

PAIRING DYNAMICS AND TIME-DEPENDENT DENSITY FUNCTIONAL THEORY*

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We discuss issues related to pairing dynamics in nuclear large amplitude collective motion. The examples of effects which are not properly described within BCS theory are presented. In the second part, we review properties of time-dependent density functional theory (TDDFT) and, in particular, we discuss the time-dependent superfluid local density approximation (TD-SLDA) starting from the stationary action principle.

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1. Remarks on pairing dynamics

The theoretical description of atomic nuclei and nuclear systems in general requires superfluidity as a crucial ingredient. Although the size of the pairing gap in nuclear systems does not exceed 3% of the Fermi energy, the influence of the pairing correlations on dynamics of medium or heavy nuclei is essential. As one of the best examples serves the nuclear induced fission process, which cannot be understood without taking into account pairing correlations [1]. Their role, both in the ground state as well as in excited states, has been studied and analysed for decades (see, *e.g.*, Refs. [2–6] and references therein). Still, dynamical aspects of the pairing field in large amplitude nuclear motion are usually not taken into account. To be precise, most of the effects related to superfluidity are described within the single-particle picture, where only one aspect of the pairing field is manifested, namely, the appearance of the energy gap at the Fermi level. Within the BCS theory, it is interpreted as the energy associated with the Cooper pair formation. This clearly produces a noticeable effect for large amplitude collective motion, being responsible for decreasing the one-body dissipation.

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Indeed, the collective energy dissipation can be traced back to the single-particle level crossings at the Fermi level. If the pairing correlations are active, the crossings will disappear and, consequently, the probability of the single-particle excitation process will be decreased. The Landau–Zener formula tells us that it will decrease exponentially with the square of the pairing gap magnitude. Consequently, the nuclear motion will become closer to the adiabatic limit and sometimes it may even justify the usage of a single adiabatic potential energy surface which becomes effectively decoupled from other degrees of freedom. This decoupling is also revealed in the behaviour of mass parameters which in the vicinity of level crossings behave as $1/\Delta$. It is therefore assumed that the pairing field is constant or changes adiabatically as a function of the density variations. This simplified description of the pairing field in nuclear dynamics is quite common as it can be applied within a relatively simple theoretical framework. It reduces the manifestation of the pairing correlations to the single complex number — the pairing gap — which is determined through the nuclear density. This is in general not correct, since dynamical aspects of the pairing field are then completely neglected. It is believed, however, that the pairing field dynamics will produce only small corrections to the commonly accepted picture of nuclear dynamics. Moreover, the proper treatment of the pairing field dynamics requires to use more advanced approaches leading to a rapid increase of computational complexity.

In order to understand better this distinction of the pairing treatments, it is instructive to start with reminding the differences between two theoretical frameworks, namely, BCS and Hartree–Fock–Bogoliubov (HFB) approaches. Formally, the difference originates from the fact that in the former case, the third transform of the Bloch–Messiah decomposition (of the Bogoliubov transformation) is equal to unity [7]. This requirement, which is responsible for a significant simplification, has serious consequences in the pairing description. It means that one cannot describe processes due to the quasiparticle scattering and, therefore, the phenomena originating from the interaction of quasiparticles with a nonuniform pairing field (scattering on the pairing potential). These phenomena, although not so well pronounced in nuclear ground states, can have an impact on the dynamics of nuclear systems. Hence, effects related to the nonuniformity of the pairing field, such as the existence of Andreev states or Andreev reflection [8, 9], which are well-known in condensed matter physics, cannot be described within the so-called HF+BCS approach. In this framework, the pairing field is expressed as $\Delta(\mathbf{r}) = g(\mathbf{r}) \sum_k v_k^* u_k |\psi_k(\mathbf{r})|^2$ and thus it resembles the density profile, even when g is coordinate-dependent. This is due to the fact that the occupation numbers of HF orbitals are just numbers associated with each orbital and, therefore, one cannot describe a configuration with

position-dependent occupation numbers. It implies that *e.g.* a quantum vortex solution of HF+BCS equations does not exist, as it requires variations of occupation numbers as a function of the distance from the vortex core, where the system is normal [10]. This prevents applications of HF+BCS theory to describe *e.g.* the inner crust of neutron stars, where various vortex-impurity configurations may exist and their properties (pinning energies) are expected to be crucial for understanding the pulsar glitch phenomenon [11].

