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Time-dependent density-functional theory for superfluids

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Abstract. – A density-functional theory is established for inhomogeneous superfluids at finite temperature, subject to time-dependent external fields in isothermal conditions. After outlining parallelisms between a neutral superfluid and a charged superconductor, Hohenberg-Kohn-Sham–type theorems are proved for gauge-invariant densities and a set of Bogolubov-Popov equations including exchange and correlation is set up. Earlier results applying in the linear-response regime are recovered.

Experiments on confined Bose-condensed gases have revealed a rich variety of dynamical behaviours. These include elementary excitations of low-lying shape deformation modes [1], propagation of sound waves in both the condensate and the thermal cloud [2], Josephson-like oscillations in double condensates [3], creation of vortices [4], phase dynamics from various atom-laser configurations [5] and Bloch oscillations of a condensate in an optical lattice [6].

While mean-field theories suffice in most cases to describe the observed behaviours, condensates can now be created where effects beyond mean field can be explored, by tuning almost at will the scattering length and hence the condensate self-interaction energy [7] or else by approaching the critical temperature for Bose-Einstein condensation. Along these lines a Time-Dependent Density-Functional Theory (TD-DFT) for superfluids is a suitable framework to treat their dynamics with inclusion of exchange and correlation.

For a many-electron system in the normal state the foundations of the theory come from a set of theorems by Runge and Gross [8,9], which have been extended to superconductors at zero temperature by Wacker, Kümmel and Gross (WKG) [10]. In applications to normal electron systems in the linear-response regime, the limitations to low-frequency phenomena have been conceptually overcome by Vignale and Kohn [11]. Their current-density formulation of TD-DFT embodies plasmon dispersion and damping as well as transverse-current fluctuations, allows a unified treatment of the damping of collective excitations from the Landau and mode-coupling mechanisms and yields microscopic generalized-hydrodynamic equations [11, 12].

A similar scheme has already been developed for the dynamic linear response of superfluids [13], extending to inhomogeneous systems and to finite-frequency phenomena Landau's hydrodynamic equations in the two-fluid model. The present letter concerns the underlying foundations of TD-DFT for superfluids. The proof of the relevant Hohenberg-Kohn-Sham–type theorems parallels the WKG derivation for superconductors and one of our results is a "dictionary" which translates vector and scalar potentials, Maxwell equations and the like from a charged to a neutral fluid characterized by spontaneous symmetry breaking. We also allow for finite temperature in isothermal conditions. This preludes to a specific choice of the reference system for the TD-DFT mapping, which is described by a set of Bogolubov-Popov equations including the non-condensate density.

Introductory material. – The dynamics of a system of interacting spinless bosons confined in a static potential and evolving from an initial equilibrium state at time t_0 is driven by the Hamiltonian

$$\hat{H}(t) = \hat{T}_{\boldsymbol{A}}(t) + \hat{V}_V(t) + \hat{S}_\eta(t) + \hat{W}(t)\ . \tag{1}$$

The system is subject to an external vector potential $\boldsymbol{A}$ and to scalar fields V and η. We have $\hat{T}_{\boldsymbol{A}} = -(1/2m)\int \mathrm{d}\boldsymbol{r}\hat{\psi}^\dagger(\boldsymbol{r},t)\left[\hbar\boldsymbol{\nabla} - i\boldsymbol{A}(\boldsymbol{r},t)\right]^2\hat{\psi}(\boldsymbol{r},t)$, $\hat{V}_V = \int \mathrm{d}\boldsymbol{r}V(\boldsymbol{r},t)\hat{\psi}^\dagger(\boldsymbol{r},t)\hat{\psi}(\boldsymbol{r},t)$ and $\hat{S}_\eta = \int \mathrm{d}\boldsymbol{r}\left[\eta(\boldsymbol{r},t)\hat{\psi}^\dagger(\boldsymbol{r},t) + \eta^*(\boldsymbol{r},t)\hat{\psi}(\boldsymbol{r},t)\right]$ [14]. $\hat{W}(t)$ is the interaction term, given in terms of the field operators by $\hat{W}(t) = (1/2)\int \mathrm{d}\boldsymbol{r}_1\mathrm{d}\boldsymbol{r}_2\hat{\psi}^\dagger(\boldsymbol{r}_1,t)\hat{\psi}^\dagger(\boldsymbol{r}_2,t)w(\boldsymbol{r}_1,\boldsymbol{r}_2)\hat{\psi}(\boldsymbol{r}_2,t)\hat{\psi}(\boldsymbol{r}_1,t)$.

