractive interactions. In this case, it is possible to find an analytical N-body wave function, which is used to evaluate the mean spatial density of the particles knowing the position of center of mass. The authors show that for a sufficiently high number of atoms the conditioned density is consistent with the mean-field broken-symmetry solution. The effect of a small symmetry breaking potential on the many-body wave function has been recently studied in Ref. [11]and related arguments have been considered in Ref. [12]. A similar behavior occurs also in the interference of two condensates. If the condensates are in number states, their phase is not defined and the average atomic distribution over many experiments does not display fringes. However a single realization yields interference [13,14], that is, in each single experiment the fringes are present, as expected in the mean-field approximation, but their maximum position is not the same. The measurement of atomic distribution of two overlapping condensates fixes their relative phase.

In Sec. II, we evaluate the one-particle density matrix under the condition that the barycenter of $\tilde{N}$ measured particles is at the zero position. The studied system is the finite one-dimension system of Ref. [9]. We show that the conditional measurement increases the purity of the one-particle state above the symmetry breaking point. This suggests that we can describe the ground state with a superposition of Hartree-Fock states that differ by the barycenter position. With this ansatz, we introduce in Sec. III a modified Gross-Pitaevskii equation that gives results in agreement with a few-mode calculation. The superposition of Hartree-Fock states is considered also in Ref. [10], but in that case the Hartree-Fock state is evaluated by the Gross-Pitaevskii equation.

II. CONDITIONED ONE-PARTICLE DENSITY MATRIX

A finite one-dimensional system of free bosons with periodic boundary conditions can be obtained confining N bosons in a toroidal region, whose cross section S has a radius much smaller than the torus radius R. In the condensation regime, the particle interaction is well described by a contact potential, which is characterized by the s-wave scattering length a. We consider attractive interactions, i.e., a negative scattering length. The Hamiltonian is

$$\hat{\mathcal{H}} = \int_{-\pi}^{\pi} d\theta \left[-\hat{\psi}^\dagger(\theta)\frac{\partial^2}{\partial\theta^2}\hat{\psi}(\theta) + \frac{U}{2}\hat{\psi}^\dagger(\theta)\hat{\psi}^\dagger(\theta)\hat{\psi}(\theta)\hat{\psi}(\theta)\right], \tag{1}$$

where $U=8\pi aR/S$, θ is the azimuthal angle and the energy is measured in units of $\hbar^2/(2mR^2)$. The system is characterized by the parameter U. In the mean-field approximation, the condensate undergoes a symmetry breaking transition at $U=-\pi/N$. Introducing the rescaled parameter $\gamma\equiv UN/2\pi$, the transition occurs at $\gamma=-0.5$ [9].

Let us perform a position measurement on $\tilde{N}$ particles, denoting with x_0 the barycenter of the resulting values. We call $\hat{\rho}_{\tilde{N}}$ the conditioned density matrix of the remaining particles for $x_0=0$. To evaluate $\hat{\rho}_{\tilde{N}}$ we use a few-mode approximation. We consider, in this section, five modes, which give qualitatively good results for $|\gamma|\simeq 1$ [9]. Since the system is periodic with respect to the position variable θ, the definition of the barycenter is not trivial. Using the standard definition, the barycenter depends on the interval of definition of θ. Thus, we use an alternative approach. Let $\theta_{1,\ldots,\tilde{N}}$ be a set of values of θ, with $\theta_1\leqslant\theta_2\leqslant\cdots\theta_{\tilde{N}}$, and $\bar{\theta}_k$ their mean value, with the first k values shifted by 2π. The barycenter of $\theta_{1,\ldots,\tilde{N}}$ is, by definition, $\bar{\theta}\equiv(\bar{\theta}'+\pi)\mathrm{mod}(2\pi)-\pi$, where $\bar{\theta}'$ is the value $\bar{\theta}_k$ with smallest mean square distance from $\theta_1+2\pi,\ldots,\theta_k+2\pi,\theta_{k+1},\ldots,\theta_{\tilde{N}}$. If two or more values $\bar{\theta}_k$ minimize this distance, then the barycenter is not defined. The outcomes with undefined barycenter do not contribute to $\hat{\rho}_{\tilde{N}}$. It is clear that if a bright soliton is present, then the barycenter of $\tilde{N}$ measured values $\theta_{1,\ldots,\tilde{N}}$ is a good estimate of the soliton center. This is not true in case of the standard definition. Consider, for example, an atomic distribution centered in π; then $\tilde{N}$ measured values $\theta_{1,\ldots,\tilde{N}}$ have a mean value around zero, not π or, equivalently, $-\pi$.