In the case of time-dependent phenomena in nuclear systems, the aforementioned limitations of the HF+BCS approach lead to an effective “freezing” of excited modes of the pairing field. Consequently, the nuclear dynamics is governed by the nucleon density evolution only, with the pairing gap adjusting each time to a given nuclear configuration. It is easily seen from the equations

$$i\hbar \frac{\partial}{\partial t} \psi_k(\mathbf{r}, t) = \hat{h} \psi_k(\mathbf{r}, t), \quad (1)$$

which define the evolution of HF orbitals according to the mean-field \hat{h} . They are used to set the basis for the evolution of the diagonal density matrix and the pairing tensor (see Refs. [12, 13])

$$\frac{d}{dt} \rho_{kk}(t) = \Delta_{k\bar{k}}(t) \nu_{k\bar{k}}^*(t) - \Delta_{k\bar{k}}^*(t) \nu_{k\bar{k}}(t), \quad (2)$$

$$\frac{d}{dt} \nu_{k\bar{k}}(t) = \Delta_{k\bar{k}}(t) (1 - 2\rho_{kk}(t)). \quad (3)$$

Clearly, the spatial dependence of the pairing field cannot be described within this framework.

It is instructive to consider the following process: suppose, we deal with a uniform system which is superfluid and the time evolution is triggered by an external spatially modulated pairing field $\Delta_{\text{ext}}(\mathbf{r})$. Note that before the external field is switched on, the HF+BCS approach is equivalent to HFB equations, since initially, there is no quasiparticle scattering and the canonical basis corresponds simply to plane waves. However, when the system is perturbed by the external pairing field, the translational invariance is lost and the density waves may be excited. This process cannot be described within TDHF+BCS treatment, as one can easily infer from Eq. (1). Namely, the system is initially described by $\psi_k(\mathbf{r}) \propto \exp(i\mathbf{k} \cdot \mathbf{r})$, which are eigenstates of \hat{h} , and there is no mechanism to break the translational invariance by the spatially modulated pairing field. Thus, the perturbation induced by the external pairing field will result in a modification of the magnitude of the pairing gap only

$$\Delta_{k\bar{k}} \rightarrow \Delta_{k\bar{k}} + \Delta_{k\bar{k}}^{\text{ext}} \quad (4)$$

leading to oscillations of the uniform pairing field. Since the density reads

$$\rho(\mathbf{r}, t) = \sum_k \rho_{kk}(t) |\psi_k(\mathbf{r}, t)|^2, \quad (5)$$

the translational symmetry breaking may occur through the symmetry breaking terms in the mean-field Hamiltonian, but these are absent, according to our initial assumption. Consequently, the spatial modulation of the pairing field in the TDHF+BCS dynamics may be generated only as a consequence of the evolution of the normal density ρ . Last but not least, it turns out that TDHF+BCS equations violate the continuity equation producing various unwanted effects (see Ref. [12]).

On the contrary, the TDHFB framework offers a possibility to take into account excitation modes of the pairing field $\Delta(\mathbf{r}, t)$ itself (*e.g.* Bogoliubov phonons). These modes are treated on the same footing as the normal degrees of freedom described by $\rho(\mathbf{r}, t)$. Within this approach, an external, inhomogeneous pairing field will induce various processes in the initially uniform system due to the quasiparticle scattering. Two examples of results, where the pairing dynamics played a crucial role, comprise the induced fission of ^{240}Pu [1] and the collisions of two superfluid nuclei [14–16]. In the former case, the dynamics of the pairing field causes much longer fission times than expected, based on the simplified pairing treatment. In the latter case, the dynamics of the pairing field lead to the soliton-like excitation of the pairing field of two colliding nuclei resulting in the modification of the kinetic energy of the fragments and the capture cross section.

Summarizing, in this section, we described differences between TDSLDA and TDHF+BCS-type approaches, discussing an example of the process which cannot be described within TDHF+BCS framework. Still the advantage of pure TDHF [17] or TDHF+BCS lies in their relative simplicity and the description they offer is correct if magic nuclei or relatively high energies are considered. There are indications however that the induced fission or collisions of nonmagic nuclei may require to consider more advanced approach, which takes pairing dynamics into account.

2. Time-dependent density functional theory

In this section, we review briefly the developments in density functional theory (DFT) extended to superfluid systems, which allow to overcome difficulties described in the previous section resulting from the incorrect treatment of pairing dynamics (see also Refs. [18, 19]). DFT has become a standard theoretical tool as it offers a universal and formally exact approach, which had enormous practical successes [20–23]. It is widely used in the field of condensed matter and, in particular, well-suited to determine properties of electronic systems [24–27].