$\boldsymbol{A}$ couples to the total current density and V to the total particle density. After writing the ensemble average of the field operator as $\langle\hat{\psi}(\boldsymbol{r},t)\rangle = \sqrt{n_\mathrm{c}(\boldsymbol{r},t)}\exp[i\varphi(\boldsymbol{r},t)]$, we see that the symmetry-breaking source field η drives both the density of condensate $n_\mathrm{c}(\boldsymbol{r},t)$ and its phase $\varphi(\boldsymbol{r},t)$; the latter determines the irrotational part $\boldsymbol{v}_\mathrm{s}(\boldsymbol{r},t)$ of the velocity field through $\boldsymbol{v}_\mathrm{s}(\boldsymbol{r},t) = (\hbar/m)\boldsymbol{\nabla}\varphi(\boldsymbol{r},t)$. In the linear regime $\hat{S}_\eta$ we can write $\hat{S}_\eta = \int \mathrm{d}\boldsymbol{r}[\boldsymbol{\lambda}(\boldsymbol{r},t)\cdot\delta\hat{\boldsymbol{v}}_\mathrm{s}(\boldsymbol{r},t) + \alpha(\boldsymbol{r},t)\delta\hat{n}_\mathrm{c}(\boldsymbol{r},t)]$ in terms of the condensate-density operator $\delta\hat{n}_\mathrm{c}(\boldsymbol{r},t) = 2\mathrm{Re}[\langle\hat{\psi}(\boldsymbol{r},t_0)\rangle\delta\hat{\psi}^\dagger(\boldsymbol{r},t)]$ and of the irrotational-flow operator $\delta\hat{\boldsymbol{v}}_\mathrm{s}(\boldsymbol{r},t) = (\hbar/m)\boldsymbol{\nabla}\delta\hat{\varphi}$ with $\delta\hat{\varphi}(\boldsymbol{r},t) = -\mathrm{Im}[\delta\hat{\psi}^\dagger(\boldsymbol{r},t)/\langle\hat{\psi}^\dagger(\boldsymbol{r},t_0)\rangle]$. The (real) fields α and $\boldsymbol{\lambda}$ are then related to η by $\alpha(\boldsymbol{r},t) = [n_\mathrm{c}(\boldsymbol{r},t_0)]^{-1}\cdot \mathrm{Re}[\langle\hat{\psi}^\dagger(\boldsymbol{r},t_0)\rangle\eta(\boldsymbol{r},t)]$ and $\boldsymbol{\nabla}\cdot\boldsymbol{\lambda}(\boldsymbol{r},t) = -2m\mathrm{Im}[\langle\hat{\psi}^\dagger(\boldsymbol{r},t_0)\rangle\eta(\boldsymbol{r},t)]$ (see [14]).

The quantity needed to deal with time-dependent phenomena in DFT is the quantal action [8]. According to WKG, this is

$$Q \equiv \int_{t_0}^{\tau}\mathrm{d}t\left\langle\frac{i\hbar}{2}\int\mathrm{d}\boldsymbol{r}\left[\hat{\psi}^\dagger(\boldsymbol{r},t)\frac{\partial\hat{\psi}(\boldsymbol{r},t)}{\partial t} - \frac{\partial\hat{\psi}^\dagger(\boldsymbol{r},t)}{\partial t}\hat{\psi}(\boldsymbol{r},t)\right] - \hat{H}\right\rangle . \tag{2}$$

Following the well-known DFT argument, we shall prove below that the potentials are in one-to-one correspondence with appropriate gauge-invariant densities (Theorem I); that the action functional can be written in terms of these densities (Theorem II); and that a practical scheme can be given to map the interacting system into a non-interacting one driven by effective potentials which include exchange and correlation (Theorem III).