The conditioned one-particle density matrix is

$$\rho_{\tilde{N}}(x_1,x_2) \equiv K_0\int_{-\pi/2}^{\pi/2} d\theta_1\cdots\int_{-\pi/2}^{\pi/2} d\theta_{\tilde{N}}\langle\Psi|\hat{\psi}^\dagger[x_1-B(\vec{\theta})] \times[\Pi_{k=1}^{\tilde{N}}\hat{\psi}^\dagger(\theta_k)][\Pi_{l=1}^{\tilde{N}}\hat{\psi}(\theta_l)]\hat{\psi}[x_2-B(\vec{\theta})]|\Psi\rangle, \tag{2}$$

where $B(\vec{\theta})$ is the barycenter of $\theta_1,\ldots,\theta_{\tilde{N}}$, as defined previously, and K_0 is a normalization constant.

This density matrix is obtained when the position of $\tilde{N}$ particles is measured and only their barycenter position is retained. We want to evaluate the highest eigenvalue λ_0 of $\rho_{\tilde{N}}(x_1,x_2)$ in order to know the degree of purity of the matrix conditioned by the barycenter measurement of $\tilde{N}$ particles. We could also be interested in the highest eigenvalue of the reduced density matrix when every measured position is retained. In general, the average of these eigenvalues, say $\bar{\lambda}$, is not equal to λ_0. However, it is possible to demonstrate that $\bar{\lambda}\geqslant\lambda_0$.

Let θ_B be the barycenter of the $\tilde{N}$ measured particles and $\vec{y}$ the remaining independent variables. We can write the density operator as follows:

$$\hat{\rho} = \int dy_1\, d\theta_B^1\, dy_2\, d\theta_B^2 c_{\vec{y}_1,\theta_B^1} c^*_{\vec{y}_2,\theta_B^2}\hat{\chi}(\vec{y}_1,\vec{y}_2,\theta_B^1,\theta_B^2),$$

where

$$\hat{\chi}(\vec{y}_1,\vec{y}_2,\theta_B^1,\theta_B^2) = |\theta_B^1\rangle|\vec{y}_1\rangle|\psi(\vec{y}_1,\theta_b^1)\rangle\langle\psi(\vec{y}_2,\theta_b^2)|\langle\vec{y}_2|\langle\theta_B^2|.$$

We have that

$$\rho_{\tilde{N}} = \mathrm{Tr}_{\vec{y}}\,\mathrm{Tr}_R[\langle\theta_B=0|\hat{\rho}|\theta_B=0\rangle] = \int dy c_{\vec{y},0}c^*_{\vec{y},0}\hat{\rho}(\vec{y}),$$

where $\hat{\rho}(\vec{y})=K_2\,\mathrm{Tr}_R[|\psi(\vec{y},0)\rangle\langle\psi(\vec{y},0)|]$ and $K_2\equiv[\mathrm{Tr}\langle\theta_B=0|\hat{\rho}|\theta_B=0\rangle]^{-1}$. Tr_R is the trace on all the unmeasured variables except one. The highest eigenvalue is λ_0. We indicate the highest eigenvalue of $\hat{\rho}(\vec{y})$ with $\lambda[\hat{\rho}(\vec{y})]$. Let $|\lambda_0\rangle$ be the eigenvector of $\hat{\rho}_{\tilde{N}}$ with eigenvalue λ_0. It follows that

$$\lambda_0 = \langle\lambda_0|\hat{\rho}_{\tilde{N}}|\lambda_0\rangle = \int dy\, c_{\vec{y},0}c^*_{\vec{y},0}\langle\lambda_0|\hat{\rho}(\vec{y})|\lambda_0\rangle \leqslant \int dy\, c_{\vec{y},0}c^*_{\vec{y},0}\lambda[\hat{\rho}(\vec{y})] = \bar{\lambda}.$$

This result is intuitive, since $\rho_{\tilde{N}}$ is obtained by retaining only the barycenter information, whereas the information on the other variables would increase the purity of the reduced matrix. We will show that the information on the barycenter is sufficient to remarkably increase the purity of the system.

