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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 $V_{\text{ext}}$. Assuming that our system is in local thermal equilibrium at each position $\vec{r}$ with the local energy per particle $\epsilon(n)$ (which 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]

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

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

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

Adding the kinetic energy pressure term, we have

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

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

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 $V_{\text{ext}}$ 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 $\mu$ is the chemical potential, and $\Phi$ is normalized to the total number of particles, $\int d\vec{r} |\Phi|^2 = N$. Then Eq. (4) becomes

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

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

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

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 $\delta$-function potential $\bar{g} \delta(x)$, $\epsilon(n)$ is given by [26] $\epsilon(n) = (\hbar^2/2m)n^2 \epsilon(\gamma)$, where $\gamma = mg/(\hbar^2 n)$ and for small val-
ues of $\gamma$, the following expression for $\epsilon(n)$: $\epsilon(n) = (\bar{g}/2)[n - (4/3\pi)\sqrt{m\bar{g}n/\hbar^2} + \cdots]$ is adequate up to approximately $\gamma = 2$ [26].

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

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

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

For the 1D impenetrable boson case ($\bar{g} \to \infty$) and for the dilute 2D boson case [$\ln(n\bar{a}^2_0) \to \infty$], 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 $n(\bar{r})$ is positive and $n(\bar{r}) = 0$ 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 $4\pi\hbar^2/m\ln(n\bar{a}^2_0)/n!$. This result agrees with energy-dependent $T$-matrix approach [27].

Now we turn our attention to elementary excitations, corresponding to small oscillations of $\Psi(\bar{r}, t)$ 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):

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

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

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

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

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

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

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

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

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

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

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 $n_\pm = u \pm v$.

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

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

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

$$\epsilon(n) \approx n\delta, \quad (16)$$

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

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

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

$$i\hbar \frac{d\Psi}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}} + \frac{\hbar^2\pi^2}{2m}|\Psi|^4\right] \Psi, \quad (18)$$

with $f^{+\pm}_\omega |\Psi(x, t)|^2dx = N$.

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

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

$$\Psi(x,t) = \left( \Phi \left[ x/\lambda(t) \right] / \sqrt{\lambda(t)} \right) e^{-i\beta(t) + i m (x^2/2\hbar)(\lambda/\hbar)},$$

we obtain the following equations for $\lambda$ and $\beta$ after inserting Eq. (20) into Eq. (18):

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

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

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

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 $\lambda$ and $\beta$: $\lambda(t) = \sqrt{1 + \omega^2(0)t^2}$, $\beta(t) = \mu/\hbar\omega(0)|\text{arctan}(|\omega(0)t)|$. We note that 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

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

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

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

where $\bar{\lambda}(t) = \{\hbar/|m\omega(0)|\}^{1/2}\lambda(t)$ 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] $|\Psi_B(x_1,x_2,\ldots,x_N,t)\rangle = |\Psi_F(x_1,x_2,\ldots,x_N,t)\rangle$, where $\Psi_F$ 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 $\Psi_F(x_1,x_2,\ldots,x_N,0) = \Phi_F(x_1,x_2,\ldots,x_N)$, where $\Phi_F(x_1,x_2,\ldots,x_N)$ is the fermionic ground-state solution of the time-independent Schrödinger equation

$$-\hbar^2 \frac{\partial^2}{\partial x_i^2} + \frac{m\omega^2(x_i^2)}{2} \Phi_F = E \Phi_F. \quad (26)$$

Therefore, for the exact density $n_B(x,t)$

$$n_B(x,t) = \int_{-\infty}^{\infty} dx_2 \cdots dx_N |\Psi_B(x,x_2,\ldots,x_N,t)|^2,$$

we have

$$n_B(x,t) = \frac{1}{\bar{\lambda}(t)} \sum_{l=0}^{N-1} \left| \Phi_l \left( \frac{x}{\bar{\lambda}(t)} \right) \right|^2 \quad (27)$$

with $\Phi_l(x) = c_l \exp(-x^2/2)H_l(x)$, $c_l = (-1)^{l/2}(2l)!^{-1/2}$, and $H_l(x)$ 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 $n_{TF}(x,t)$ one can evaluate the radii $r(t) = \{(\int_{-\infty}^{\infty} n_B(x,t)x^2 dx)^{-1/2} \}$ and $r_{TF}(t) = \{(\int_{-\infty}^{\infty} n_{TF}(x,t)x^2 dx)^{-1/2} \}$ and the ratio $r(t)/r_{TF}(t)$. 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 $N\approx 10$.

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]

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

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

$$n_B(x,t) = [1/2\bar{\lambda}(t)] c_{n-1} e^{-x^2/2\bar{\lambda}^2(t)} \left[ H_n(x/\bar{\lambda}(t)) \right]^2 - H_{n-1}(x/\bar{\lambda}(t))H_{n+1}(x/\bar{\lambda}(t)). \quad (28)$$

Then the Fourier transform is given by

$$n_B(k,t) = \frac{1}{\sqrt{2\pi}} e^{-\bar{\lambda}^2(t)k^2/2} \int \left[ N L_N^{(0)}(\bar{\lambda}^2(t)k^2/2) \right] \quad (29)$$

where $L_N^{(a)}$ 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 $N\to\infty$:

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

which is valid uniformly in any bounded region of $k\bar{\lambda}(t)$. 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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[18] See, for example, V. E. Barletta et al., Am. J. Phys. 69, 1010 (2001); S. K. Adhikari, ibid. 54, 362 (1986).
[38] P. Öhberg and L. Santos, e-print cond-mat/0204611.