The action (2) is invariant under the gauge transformation $\boldsymbol{A}(\boldsymbol{r},t)\to\boldsymbol{A}(\boldsymbol{r},t)+\hbar\boldsymbol{\nabla}\Lambda(\boldsymbol{r},t)$ and $V(\boldsymbol{r},t)\to V(\boldsymbol{r},t)-\hbar\partial\Lambda(\boldsymbol{r},t)/\partial t$, where $\Lambda(\boldsymbol{r},t)$ is a real scalar function such that $\Lambda(\boldsymbol{r},t_0) = 0 \bmod (2\pi)$. The source function $\eta(\boldsymbol{r},t)$ transforms into $\eta(\boldsymbol{r},t)\exp[i\Lambda(\boldsymbol{r},t)]$, so that $\hat{S}_\eta$ is gauge invariant. The operators transform according to

$$\hat{\psi}(\boldsymbol{r},t)\to\hat{\psi}(\boldsymbol{r},t)\exp[i\Lambda(\boldsymbol{r},t)] \tag{3}$$

and

$$\hat{\boldsymbol{j}}(\boldsymbol{r},t)\to\hat{\boldsymbol{j}}(\boldsymbol{r},t)+(\hbar/m)\hat{\psi}^\dagger(\boldsymbol{r},t)\hat{\psi}(\boldsymbol{r},t)\boldsymbol{\nabla}\Lambda(\boldsymbol{r},t)\ , \tag{4}$$

with $\hat{\boldsymbol{j}}$ the paramagnetic current-density operator. We choose the following gauge-invariant densities: the current density $\boldsymbol{j}(\boldsymbol{r},t) = \langle\hat{\boldsymbol{j}}(\boldsymbol{r},t)\rangle - n(\boldsymbol{r},t)\boldsymbol{A}(\boldsymbol{r},t)/m$, the condensate density $n_\mathrm{c}(\boldsymbol{r},t) = |\langle\hat{\psi}^\dagger(\boldsymbol{r},t)\rangle|^2$ and the velocity field $\boldsymbol{v}_\mathrm{s}(\boldsymbol{r},t) = (\hbar/m)\boldsymbol{\nabla}\varphi(\boldsymbol{r},t) - \boldsymbol{A}(\boldsymbol{r},t)/m$. The total density $n(\boldsymbol{r},t)$ is not an independent quantity, since it is determined by the continuity equation. The pair of physical quantities $n_c(\boldsymbol{r},t)$ and $\boldsymbol{v}_s(\boldsymbol{r},t)$ can be replaced by the gauge-invariant order parameter $\Phi(\boldsymbol{r},t) = \langle\hat{\psi}(\boldsymbol{r},t)\rangle \exp[-(i/\hbar)\int_{t_0}^{t} dt' V(\boldsymbol{r},t')]$: we shall exploit this fact whenever convenient. Finally, we stress that $\boldsymbol{v}_s$ is the *irrotational* part of the velocity field.

The role of $\boldsymbol{A}$ *and* V. – We have already discussed the role of the source field η, which is characteristic of a neutral superfluid. Before proceeding to prove the TD-DFT theorems, we pause to discuss the physical import of the fields $\boldsymbol{A}$ and V entering the Hamiltonian (1). Their meaning is obvious for a superconductor, but needs elaboration for a superfluid. We use as a guideline for this purpose the linearized two-fluid model below threshold for vortex formation.