The ground state $|\Psi\rangle$ is evaluated using a few modes in the momentum space. The field operator $\hat{\psi}$ can be written as a function of the annihilation operators of the momentum modes. The reduced density matrix ρ can be evaluated with a Monte Carlo integration [15], but this method is inefficient for large $\tilde{N}$ and far from the symmetry breaking point, since

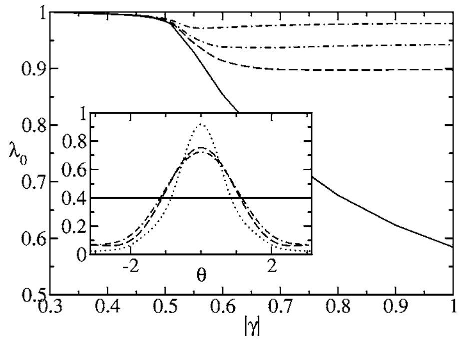

FIG. 1. The largest eigenvalue of the conditioned one-particle matrix as a function of $|\gamma|$ for $N=100$, with the conditional measurement of $\tilde{N}=0$ (solid line), 2 (dashed line), 4 (dotted-dashed line) and 12 (dotted-dashed-dashed line) atoms. In the inset, we report the corresponding eigenvectors for $|\gamma|=1$ and for $\tilde{N}=0$ (uniform distribution), $\tilde{N}=2$ (dotted-dashed-dashed line) and $\tilde{N}=12$ (dashed line). We also report the wave function evaluated with the Gross-Pitaevskii equation (dotted line).

the region of the parameter space where the integrand is not nearly zero is very small. In order to evaluate $\rho_{\tilde{N}}$, first we calculate the conditioned density matrix $\rho_{\tilde{N}}$ for $\tilde{N}=1$ and $\theta_1=0$. The diagonal elements give the probability density, say $D_1(\theta)$, of a particle when one atom is found in 0. At this point we generate stochastically the value θ_2 with the probability distribution D_1 and we evaluate the conditioned density matrix for $\tilde{N}=2$. The diagonal elements $D_2(\theta)$ are again used to generate the value θ_3. The difference between D_n and D_{n+1} is already small for $n=2$, thus, we have used, in practice, D_2 for θ_n, with $n>2$. The generated values for θ_i are put in the expression (2) with the weight $[D_1(\theta_2)D_2(\theta_3)\cdots]^{-1}$. The average of the obtained quantity over many realizations gives, with a suitable normalization, $\rho_{\tilde{N}}$.

In Fig. 1, we report the largest eigenvalue λ_0 of the conditioned density matrix as a function of $|\gamma|$, for $\tilde{N}=0$, 2, 4, and 12. The total number of atoms is 100. In the inset, we plot the corresponding eigenvectors for $\tilde{N}=0$, 2, and 12, and the wave function evaluated with the Gross-Pitaevskii equation. Below $|\gamma|=0.5$, λ_0 is nearly equal to 1, i.e., there is a macroscopically populated state whose relative population is nearly equal to 1. For $\tilde{N}=0$, the eigenvalue decreases above $|\gamma|=0.5$, i.e., the condensate disappears. However, the conditional measurement partially restores the macroscopic state. Around $|\gamma|=0.5$ the barycenter measurement has nearly no effect on λ_0. Indeed, the soliton being quasiuniform, the conditional measurement is less selective. Furthermore, around $|\gamma|=0.5$ large fluctuations of the width cannot be lowered by a barycenter measurement. Since there is an entanglement between the atoms, the measurement of the barycenter of $\tilde{N}$ atoms determines the position of the remaining ones with an uncertainty, shrinking increasing $\tilde{N}$. For this reason, the purity of the conditioned density matrix increases when a higher number of atoms is measured.

Thus, the one-dimensional boson gas with attractive interaction and above the critical symmetry breaking point, has no long-range order, however, the state can be considered a superposition of many condensates with different barycenter. If we perform a measurement on the system, we find a coherent soliton and if we split it, the daughter solitons exhibit interference when they overlap. In this sense, the condensate is present, even though the one-particle density matrix is not pure.

