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Density-functional theory of bosons in a trap

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A time-dependent Kohn-Sham-(KS)-like theory is presented for N bosons in three- and lower-dimensional traps. We derive coupled equations, which allow us to calculate the energies of elementary excitations. A rigorous proof is given to show that the KS-like equation correctly describes the properties of one-dimensional impenetrable bosons in a general time-dependent harmonic trap in the large- N limit.

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The recently reported Bose-Einstein condensates (BEC's) of weakly interacting alkali-metal atoms [1] stimulated a large number of theoretical investigations (see recent reviews [2]). Most of this work is based on the assumption that the properties of the BEC are well described by the Gross-Pitaevskii (GP) mean-field theory [3]. The validity of the GP equation is nearly universally accepted.

The experimental realization of quasi-one-dimensional (1D) and quasi-two-dimensional (2D) trapped gases [4–6] stimulated much theoretical interest. The theoretical aspects of BEC's in quasi-1D and quasi-2D traps have been reported in many papers [7–17]. For the case of dimensions $d < 3$, it is known that the quantum-mechanical two-body t matrix vanishes [18] at low energies. Therefore, the replacement of the two-body interaction by the t matrix, as is done in deriving the GP mean-field theory, is not correct in general for $d < 3$ [12,19].

The density-functional theory (DFT), originally developed for interacting systems of fermions [20], provides a rigorous alternative approach to interacting inhomogeneous Bose gases [21,22]. The main goal of this Brief Report is to develop a Kohn-Sham-(KS)-like time-dependent theory for bosons.

We consider a system of N interacting bosons in a trap potential V_{ext} . Assuming that our system is in local thermal equilibrium at each position $\vec{r}$ with the local energy per particle $\epsilon(n)$ (ϵ is the ground-state energy per particle of the homogeneous system and n is the density), we can write a zero-temperature classical hydrodynamics equation as [8]

$$\partial n / \partial t + \vec{\nabla} \cdot (n \vec{v}) = 0, \quad (1)$$

$$\partial \vec{v} / \partial t + (1/m) \vec{\nabla} (V_{\text{ext}} + \partial[n\epsilon(n)]/\partial n + \frac{1}{2} m v^2) = 0, \quad (2)$$

where $\vec{v}$ is the velocity field.

Adding the kinetic energy pressure term, we have

$$\frac{\partial \vec{v}}{\partial t} + \frac{1}{m} \vec{\nabla} \left(V_{\text{ext}} + \frac{\partial[n\epsilon(n)]}{\partial n} + \frac{1}{2} m v^2 - \frac{\hbar^2}{2m} \frac{1}{\sqrt{n}} \nabla^2 \sqrt{n} \right) = 0. \quad (3)$$

We define the density of the system as $n(\vec{r}, t) = |\Psi(\vec{r}, t)|^2$, and the velocity field $\vec{v}$ as $\vec{v}(\vec{r}, t) = \hbar(\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) / [2imn(\vec{r}, t)]$.

From Eqs. (1) and (3), we obtain the following KS-like time-dependent equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V_{\text{ext}} \Psi + \frac{\partial[n\epsilon(n)]}{\partial n} \Psi \quad (4)$$

in the adiabatic local-density approximation (ALDA).

We note here that the current-density-functional theory (CDFT) for fermions, which goes beyond the ALDA, was formulated in Ref. [23]. In our future work, we will also consider the CDFT for bosons.

If the trap potential V_{ext} is independent of time, one can write the ground-state wave function as $\Psi(\vec{r}, t) = \Phi(\vec{r}) \exp(-i\mu t/\hbar)$, where μ is the chemical potential, and Φ is normalized to the total number of particles, $\int d\vec{r} |\Phi|^2 = N$. Then Eq. (4) becomes

$$\{-\hbar^2/2m \nabla^2 + V_{\text{ext}} + \partial[n\epsilon(n)]/\partial n\} \Phi = \mu \Phi, \quad (5)$$

where the solution of Eq. (5) minimizes the KS energy functional in the local-density approximation $E = N \langle \Phi | (\hbar^2/2m) \nabla^2 + V_{\text{ext}} + \epsilon(n) | \Phi \rangle$, and the chemical potential μ is given by $\mu = \partial E / \partial N$. Equation (5) has the form of the KS equation.