We consider first the vector potential $\boldsymbol{A}$. As pointed out by Baym while discussing the rotating-bucket experiment [15], what may create transverse currents in a superfluid is a spoon-stirring mechanism. Let $\boldsymbol{\omega}$ be the stirring angular velocity, with magnitude below the threshold ω_c for vortex formation. If $\boldsymbol{L} = m\boldsymbol{r}\times\boldsymbol{j}$ is the angular momentum, the corresponding Hamiltonian term can be written as $\int d\boldsymbol{r}\; \boldsymbol{\omega}\cdot\boldsymbol{L} = \int d\boldsymbol{r}\; \boldsymbol{j}\cdot(\boldsymbol{\omega}\times\boldsymbol{r})$. Comparing with the minimal coupling form $\boldsymbol{j}\cdot\boldsymbol{A}$ in the Hamiltonian (1), the component of $\boldsymbol{A}$ parallel to $\boldsymbol{j}$ is $\boldsymbol{A} = m\boldsymbol{\omega}\times\boldsymbol{r}$, namely with m times the rigid-body rotational velocity of the fluid. Since that part of the fluid which can respond to a transverse probe is by definition the normal-fluid component, $\boldsymbol{\omega}\times\boldsymbol{r}$ is the normal-fluid velocity $\boldsymbol{v}_n$ and thus $\boldsymbol{A} = m\boldsymbol{v}_n$. This result remains true for a non-rotating fluid, as demonstrated by Hohenberg and Martin by means of a Galileian transformation [14].

Let us turn to the scalar potential V. The quantity $V + \hbar\partial\varphi/\partial t$, with φ being the phase of the condensate, is gauge invariant. Therefore, writing the equations in the gauge in which the scalar potential vanishes corresponds to a Galileian transformation to a reference frame moving with velocity $\boldsymbol{v}_s$. This fact will be used in the proof of Theorem I below.

From the above arguments regarding the potentials $\boldsymbol{A}$ and V, it follows that $\partial(\boldsymbol{v}_n - \boldsymbol{v}_s)/\partial t = \partial\boldsymbol{A}/\partial t + \boldsymbol{\nabla}V/m$ and therefore is gauge invariant. In fact, in the two-fluid model (with $n = \rho_s + \rho_n$, ρ_s and ρ_n being the super- and normal-fluid densities) the gauge-invariant current density is $\boldsymbol{j}_r = \rho_s\boldsymbol{v}_s + \rho_n\boldsymbol{v}_n - n\boldsymbol{v}_n = \rho_s(\boldsymbol{v}_s - \boldsymbol{v}_n)$. This is the current as seen in a reference frame which moves with the normal-fluid component and determining one of the driving forces in the Landau-Khalatnikov equations [16].

We conclude by remarking that a parallel can be made between the two-fluid equations for neutral superfluids and Maxwell's equations for charged superconductors. From the above analysis it turns out that the equation $\boldsymbol{\nabla}\times(\boldsymbol{E}+c^{-1}\partial\boldsymbol{A}/\partial t) = 0$ or else $\boldsymbol{E}+c^{-1}\partial\boldsymbol{A}/\partial t = -\boldsymbol{\nabla}V$ is just the condition for irrotational flow. The "electric field" $\boldsymbol{E}$ is identified with $(m/\rho_s)\partial\boldsymbol{j}_r/\partial t$. As expected, the Maxwell equation for $\boldsymbol{\nabla}\times\boldsymbol{B}$ expresses the relation of continuity between particle and current densities.

After this excursus we return to the basic theorems of TD-DFT for neutral superfluids.

Theorem I. – It states that the densities $\{d\} \equiv \{\boldsymbol{j}(\boldsymbol{r},t), \Phi(\boldsymbol{r},t)\}$ are uniquely related to the potentials $\{p\} \equiv \{\boldsymbol{A}(\boldsymbol{r},t), V(\boldsymbol{r},t), \eta(\boldsymbol{r},t)\}$. One has to show that two sets of potentials $\{p\}$ and $\{p'\}$, which differ by more than a gauge transformation and can be expanded in Taylor series around t_0, determine two different sets of densities $\{d\}$ and $\{d'\}$ evolving from a common initial equilibrium state. While the statement is trivially true at time t_0, it is sufficient to prove it at some time t infinitesimally later than t_0 by relating the coefficients of the Taylor series for the densities to those for the potentials [8].