III. SUPERPOSITION OF HARTREE-FOCK STATES

The previous results suggest that the ground state of the system can be described by the superposition of Hartree-Fock states that differ by the barycenter position. We consider the following N-body wave function:

$$\Psi(x_1,x_2,\ldots,x_N) = \int \phi(y)\psi(x_1-y)\psi(x_2-y)\cdots\psi(x_N-y)d^3y, \quad (3)$$

where ϕ is a suitable function. For the ground state, it is reasonable to take ϕ as a constant. Note that the whole set of Hartree-Fock functions is an overcomplete basis of the N-particle Hilbert space [16]. With Eq. (3), we have chosen to represent the state as a superposition of products of functions that differ only in position; it amounts to assuming that the absence of a pure condensate is due mainly to quantum fluctuations of the barycenter. This ansatz is also considered in Ref. [10] for an infinite system, but in that case ψ is evaluated by the Gross-Pitaevskii equation. Here, the function ψ is obtained minimizing the expectation value of energy and it is a solution of a modified Gross-Pitaevskii equation.

The Hamiltonian (1) becomes, in the particle representation,

$$H=\sum_{i=1}^{N}\frac{\partial^2}{\partial\theta_i^2}+\frac{U}{2}\sum_{i\neq j}\delta(\theta_i-\theta_j). \quad (4)$$

The energy expectation value of the state (3) is

$$\langle H\rangle = -NK\int_{-\pi}^{\pi}dy\int_{-\pi}^{\pi}dx\,\psi''(x)\psi(x-y)g_{N-1}(y) + N(N-1)K\frac{U}{2}\int_{-\pi}^{\pi}dy\int_{-\pi}^{\pi}dx\,\psi^2(x)\psi^2(x-y)g_{N-2}(y), \quad (5)$$

where $g_k(y)=[\int_{-\pi}^{\pi}dx_1\psi^*(x_1)\psi(x_1-y)]^k$ and

$$K=\left[\int_{-\pi}^{\pi}dy\,g_N(y)\right]^{-1}. \quad (6)$$

$[K/(2\pi)]^{1/2}$ is the normalization factor of the state (3) when $\phi(y)\equiv 1$.

The state with minimum energy satisfies the equation

$$\int_{-\pi}^{\pi} dy \Bigg\{ -\psi''(\theta-y) g_{N-1}(y) - (N-1)\psi(\theta-y) g_{N-2}(y) \times \int_{-\pi}^{\pi} dx_1\, \psi^*(x_1)\psi''(x_1-y) + (N-1) g \Bigg[\psi(\theta-y)^2 \times \psi^*(\theta) g_{N-2}(y) + \frac{N-2}{2}\psi(\theta-y)\int_{-\pi}^{\pi} dx_1\, \psi^*(x_1)^2 \times \psi(x_1-y)^2 g_{N-3}(y) \Bigg] - \epsilon\psi(\theta-y) g_{N-1}(y) \Bigg\} = 0, \quad (7)$$

where ϵ is a Lagrange multiplier, introduced because of the normalization condition of the N-particle wave function. In the presence of a soliton, $g_k(y)$ becomes a Dirac delta for $k\to\infty$, apart from a normalization constant. Thus, in the limit $N\to\infty$, $\langle H\rangle$ approaches the mean-field value and the minimal energy function is given by the Gross-Pitaevskii equation. In order to find the minimal energy state, we have used the conjugate gradient method of Ref. [15] (see Sec. 10.6, p. 317).

The first-order correlation function is

$$C(\theta,\theta') \equiv \frac{1}{2\pi}\int_{-\pi}^{\pi} dx_0 \int_{-\pi}^{\pi} dy_0\, \psi^*(\theta-x_0) \times \psi(\theta'-x_0-y_0) g_{N-1}(y_0) \Bigg/ \int_{-\pi}^{\pi} dy_1\, g_N(y_1). \quad (8)$$

We have evaluated the eigenvalues of the one-particle density matrix with the state (3). In Fig. 2 the highest eigenvalue is reported as a function of U for $N=5$, 10, and 15. We have also evaluated the values with a few-mode approach (circles), that is, we have considered a few modes of the field in the momentum space and we have found the minimal energy state in the corresponding Hilbert subspace. Also in this case, we have used the conjugate gradient method. From the ground state, we have obtained the one-particle density matrix and we have found its eigenvalues (the matrix rank is equal to the number of modes). The number of modes is between 11 and 15 for $N=10,15$. For $N=5$ and high values of U, we have used up to 17–19 modes. The dashed lines have been obtained with a superposition of Hartree-Fock states that have been evaluated via the Gross-Pitaevskii equation

$$-\psi''_{GP}(\theta) + (N-1)U|\psi_{GP}(\theta)|^2\psi_{GP}(\theta) = E\psi_{GP}(\theta), \quad (9)$$