The ground-state energy per particle of the homogeneous system $\epsilon(n)$ for dilute 3D [24] and dilute 2D [25] Bose gases is

$$\begin{aligned} \epsilon(n) = & (2\pi\hbar^2/m) a_{3D} n [1 + (128/15\sqrt{\pi}) (na_{3D}^3)^{1/2} \\ & + 8(4\pi/3 - \sqrt{3}) na_{3D}^3 \ln(na_{3D}^3) + \dots], \end{aligned} \quad (6)$$

and

$$\epsilon(n) = \frac{2\pi\hbar^2 n}{m} |\ln(na_{2D}^2)|^{-1} [1 + O(|\ln(na_{2D}^2)|^{-1/5})], \quad (7)$$

where a_{3D} and a_{2D} are the 3D and 2D scattering lengths, respectively.

For a 1D Bose gas interacting via a repulsive δ -function potential $\tilde{g}\delta(x)$, $\epsilon(n)$ is given by [26] $\epsilon(n) = (\hbar^2/2m) n^2 e(\gamma)$, where $\gamma = m\tilde{g}/(\hbar^2 n)$ and for small val-

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ues of γ , the following expression for $\epsilon(n)$: $\epsilon(n) = (\tilde{g}/2)[n - (4/3\pi)\sqrt{m\tilde{g}n/\hbar^2} + \dots]$ is adequate up to approximately $\gamma = 2$ [26].

For a large coupling strength $\tilde{g}$ [26],

$$\epsilon(n) = (\hbar^2 \pi^2 n^2 / 6m) (1 + 2\hbar^2 n / m\tilde{g})^{-2}. \quad (8)$$

Equation (8) is accurate to 1% for $\gamma \geq 10$ [26].

For the 1D impenetrable boson case ($g \rightarrow \infty$) and for the dilute 2D boson case [$|\ln(na_{2D}^2)| \rightarrow \infty$], Eq. (4) is equivalent to the low-dimensional modifications of the GP equations, given by Ref. [12].

In the limit of large N , by neglecting the kinetic energy term in the KS equation (5), we obtain an equation corresponding to the Thomas-Fermi (TF) approximation

$$V_{\text{ext}} + \partial[n\epsilon(n)]/\partial n = \mu \quad (9)$$

in the region where $n(\vec{r})$ is positive and $n(\vec{r})=0$ outside this region.

Equation (5) can be written as the stationary GP equation with density-dependent coupling parameter $\{\partial[n\epsilon(n)]/\partial n\}/n$, and, for example, for a dilute 2D Bose gas, Eq. (7), the coupling parameter is $4\pi\hbar^2|m\ln(na_{2D}^2)|^{-1}$. This result agrees with energy-dependent T -matrix approach [27].

Now we turn our attention to elementary excitations, corresponding to small oscillations of $\Psi(\vec{r}, t)$ around the ground state. Elementary excitations can be obtained by standard linear response analysis [28,29] of Eq. (4), as resonances in the linear response. We add a weak sinusoidal perturbation to the time-dependent equation (4):

$$i\hbar \frac{\partial \Psi}{\partial t} = \left\{ -(\hbar^2/2m) \nabla^2 + V_{\text{ext}} + \partial[n\epsilon(n)]/\partial n + f_+ e^{-i\omega t} + f_- e^{i\omega t} \right\} \Psi, \quad (10)$$

and assume that the solution of Eq. (10) has the following form:

$$\Psi(\vec{r}, t) = e^{-i\mu t/\hbar} [\Phi(\vec{r}) + u(\vec{r})e^{-i\omega t} + v^*(\vec{r})e^{i\omega t}], \quad (11)$$

where $\Phi(\vec{r})$ is the ground-state solution of Eq. (5).