The case of atomic nuclei is more complicated, however, since two types of particles, neutrons and protons, need to be taken into account in the description of the system. Moreover, the nuclear interaction involves many terms, including also the three-body force, without a clear recipe concerning its functional form. Consequently, the nuclear energy density functionals have various forms, the most popular being the Skyrme functional, which despite of known shortcomings is still widely used (see, *e.g.*, Refs. [28–33] and references therein). For nonsuperfluid systems, the simple scheme offered by the energy density functional theory is very attractive, as instead of searching for the wave function of an N -particle system which depends on $3N$ variables, one solves a system of N nonlinear, coupled partial differential equations. It can be achieved through the application of the Kohn–Sham (K–S) scheme, in which the interacting system is replaced by the equivalent (*i.e.* of the same density distribution) noninteracting system defined through the set of orbitals. These orbitals are, in turn, determined from variational principle [34], which is equivalent to the minimization of the functional and generates the set of nonlinear equations defining the density distribution. The formulation of DFT limits its applicability to the ground-state properties of the system. In order to address the excited states and, in particular, nonequilibrium processes such as nuclear fission or reactions, an extension of the DFT is necessary to include the time evolution.

This can be achieved through the time-dependent density functional theory (TDDFT), which can be used to describe nonstationary situations in systems consisting of nuclei, atoms, molecules, solids, or nanostructures (see Refs. [35–37] and references therein). Whereas DFT is based on the Hohenberg–Kohn theorem proving the existence of the unique density functional, TDDFT relies on the Runge–Gross mapping which ensures that the evolution of the quantum system, *i.e.* its wave function, can be determined through the density (up to an arbitrary phase) [38]. Despite these similarities with the static DFT, the time-dependent theory may exhibit nonlocality in time, which leads to various problems related to causality principle. The so-called causality paradox has been resolved in a series of papers [39–43]. Nonlocality in time is responsible for memory effects, which means that the behaviour of the system is dependent on the densities at earlier times [44, 45]. This memory is, in principle, infinitely long-ranged and very little is known about its behaviour. This fact, together with a serious complication of resulting time-dependent equations, which would become integro-differential equations, results in the most common approximation in TDDFT ignoring memory effects. The price which one pays for this simplification is an incorrect treatment of energy dissipation processes [35].

The existence of superfluidity and its incorporation in TDDFT leads to additional complications. The first attempt to develop the formal framework of DFT for superconductors has been triggered by the discovery of high-temperature superconductivity [46, 47]. Namely, it can be achieved through the introduction of an anomalous density $\chi(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \langle \hat{\psi}_{\sigma'}(\mathbf{r}') \hat{\psi}_{\sigma}(\mathbf{r}) \rangle$ (σ denotes the spin degrees of freedom), which plays the role of the superconducting order parameter. The pairing potential is then defined as a functional derivative of the energy functional with respect to χ

$$\Delta(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \frac{\delta E(\rho, \chi)}{\delta \chi^*(\mathbf{r}\sigma, \mathbf{r}'\sigma')}. \quad (6)$$

Introducing the Bogoliubov transformation (see below), which allows to express both normal and anomalous densities in a form similar to the orbital expansion in conventional DFT, one arrives at the Kohn–Sham scheme for superfluid Fermi systems, which formally resemble the Bogoliubov–de Gennes equations. Unfortunately, this set of equations is of the integro-differential form and, therefore, the above formulation has rarely been used in practice. This complication comes from the nonlocality of the pairing potential $\Delta(\mathbf{r}\sigma, \mathbf{r}'\sigma')$. It turned out, however, to be possible to formulate the problem using a local pairing field [48]. The justification for the so-called SLDA (Superfluid Local Density Approximation) has been developed in a series of papers (see Refs. [49–54]) and was shown to be very accurate for nuclei and cold atomic gases. The prescription involves the renormalization of the pairing coupling constant, which is a function of the momentum cutoff. In the case of the spherical cutoff, the analytic formula can be derived (spin indices are omitted for clarity)

$$\Delta(\mathbf{r}) = -g_{\text{eff}}(\mathbf{r})\chi_c(\mathbf{r}), \quad (7)$$

$$\frac{1}{g_{\text{eff}}(\mathbf{r})} = \frac{1}{g(\mathbf{r})} - \frac{mk_c(\mathbf{r})}{2\pi^2\hbar^2} \left(1 - \frac{k_F(\mathbf{r})}{2k_c(\mathbf{r})} \ln \frac{k_c(\mathbf{r}) + k_F(\mathbf{r})}{k_c(\mathbf{r}) - k_F(\mathbf{r})} \right), \quad (8)$$

where anomalous density χ_c is defined within the truncated space and k_c is the momentum cutoff. This prescription works in the case of static DFT extended to superfluid system, but is only of a little help in the case of TDDFT, for the reasons which are discussed below (see also [19]).