We thus consider the Heisenberg equations of motion for the densities. The potentials contribute to the equation for the induced current j_α with terms including $n\nabla_\alpha V$, $A_\beta\nabla_\beta j_\alpha$, $j_\beta\nabla_\alpha A_\beta$, $j_\alpha\nabla_\beta A_\beta$, and $(\hbar n/m)A_\beta\nabla_\alpha A_\beta$. It is evident that the proof will be easier in a reference frame moving with velocity $\mathbf{v}_s$: in this gauge, as already remarked, the scalar potential vanishes and $\boldsymbol{j}$ and $\boldsymbol{A}$ are both transverse, so that all the above terms vanish. We proceed within this gauge, signalled henceforth by a tilde on the potentials.

Since the two sets of potentials are different, their Taylor-expansion coefficients must differ at some order, say l for $\tilde{A}$ and $\tilde{A}'$ and l' for $\tilde{\eta}$ and $\tilde{\eta}'$. It is then sufficient to show, for the lower among l and l', that different coefficients in the expansion of the potentials imply different coefficients in the expansion of the densities [8–10]. In the case $l < l'$ we have

$$\frac{\partial^l}{\partial t^l}\left[\boldsymbol{j}(\boldsymbol{r},t)-\boldsymbol{j}'(\boldsymbol{r},t)\right]_{t=t_0}=\frac{n(\boldsymbol{r},t_0)}{m}\frac{\partial^l}{\partial t^l}\left[\tilde{A}(\boldsymbol{r},t)-\tilde{A}'(\boldsymbol{r},t)\right]_{t=t_0}, \tag{5}$$

while in the case $l > l'$ we have

$$i\hbar\frac{\partial^{l'+1}}{\partial t^{l'+1}}\left[\Phi(\boldsymbol{r},t)-\Phi'(\boldsymbol{r},t)\right]_{t=t_0}=\frac{\partial^{l'}}{\partial t^{l'}}\left[\tilde{\eta}(\boldsymbol{r},t)-\tilde{\eta}'(\boldsymbol{r},t)\right]_{t=t_0}. \tag{6}$$

As a consequence of eqs. (5) and (6), the set of densities $\{d\}$ will differ from $\{d'\}$ at times infinitesimally later than t_0. Hence they are different. This proves Theorem I.

The conclusion thus is that in a superfluid the potentials are unique functionals of the densities. Since from the Heisenberg equations of motion the field operators are functionals of the potentials, we may state that the ensemble expectation value of any gauge-invariant operator is a unique functional of the chosen set of densities.

Theorem II. – It states that i) the action Q in given external potentials can be expressed as a unique functional $Q^0[\{d\}]$ of the densities $\{d\}$ where the superscript 0 indicates the external potentials; and ii) $Q^0[\{d\}]$ is stationary with respect to the actual densities $\{d^0\}$ of the interacting system. The proof precisely parallels that given by WKG for superconductors, once their complex gap function $\Delta(\boldsymbol{r},t)$ is replaced by $\Phi(\boldsymbol{r},t)$ or by the subset $\{n_c(\boldsymbol{r},t),\boldsymbol{v}_s(\boldsymbol{r},t)\}$.

The functional is given by

$$Q^0[\{d\}]=R[\{d\}]-W[\{d\}]-P^0[\{d\}]-S^0[\{d\}], \tag{7}$$

where

$$R[\{d\}]\equiv(1/2)\int_{t_0}^{t}\mathrm{d}t'\int\mathrm{d}\boldsymbol{r}\langle\hat{\psi}^\dagger[\{d\}]\left[(i\hbar\partial/\partial t')-(\hbar^2/2m)\nabla^2\right]\hat{\psi}[\{d\}]\rangle+\text{c.c.} \tag{8}$$

and $W[\{d\}]\equiv\int_{t_0}^{t}\mathrm{d}t'\langle\hat{W}[\{d\}](t')\rangle$ are its universal parts, while