Linearization in the small amplitudes u and v yields the inhomogeneous equations

$$(L - \hbar\omega)u + \{\partial^2[n\epsilon(n)]/\partial n^2\} \Phi^2 v = -f_+ \Phi, \quad (12)$$

$$(L + \hbar\omega)v + \{\partial^2[n\epsilon(n)]/\partial n^2\} \Phi^{*2} u = -f_- \Phi,$$

where $n = |\Phi(\vec{r})|^2$ and

$$L = -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}} - \mu + \frac{\partial[n\epsilon(n)]}{\partial n} + \frac{\partial^2[n\epsilon(n)]}{\partial n^2} n. \quad (13)$$

Setting $f_{\pm}$ to zero in Eq. (12), we obtain the coupled equations

$$Lu + \{\partial^2[n\epsilon(n)]/\partial n^2\} \Phi^2 v = \hbar\omega u,$$

$$Lv + \{\partial^2[n\epsilon(n)]/\partial n^2\} \Phi^{*2} u = -\hbar\omega v, \quad (14)$$

which can be used to calculate the energies $\mathcal{E} = \hbar\omega$ of the elementary excitations. Equations (14) are reduced to the fourth-order differential equations for the functions $\eta_{\pm} = u \pm v$.

For the remainder of this paper, we will focus solely on the one-dimensional case. For low-energy excitations, $\mathcal{E} \ll \mu$, of a Bose gas in a 1D harmonic trap $V_{\text{ext}} = m\tilde{\omega}^2 x^2/2$, we obtain in the case of large N

$$\left(\frac{\partial^2[n\epsilon(n)]}{\partial n^2} n \right)^{1/2} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{\hbar^2}{2m} n^{-1/2} \frac{d^2 n^{1/2}}{dx^2} \right) \times \left(\frac{\partial^2[n\epsilon(n)]}{\partial n^2} n \right)^{1/2} \chi = \mathcal{E}^2 \chi, \quad (15)$$

where n is the solution of Eq. (9) and $\eta_{\pm} = \{n\partial^2[n\epsilon(n)]/(\partial n^2)\}^{\pm 1/2} \chi$. If

$$\epsilon(n) \propto n^{\delta}, \quad (16)$$

the solution of Eq. (15) has the form $\chi(\tilde{x}) = (1 - \tilde{x}^2)^{-1/2-1/(2\delta)} P(\tilde{x})$, where $\tilde{x} = x\sqrt{m\tilde{\omega}^2/(2\mu)}$ and $P(\tilde{x})$ satisfies the hypergeometric differential equation $\delta(1 - \tilde{x}^2)P'' - 2\tilde{x}P' + 2[\mathcal{E}/(\hbar\tilde{\omega})]^2 P = 0$. The solution of this equation can be written as the expansion $P(\tilde{x}) = \sum_{i=0}^{\infty} c_i \tilde{x}^i$, where the coefficients c_i satisfy the recurrence relation $c_{i+2} = c_i \{i(i-1)\delta + 2i - 2[\mathcal{E}/(\hbar\tilde{\omega})]^2\} / [(i+2)(i+1)\delta]$. The convergence condition at $\tilde{x}=1$ requires the termination of the expansion at $i=j$, and for the energy spectrum we have

$$(\mathcal{E}/\hbar\tilde{\omega})^2 = j/2[2 + \delta(j-1)]. \quad (17)$$

The spectrum Eq. (17) agrees with Ref. [30] where a similar expression was obtained based on the hydrodynamics approximation. In the case of $j=1$, we find $\mathcal{E} = \hbar\tilde{\omega}$ from Eq. (17), in agreement with the generalized Kohn theorem [31]. Note that, for impenetrable bosons $\delta=2$, Eq. (17) reduces to the exact excitation spectrum of the harmonically trapped 1D ideal Fermi gas, $\mathcal{E} = j\hbar\tilde{\omega}$.

Now we describe the application of the time-dependent equation (4) to the case of nonlinear dynamics. We turn to the limit of very strong coupling between the interacting bosons in 1D, the so-called Tonks-Girardeau gas [32]. In this impenetrable boson case, the energy density $\epsilon(n)$ reduces to $\epsilon(n) = \hbar^2 \pi^2 n^2 / 6m$, and Eq. (4) reads [12]

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_{\text{ext}} + \frac{\hbar^2 \pi^2}{2m} |\Psi|^4 \right) \Psi, \quad (18)$$

with $\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx = N$.

For a general time-dependent harmonic trap $V_{\text{ext}} = m\omega^2(t)x^2/2$, with the initial condition $\Psi(x, 0) = \Phi(x)$, where $\Phi(x)$ is the ground-state solution of the time-independent equation

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2(0)x^2}{2} + \frac{\hbar^2 \pi^2}{2m} |\Phi|^4 \right) \Phi = \mu \Phi, \quad (19)$$

Eq. (18) reduces to the ordinary differential equation, which can provide the exact solution of Eq. (18).