as done in Ref. [10] for an infinite system. Note that in the nonlinear term $N-1$ is present, not N, and the symmetry breaking for ψ_{GP} is at $|\gamma|=0.5N/(N-1)$. Below this value, the ψ_{GP} is constant and, consequently, the superposition of Hartree-Fock states is a constant N-body function. The one-particle density matrix has an eigenvalue equal to 1. Indeed, the few-mode approach shows that it is not the case. The macroscopic population begins to decrease when the attractive interaction grows, also below the critical point. The variation approach with the ansatz (3) is able to reproduce this behavior with good precision. The number of used modes is less than 20 in the few-mode approach; above this value the required computer memory and evaluation time become too large. Thus, it is not possible to use the few-mode approximation for $|\gamma|>1$. Around the transition point the two approaches give slightly different results. We have noted that this discrepancy increases for a high number of atoms. It is likely due to fluctuations of the soliton shape. We have also tested the variational approach for repulsive interactions. It gives constant wave functions and the one-particle density matrix has one eigenvalue equal to 1 (pure matrix). Indeed, the ansatz in Eq. (3) is a bunched state, but with repulsive interactions the ground state is antibunched. Thus, the considered ansatz is not suitable in the repulsive case.

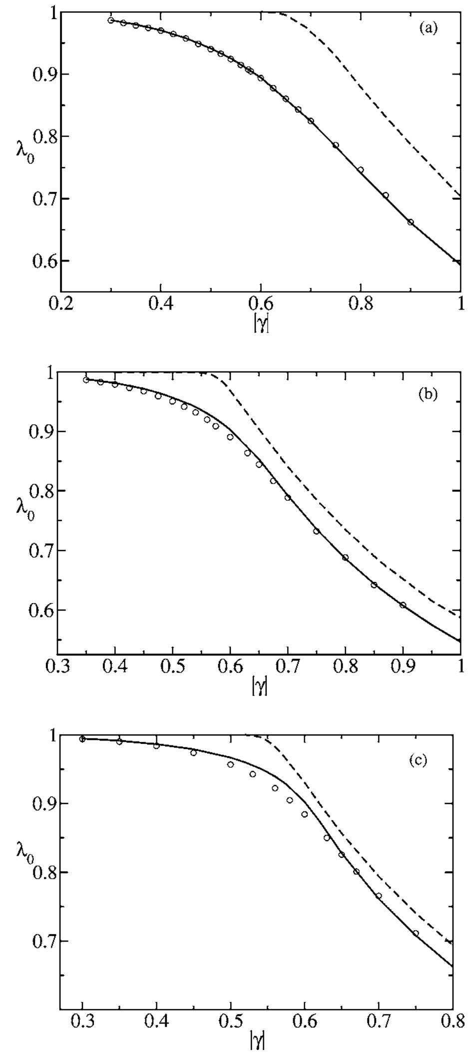

FIG. 2. The highest eigenvalue of the one-particle density matrix as a function of $|\gamma|$, evaluated using the modified Gross-Pitaevskii (solid line), the Gross-Pitaevskii (dashed line) and the few-mode approach (circles). (a) $N=5$, (b) $N=10$, (c) $N=15$.

IV. CONCLUSION

Above a critical interaction strength, a one-dimensional condensate with attractive interaction undergoes a symmetry breaking with the formation of a spatial bright soliton in the mean-field framework. This transition implies that for the many-body ground state the macroscopic population of a single one-particle state decreases above the critical point and the condensate disappears. We have shown that, in a certain sense, the condensate is present, even above the critical point, i.e., the ground state is given approximatively by the superposition of peaked condensates with different central positions. A conditional measurement selects one soliton of the superposition. We have shown that the system conditioned by the barycenter measurement has a long-range order and the one-particle density matrix is nearly pure, even above the critical point. Then, we have considered a superposition of Hartree-Fock states that differ in the barycenter position and have evaluated the minimal energy state. This state is given by a modified Gross-Pitaevskii equation. Our simulations are in very good agreement with a few-mode approach. The superposition state is given by the many-body function of Eq. (3). It is remarkable that a variational approach where the parameter is a one-dimensional field is able to describe a many-body problem that has no macroscopic order parameter. Near the transition point there is a slight difference between the results of the few-mode calculations and the variational approach. This discrepancy increases for large numbers of atoms. It is likely due to fluctuations of the soliton shape. A superposition of Hartree-Fock states that differ also in their width can increase the precision of the variational approach.

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