$$\begin{aligned}P^0[\{d\}] \equiv& \int_{t_0}^{t}\mathrm{d}t'\int\mathrm{d}\boldsymbol{r}\left[\left(V^0(\boldsymbol{r},t')+\frac{1}{2m}{A^0}^2(\boldsymbol{r},t')\right)n[\{d(\boldsymbol{r},t')\}]+\right.\\ &\left.+\boldsymbol{A}^0(\boldsymbol{r},t')\cdot(\boldsymbol{j}(\boldsymbol{r},t')-n[\{d(\boldsymbol{r},t')\}]\boldsymbol{A}[\{d(\boldsymbol{r},t')\}]/m)\right]\end{aligned} \tag{9}$$

and

$$S^0[\{d\}]\equiv\int_{t_0}^{t}\mathrm{d}t'\int\mathrm{d}\boldsymbol{r}\left[\eta_{\mathrm{g}}^0(\boldsymbol{r},t')\Phi^*(\boldsymbol{r},t')+\eta_{\mathrm{g}}^{0*}(\boldsymbol{r},t')\Phi(\boldsymbol{r},t')\right], \tag{10}$$

depend on the external potentials. The gauge has been chosen so that the functional $V[\{d\}]$ equals the external scalar potential $V^0(\boldsymbol{r},t)$ and η_{g}^0 is defined by $\eta_{\mathrm{g}}^0\equiv\eta^0\exp[-(i/\hbar)\cdot\int_{t_0}^{t}\mathrm{d}t'V^0(\boldsymbol{r},t')]$.

Along with the basic idea underlying DFT, Theorem II admits a map of the densities in the real system onto those of a reference system subject to appropriate potentials. This map is proven in Theorem III, which defines the so-called Kohn-Sham scheme needed to implement TD-DFT.

Theorem III. – It states that there exist unique reference-potential functionals $\{p^{\mathrm{R}}[\{d\}]\}$ such that the densities $\{d^{\mathrm{R}}\}$ calculated within the chosen reference system coincide with the densities $\{d^0\}$ of the real interacting system.

Following again WKG, we first define the action functional $Q^{\mathrm{R}}[\{d\}] \equiv R^{\mathrm{R}}[\{d\}] - P^{\mathrm{R}}[\{d\}] - S^{\mathrm{R}}[\{d\}]$ for the reference system as in eq. (7) for its interacting analogue. The functional $Q^0[\{d\}]$ is written as

$$Q^0[\{d\}] = R^{\mathrm{R}}[\{d\}] - P^0[\{d\}] - S^0[\{d\}] - Q_{\mathrm{xc}}[\{d\}]\ , \tag{11}$$

thereby defining the exchange-correlation functional $Q_{\mathrm{xc}}[\{d\}]$. We can now exploit the stationarity of both $Q^{\mathrm{R}}[\{d\}]$ and $Q^0[\{d\}]$ to obtain a set of equations relating the potentials $\{p^{\mathrm{R}}[\{d\}]\}$ to the original external potentials $\{p^0\}$.

The resulting equations, in addition to $V^{\mathrm{R}}\left[\{d^0(\boldsymbol{r},t)\}\right] = V^0(\boldsymbol{r},t)$ are as follows:

$$\left[\frac{\delta P^{\mathrm{R}}[\{d\}]}{\delta \boldsymbol{j}(\boldsymbol{r},t)}\right]_{\{d^0\}} = \left[\frac{\delta P^0[\{d\}]}{\delta \boldsymbol{j}(\boldsymbol{r},t)}\right]_{\{d^0\}} + \left[\frac{\delta Q_{\mathrm{xc}}[\{d\}]}{\delta \boldsymbol{j}(\boldsymbol{r},t)}\right]_{\{d^0\}} \tag{12}$$

and

$$\eta_{\mathrm{g}}^{\mathrm{R}}(\boldsymbol{r},t) + \left[\frac{\delta P^{\mathrm{R}}[\{d\}]}{\delta \Phi^*(\boldsymbol{r},t)}\right]_{\{d^0\}} = \eta_{\mathrm{g}}^0(\boldsymbol{r},t) + \left[\frac{\delta P^0[\{d\}]}{\delta \Phi^*(\boldsymbol{r},t)}\right]_{\{d^0\}} + \left[\frac{\delta Q_{\mathrm{xc}}[\{d\}]}{\delta \Phi^*(\boldsymbol{r},t)}\right]_{\{d^0\}} \tag{13}$$

with its complex conjugate. These equations define the effective exchange-correlation potentials.