Indeed, if we assume that the solution $\Psi(x, t)$ can be expressed as

$$\Psi(x, t) = \{\Phi[x/\lambda(t)]/\sqrt{\lambda(t)}\} e^{-i\beta(t) + im(x^2/2\hbar)(\dot{\lambda}/\lambda)}, \quad (20)$$

we obtain the following equations for λ and β after inserting Eq. (20) into Eq. (18):

$$\begin{aligned} \ddot{\lambda} + \omega^2(t)\lambda &= \omega^2(0)/\lambda^3, \quad \lambda(0)=1, \quad \dot{\lambda}(0)=0, \\ \dot{\beta} &= \mu/\hbar\lambda^2, \quad \beta(0)=0. \end{aligned} \quad (21)$$

Thus, the ordinary differential equations Eqs. (19) and (21) give the exact solution of Eq. (18), and the evolution of the density can be written exactly as

$$n(x, t) = [1/\lambda(t)]n(x/\lambda(t), 0). \quad (22)$$

For the case of free expansion, the confining potential is switched off at $t=0$ and the atoms fly away. In this case, Eqs. (21) can be integrated analytically, leading to the following solutions for λ and β : $\lambda(t) = \sqrt{1 + \omega^2(0)t^2}$, $\beta(t) = [\mu/\hbar\omega(0)]\arctan[\omega(0)t]$. We note that self-similar solutions [33] of Eq. (18) were discussed in Ref. [34] (see also Refs. [35]).

In the large- N limit, where the kinetic energy term in Eq. (19) is dropped altogether (the so-called Thomas-Fermi limit), the corresponding density is

$$n_{\text{TF}}(x, t) = \frac{1}{\pi\tilde{\lambda}(t)} \left[\left(2N - \frac{x^2}{\tilde{\lambda}^2(t)} \right) \right]^{1/2} \theta \left(2N - \frac{x^2}{\tilde{\lambda}^2(t)} \right), \quad (23)$$

and for the Fourier transform $n(k, t) = (1/\sqrt{2\pi}) \int_{-\infty}^{+\infty} n(x, t) e^{ikx} dx$ we have

$$n_{\text{TF}}(k, t) = (N/\sqrt{2\pi}) [2J_1(\sqrt{2N\tilde{\lambda}(t)}k)/\sqrt{2N\tilde{\lambda}(t)}k], \quad (24)$$

where $\tilde{\lambda}(t) = \{\hbar/[m\omega(0)]\}^{1/2}\lambda(t)$ and J_1 is the Bessel function of first order.

The exact many-body wave function $\Psi_B(x_1, x_2, \dots, x_N, t)$, of a system of N impenetrable bosons in a time-dependent 1D harmonic trap, can be found from the Fermi-Bose mapping [15] $|\Psi_B(x_1, x_2, \dots, x_N, t)| = |\Psi_F(x_1, x_2, \dots, x_N, t)|$, where Ψ_F is the fermionic solution of the time-dependent many-body Schrödinger equation

$$i\hbar \frac{\partial \Psi_F}{\partial t} = \sum_{i=1}^N \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{m\omega^2(t)x_i^2}{2} \right) \Psi_F \quad (25)$$

with initial condition $\Psi_F(x_1, x_2, \dots, x_N, 0) = \Phi_F(x_1, x_2, \dots, x_N)$, where $\Phi_F(x_1, x_2, \dots, x_N)$ is the fermionic ground-state solution of the time-independent Schrödinger equation

$$\sum_{i=1}^N \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{m\omega^2(0)x_i^2}{2} \right) \Phi_F = E\Phi_F.$$

Therefore, for the exact density $n_B(x, t) = \int_{-\infty}^{+\infty} dx_2 \cdots \int_{-\infty}^{+\infty} dx_N |\Psi_B(x, x_2, \dots, x_N, t)|^2$, we have

$$n_B(x, t) = \frac{1}{\tilde{\lambda}(t)} \sum_{i=0}^{N-1} \left| \phi_i \left(\frac{x}{\tilde{\lambda}(t)} \right) \right|^2, \quad (26)$$

where $\phi_i(x) = c_i \exp(-x^2/2) H_i(x)$, $c_i = \pi^{-1/4} (2^i i!)^{-1/2}$, and $H_i(x)$ are Hermite polynomials. Note that the evolution of $n_B(x, t)$ can be written as Eq. (22), corresponding to a time-dependent dilatation of the length scale.