We may formulate TDDFT from the action stationarity principle, by defining the action (without including memory effects)

$$S = \int_{t_0}^{t_1} \left(\langle 0(t) | i \frac{d}{dt} | 0(t) \rangle - E[\rho(\mathbf{r}\sigma, \mathbf{r}'\sigma', t), \chi(\mathbf{r}\sigma, \mathbf{r}'\sigma', t)] \right) dt. \quad (9)$$

The energy density functional in E , in principle, also contains currents but they do not affect the derivations, so we will omit them for clarity. In the above equation, $|0(t)\rangle$ is a state which is a quasiparticle vacuum $\alpha_\mu(t)|0(t)\rangle=0$, where $\alpha_\mu(t) = \hat{B}(t)a(\mathbf{r}\sigma)\hat{B}^\dagger(t)$. It can be treated in the Kohn–Sham scheme (similarly as in the case of nonsuperfluid system) as a fictitious state describing an equivalent non-interacting system having the same densities ρ and χ as the true interacting system. The operator $\hat{B}(t)$ defines the Bogoliubov transformation (and the state $|0(t)\rangle$) and can be written as $\hat{B}(t) = \exp[i\hat{G}(t)]$, where $\hat{G}(t)$ is the Hermitian operator of the form of

$$\begin{aligned} \hat{G}(t) = & \int d\mathbf{r}d\mathbf{r}' \sum_{\sigma,\sigma'} h(\mathbf{r}\sigma, \mathbf{r}'\sigma', t) a^\dagger(\mathbf{r}\sigma)a(\mathbf{r}'\sigma') - \frac{1}{2} \int d\mathbf{r} \sum_{\sigma} h(\mathbf{r}\sigma, \mathbf{r}\sigma, t) \\ & + \int d\mathbf{r}d\mathbf{r}' \sum_{\sigma,\sigma'} \left(\frac{1}{2} \Delta^*(\mathbf{r}'\sigma', \mathbf{r}\sigma, t) a(\mathbf{r}\sigma)a(\mathbf{r}'\sigma') + \frac{1}{2} \Delta(\mathbf{r}\sigma, \mathbf{r}'\sigma', t) a^\dagger(\mathbf{r}\sigma) a^\dagger(\mathbf{r}'\sigma') \right). \end{aligned} \quad (10)$$

Although \mathbf{r} is formally a continuous variable, in practical applications one performs calculations on the lattice and thus it is discretized leading to sums instead of integrals in the above formulas. Hence, matrices h and Δ define the matrix $G(t)$

$$G(t) = \begin{pmatrix} h(t) & \Delta(t) \\ \Delta^\dagger(t) & -h^*(t) \end{pmatrix} \quad (11)$$

which define the matrix of the Bogoliubov transformation

$$B(t) = \begin{pmatrix} U(t) & V^*(t) \\ V(t) & U^*(t) \end{pmatrix} = \exp[iG(t)], \quad (12)$$

where amplitudes $U_\mu(\mathbf{r}\sigma, t)$ and $V_\mu(\mathbf{r}\sigma, t)$ (μ^{th} column of U and V , respectively) play the role of the Kohn–Sham orbitals. The matrix of the Bogoliubov transformation relates the new basis which define the state $|0(t)\rangle$ to the initial coordinate basis

$$\vec{c} = B(t)\vec{\gamma}(t), \quad (13)$$

where

$$\vec{\gamma}(t) = \begin{pmatrix} \vec{\alpha}(t) \\ \vec{\alpha}^\dagger(t) \end{pmatrix}, \quad \vec{c} = \begin{pmatrix} \vec{a} \\ \vec{a}^\dagger \end{pmatrix}. \quad (14)$$