We conclude this discussion by noticing that eqs. (12) and (13) have been derived in a previous paper [13] within a linear-response formulation of TD-DFT for superfluids. In brief, by writing the microscopic equation of motion for the order parameter in terms of the condensate self-energy, we proved that the matrix expressing the linear response of $n_{\mathrm{c}}(\boldsymbol{r},t)$ and $\boldsymbol{v}_{\mathrm{s}}(\boldsymbol{r},t)$ to the symmetry-breaking field η explicitly has the Hohenberg-Kohn-Sham structure.

Reference system. – A suitable choice of the reference system for a superfluid at finite temperature is provided by the gapless Bogolubov-Popov approximation. This accounts for the thermally excited non-condensate cloud and satisfies the Hugenholtz-Pines theorem [14]. In this approximation the densities can be written as [17]

$$n_{\mathrm{c}}(\boldsymbol{r},t) = |\Phi(\boldsymbol{r},t)|^2, \tag{14}$$

$$\boldsymbol{v}_{\mathrm{s}}(\boldsymbol{r},t) = (\hbar/m)\boldsymbol{\nabla}\varphi(\boldsymbol{r},t) - \boldsymbol{A}^{\mathrm{R}}(\boldsymbol{r},t)/m \tag{15}$$

and

$$\boldsymbol{j}(\boldsymbol{r},t) = \boldsymbol{j}_{\mathrm{c}}(\boldsymbol{r},t) + \tilde{\jmath}(\boldsymbol{r},t) - n(\boldsymbol{r},t)\boldsymbol{A}^{\mathrm{R}}(\boldsymbol{r},t)/m\ . \tag{16}$$

Here $\boldsymbol{j}_{\mathrm{c}}(\boldsymbol{r},t) \equiv n_{\mathrm{c}}(\boldsymbol{r},t)\boldsymbol{v}_{\mathrm{s}}(\boldsymbol{r},t)$ is the condensate current and

$$\tilde{\jmath}(\boldsymbol{r},t) = \frac{1}{2im}\sum_n \left[N_n U_n(\boldsymbol{r},t)\boldsymbol{\nabla}U_n^*(\boldsymbol{r},t) + (N_n+1)\,V_n(\boldsymbol{r},t)\boldsymbol{\nabla}V_n^*(\boldsymbol{r},t) - \mathrm{c.c.}\right] \tag{17}$$

is the current carried by the non-condensate. In eq. (17) U_n and V_n are the Bogolubov functions and $N_n = \left[\exp(E_n/k_{\mathrm{B}}T) - 1\right]^{-1}$ is the boson thermal factor, with E_n being the energy eigenvalues in the Bogolubov-Popov equations (see below) at the initial time t_0. Finally, $n(\boldsymbol{r},t) = n_{\mathrm{c}}(\boldsymbol{r},t) + \tilde{n}(\boldsymbol{r},t)$, with

$$\tilde{n}(\boldsymbol{r},t) = \sum_n \left[N_n\left(|U_n(\boldsymbol{r},t)|^2 + |V_n(\boldsymbol{r},t)|^2\right) + |V_n(\boldsymbol{r},t)|^2\right] \tag{18}$$

being the non-condensate density. The anomalous density is given by $\langle\hat{\psi}(\boldsymbol{r},t)\hat{\psi}(\boldsymbol{r},t)\rangle = \Phi^2(\boldsymbol{r},t) + \sum_n (2N_n+1)\, U_n(\boldsymbol{r},t)V_n^*(\boldsymbol{r},t)$.