From the knowledge of $n_B(x, t)$ and $n_{\text{TF}}(x, t)$ one can evaluate the radii $r(t) = [\int_{-\infty}^{+\infty} n_B(x, t) x^2 dx]^{1/2}$ and $r_{\text{TF}}(t) = [\int_{-\infty}^{+\infty} n_{\text{TF}}(x, t) x^2 dx]^{1/2}$ and the ratio $r(t)/n_{\text{TF}}(t)$. This quantity is equal to 1 at any t for any N . This circumstance explains why for a harmonic trap the ground-state density profile from Eq. (18) agrees well with the many-body results for systems with a rather small number of atoms $N \approx 10$ [12]. As for a general trap potential, we expect such agreement for much larger N . It was shown in Ref. [15] that Eq. (18) overestimates the interference between split condensates that are recombined at a small number of atoms ($N \approx 10$).

Using the relation [36]

$$\sum_{m=0}^n (2^m m!)^{-1} [H_m(x)]^2 = (2^{n+1} n!)^{-1} \{ [H_{n+1}(x)]^2 - H_n(x) H_{n+2}(x) \}, \quad (27)$$

we obtain an analytical formula for the exact density $n_B(x, t)$:

$$n_B(x, t) = [1/2\tilde{\lambda}(t)] c_{N-1}^2 e^{-x^2/\tilde{\lambda}^2(t)} \{ [H_N(x/\tilde{\lambda}(t))]^2 - H_{N-1}(x/\tilde{\lambda}(t)) H_{N+1}(x/\tilde{\lambda}(t)) \}. \quad (28)$$

Then the Fourier transform is given by

$$n_B(k, t) = \frac{1}{\sqrt{2\pi}} e^{-\tilde{\lambda}^2(t)k^2/4} \left[NL_N^{(0)}(\tilde{\lambda}^2(t)k^2/2) + \frac{\tilde{\lambda}^2(t)k^2}{2} L_{N-1}^{(2)}(\tilde{\lambda}(t)k^2/2) \right], \quad (29)$$

where $L_n^{(\alpha)}$ are Laguerre polynomials. Using an asymptotic formula of Hilb's type for the Laguerre polynomial [36], we have the asymptotic behavior of $n_B(k, t)$ as $N \rightarrow \infty$:

$$n_B(k, t) = (N/\sqrt{2\pi}) [2J_1(\sqrt{2N\tilde{\lambda}(t)}k)/\sqrt{2N\tilde{\lambda}(t)}k] + O(N^{1/4}), \quad (30)$$

which is valid uniformly in any bounded region of $k\tilde{\lambda}(t)$. Equation (30) for the case of $t=0$ is a rigorous justification of the Thomas-Fermi approximation [13,37] for a system of noninteracting 1D spinless fermions in harmonic trapping potentials.

Comparison of Eq. (30) with Eq. (24) shows that in the large- N limit the KS-like time-dependent theory for 1D impenetrable bosons in a time-dependent harmonic trap, Eq. (24), gives the same result as the exact many-body treatment, Eq. (30). Hence, we have rigorously proved that Eq. (24) correctly describes the properties of a 1D Bose gas in a time-dependent harmonic trap in the limit of large N . This is a *posteriori* justification of our approximations.

In conclusion, we have developed a time-dependent KS-like theory for bosons in three- and lower-dimensional traps. We have derived coupled equations that can be used to calculate the energies of elementary excitations and have shown that the energy spectrum provided by these equations for a

Bose gas in a 1D harmonic trap, Eq. (16), is the same as that found in the hydrodynamics approximation. For a one-dimensional condensate of impenetrable bosons in a general time-dependent harmonic trap, it is shown that the corresponding equation reduces to the ordinary differential equations and gives the same results as the exact many-body treatment in the large- N limit.

Note added. Recently, Ref. [38] appeared. The authors use a 1D nonlinear Schrödinger equation, which is equivalent to the 1D variant of Eq. (4), to analyze the expansion of a 1D Bose gas after removing the axial confinement.

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