Clearly, since $B^\dagger(t)B(t) = B(t)B^\dagger(t) = I$, variations of Eq. (9) with respect to U and V are not independent and the conditions

$$\frac{\delta S}{\delta U_\mu(\mathbf{r}\sigma, t)} = \frac{\delta S}{\delta V_\mu(\mathbf{r}\sigma, t)} = 0 \quad (15)$$

are not going to produce the correct equation of motion which conserves the structure of the product state $|0(t)\rangle$, unless certain constraints on variations are imposed. This can be achieved also by noticing that the functional (omitting spin indices for clarity) $E(\rho, \chi) = E[\sum_{\mu} V_{\mu}^*(\mathbf{r}, t)V_{\mu}(\mathbf{r}', t), \sum_{\mu} V_{\mu}^*(\mathbf{r}, t)U_{\mu}(\mathbf{r}', t)]$ has to be invariant under the transformation

$$\begin{aligned} & \sum_{\mu} V_{\mu}^*(\mathbf{r}, t)V_{\mu}(\mathbf{r}', t) \rightarrow \\ & \alpha \sum_{\mu} V_{\mu}^*(\mathbf{r}, t)V_{\mu}(\mathbf{r}', t) + (1 - \alpha) \sum_{\mu} (1 - U_{\mu}(\mathbf{r}, t)U_{\mu}^*(\mathbf{r}', t)), \\ & \sum_{\mu} V_{\mu}^*(\mathbf{r}, t)U_{\mu}(\mathbf{r}', t) \rightarrow \\ & \alpha \sum_{\mu} V_{\mu}^*(\mathbf{r}, t)U_{\mu}(\mathbf{r}', t) - (1 - \alpha) \sum_{\mu} U_{\mu}(\mathbf{r}, t)V_{\mu}^*(\mathbf{r}', t) \end{aligned} \quad (16)$$

for an arbitrary parameter α . This invariance is a direct consequence of the completeness of the Bogoliubov transformation: $B(t)B^{\dagger}(t) = I$. In order to get the proper equation of motion, one needs to set $\alpha = 1/2$ obtaining the symmetric form of the energy density functional. In the so-called local TDDFT, which is denoted as time-dependent local density approximation (TDSLDA), one limits to local expressions: $h(\mathbf{r}, \mathbf{r}', t) \rightarrow h(\mathbf{r}, t)$ and $\Delta(\mathbf{r}, \mathbf{r}', t) \rightarrow \Delta(\mathbf{r}, t)$. Consequently, from condition (15), one arrives at TDSLDA equations (omitting spin indices for clarity)

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} U_{\mu}(\mathbf{r}, t) \\ V_{\mu}(\mathbf{r}, t) \end{pmatrix} = \begin{pmatrix} h(\mathbf{r}, t) & \Delta(\mathbf{r}, t) \\ \Delta^*(\mathbf{r}, t) & -h^*(\mathbf{r}, t) \end{pmatrix} \begin{pmatrix} U_{\mu}(\mathbf{r}, t) \\ V_{\mu}(\mathbf{r}, t) \end{pmatrix}, \quad (17)$$

where the relation between E and h , Δ reads: $h(\mathbf{r}, \mathbf{r}', t) = \frac{\delta E}{\delta \rho(\mathbf{r}', \mathbf{r}, t)}$ and $\Delta(\mathbf{r}, \mathbf{r}', t) = \frac{\delta E}{\delta \chi^*(\mathbf{r}, \mathbf{r}', t)}$. In deriving the above formula, the following property is used:

$$\langle 0(t) | i \frac{d}{dt} | 0(t) \rangle = \frac{1}{2} i \int d^3r \sum_{\mu} \left(V_{\mu}(\mathbf{r}, t) \frac{\partial V_{\mu}^*(\mathbf{r}, t)}{\partial t} + U_{\mu}(\mathbf{r}, t) \frac{\partial U_{\mu}^*(\mathbf{r}, t)}{\partial t} \right). \quad (18)$$

Note, however, that these equations have been obtained from the stationary action principle under condition that the Bogoliubov transformation fulfills the completeness relation. Otherwise, one would not be able to define the new state $|0(t+\Delta t)\rangle$ from the previous one $|0(t)\rangle$. However, when the energy cutoff is introduced, then only certain amplitudes U_{μ} and V_{μ} are taken into account. In such a case, the expression for the energy density functional E ceases to be invariant under transform (16) and the resulting equations

are not correct. It means that although formally one may still use Eq. (17), evolving only selected amplitudes U_μ and V_μ , it does not lead to a unique determination of the state $|0(t)\rangle$. One of the manifestation of this problem is the energy nonconservation which will occur during the evolution [55]. The fact that the energy of the system is conserved is a trivial observation based on the form of action (9), but it is only the case when the Bogoliubov transformation is properly defined according to Eq. (12). Therefore, during the evolution on the spatial lattice, all amplitudes of U and V need to be evolved, unless for short time evolutions (see Ref. [55]).

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