In eq. (15) the condensate wave function $\Phi(\boldsymbol{r},t)$ satisfies the Schrödinger equation [18]

$$i\hbar\frac{\partial\Phi(\boldsymbol{r},t)}{\partial t} = \mathcal{L}^{\rm R}\Phi(\boldsymbol{r},t) + \eta_g^{\rm R}(\boldsymbol{r},t)\ , \tag{19}$$

where $\mathcal{L}^{\rm R} \equiv -(2m)^{-1}\left[\hbar\boldsymbol{\nabla} - i\boldsymbol{A}^{\rm R}(\boldsymbol{r},t)\right]^2 + V^{\rm R}(\boldsymbol{r},t)$ and $V^{\rm R}(\boldsymbol{r},t) = V^0(\boldsymbol{r},t) + 2\int {\rm d}\boldsymbol{r}' w(\boldsymbol{r}-\boldsymbol{r}')n(\boldsymbol{r}',t) + V_{\rm xc}(\boldsymbol{r},t)$, with $V_{\rm xc}(\boldsymbol{r},t)$ being determined from eq. (12). The gauge-invariant reference source field is $\eta_{\rm g}^{\rm R}(\boldsymbol{r},t) = \eta_{\rm g}^0(\boldsymbol{r},t) - \Phi(\boldsymbol{r},t)\int {\rm d}\boldsymbol{r}' w(\boldsymbol{r}-\boldsymbol{r}')|\Phi(\boldsymbol{r}',t)|^2 + \eta_{\rm xc}(\boldsymbol{r},t) = \eta_{\rm g}^0(\boldsymbol{r},t) + \delta Q_{\rm xc}/\delta\Phi^*$ (see eq. (13)). In the special case of a point-contact interaction eq. (19) becomes the well-known Gross-Pitaevskii equation.

The Bogolubov functions U_n and V_n satisfy the single-particle coupled equations

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} U_n(\boldsymbol{r},t) \\ V_n(\boldsymbol{r},t)\end{pmatrix} = \begin{pmatrix} \mathcal{L}^{\rm R} & -\int {\rm d}\boldsymbol{r}' w(\boldsymbol{r}-\boldsymbol{r}')\Phi^{*2}(\boldsymbol{r}',t) \\ -\int {\rm d}\boldsymbol{r}' w(\boldsymbol{r}-\boldsymbol{r}')\Phi^{2}(\boldsymbol{r}',t) & -\mathcal{L}^{\rm R}\end{pmatrix}\begin{pmatrix} U_n(\boldsymbol{r},t) \\ V_n(\boldsymbol{r},t)\end{pmatrix}. \tag{20}$$

We point out that, as a result of imposing gauge invariance, the reference system in eq. (19) is the same as that in eq. (20).

In summary, we have demonstrated the basic Hohenberg-Kohn-Sham–type theorems underlying TD-DFT for inhomogeneous neutral superfluids at finite temperature below threshold for vortex formation and proposed an implementation based on a reference system described by the Bogolubov-Popov theory. We have also explicitly pointed out similarities and differences with respect to charged superconductors as treated by Wacker *et al.* [10] and briefly remarked on the linear-response limit as treated by Chiofalo *et al.* [13]. A final comment is in order. For super-critical rotational velocities quantized vortices will appear in the superfluid: at that point the velocity field $\boldsymbol{v}_{\rm s}$ ceases to be irrotational and acquires a regular contribution $\boldsymbol{v}_r$ describing the velocity of each point of a vortex line as well as a singular contribution due to the quantized structure of the vortex line [19]. The regular term leads to the well-known Magnus force on a vortex line [20] and to friction forces between superfluid and normal-fluid components, which are proportional to $\boldsymbol{v}_{\rm r} - \boldsymbol{v}_{\rm n}$ [19]. Therefore, in order to account for vortices, the present TD-DFT approach will need extension to include one additional external field and one additional density variable. We hope to return to this problem in the near future.

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