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]

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

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

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

Adding the kinetic energy pressure term, we have

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

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:

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

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

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

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

$$\epsilon(n)=(2\pi\hbar^2/m)\,a_{3\text{D}}n[1+(128/15\sqrt{\pi})\,(na_{3\text{D}}^3)^{1/2}+8(4\pi/3-\sqrt{3})na_{3\text{D}}^3\ln(na_{3\text{D}}^3)+\cdots], \tag{6}$$

and

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

where $a_{3\text{D}}$ and $a_{2\text{D}}$ 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] $\epsilon(n)=(\hbar^2/2m)n^2e(\gamma)$, where $\gamma=m\tilde{g}/(\hbar^2n)$ and for small val-

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

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

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

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

For the 1D impenetrable boson case ($g\rightarrow\infty$) and for the dilute 2D boson case [$|\ln(na_{2\mathrm{D}}^2)|\rightarrow\infty$], 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

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

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 $4\pi\hbar^2|m\ln(na_{2\mathrm{D}}^2)|^{-1}$. 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):

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

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

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

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

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

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

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

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

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

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

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 $V_{\mathrm{ext}}=m\tilde{\omega}^2x^2/2$, we obtain in the case of large N

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

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

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

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 $\delta(1-\tilde{x}^2)P''-2\tilde{x}P'+2[\mathcal{E}/(\hbar\tilde{\omega})]^2P=0$. The solution of this equation can be written as the expansion $P(\tilde{x})=\Sigma_{i=0}^{\infty}c_i\tilde{x}_i$, 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

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

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 $\epsilon(n)=\hbar^2\pi^2n^2/6m$, and Eq. (4) reads [12]

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

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

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

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

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

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

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

$$\ddot{\lambda}+\omega^2(t)\lambda=\omega^2(0)/\lambda^3,\quad \lambda(0)=1,\quad \dot{\lambda}(0)=0,$$

$$\dot{\beta}=\mu/\hbar\lambda^2,\quad \beta(0)=0. \tag{21}$$

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

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

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

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

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

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

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

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

with initial condition $\Psi_F(x_1,x_2,\ldots,x_N,0)=\Phi_F(x_1,x_2,\ldots,x_N)$, where $\Phi_F(x_1,x_2,\ldots,x_N)$ 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 $n_B(x,t)=\int_{-\infty}^{+\infty}dx_2\cdots\int_{-\infty}^{+\infty}dx_N|\Psi_B(x,x_2,\ldots,x_N,t)|^2$, we have

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

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 $n_{\mathrm{TF}}(x,t)$ one can evaluate the radii $r(t)=[\int_{-\infty}^{+\infty}n_B(x,t)x^2dx]^{1/2}$ and $r_{\mathrm{TF}}(t)=[\int_{-\infty}^{+\infty}n_{\mathrm{TF}}(x,t)x^2dx]^{1/2}$ and the ratio $r(t)/n_{\mathrm{TF}}(t)$. 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 $N\approx10$ [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 ($N\approx10$).

Using the relation [36]

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

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

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

Then the Fourier transform is given by

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

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 $N\to\infty$:

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

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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