Theories and calculations

Nuclear energy density functional theory

According to the basic theorems of the density functional theory (DFT) [1], all the physical quantities at the ground state of many-body systems can be given by functionals of one-body density $\rho(\boldsymbol{r})$. In nuclei, there are two kinds of particles, protons and neutrons, thus, they are functionals of proton and neutron densities, $\rho_p(\boldsymbol{r})$ and $\rho_n(\boldsymbol{r})$. We start from a given energy density functional $E[\rho_p, \rho_n]$, and try to find the density distributions, $\rho_p(\boldsymbol{r})$ and $\rho_n(\boldsymbol{r})$, which minimize the energy. In a variational form, it is given by

$$\delta\left(E[\rho_p, \rho_n] - \mu_p \int \rho_p(r)dr - \mu_n \int \rho_n(r)dr\right) = 0\,, \tag{1}$$

where μ_p and μ_n are the Lagrange multipliers to fix the numbers of protons and neutrons. Equation $(\mathbf{1})$ is enough in principle. However, in practice, to achieve high accuracy of the calculation, we use the Kohn-Sham scheme [2] with a Bogoliubov extension [3] and replace $E[\rho_p, \rho_n]$ by $E[\rho_p, \rho_n, \tau_p, \tau_n, \overleftrightarrow{J}_p, \overleftrightarrow{J}_n; \kappa_p, \kappa_n]$ where $\tau_q(\boldsymbol{r})$ are the kinetic density and $\overleftrightarrow{J}_q$ are the spin-current density, κ_q are the pair density $(q = n, p)$. The definitions of these densities can be found in literature, e.g., [4]. Finally, this leads to the Kohn-Sham-Bogoliubov-de-Gennes equations:

$$\begin{pmatrix} h_q - \mu_q & \Delta_q \\ -\Delta_q^* & -(h_q - \mu_q)^* \end{pmatrix} \begin{pmatrix} U_\mu^q \\ V_\mu^q \end{pmatrix} = E_\mu^{(q)} \begin{pmatrix} U_\mu^q \\ V_\mu^q \end{pmatrix}, \tag{2}$$

where $q = n, p$. Here, μ_q are called "chemical potentials" to control the average numbers of protons and neutrons, $h_q(\boldsymbol{r}, \sigma)$ are the single-particle Hamiltonians, $\Delta_q(\boldsymbol{r}, \sigma)$ are the pair fields which introduce the Cooper pairs and the superfluidity in nuclei. The pair fields are coordinate-dependent in general, and their average values are often called "pairing gap energy" denoted as Δ_q. Equation (2) has solutions $\left(U_\mu^q(\boldsymbol{r}, \sigma), V_\mu^q(\boldsymbol{r}, \sigma)\right)$ with positive quasi-particle energies $E_\mu^q > 0$ and negative ones $E_n^q < 0$. In order to construct $h_q(\boldsymbol{r}, \sigma)$ and $\Delta_q(\boldsymbol{r}, \sigma)$ in the left hand side of Eq. (2), we need all the solutions $\left(U_\mu^q(\boldsymbol{r}, \sigma), V_\mu^q(\boldsymbol{r}, \sigma)\right)$ with either positive or negative E_μ^q. Thus, Eq. (2) must be self-consistently solved and the

iterative procedure is necessary. The theory is called "Hartree-Fock-Bogoliubov" (HFB) theory in nuclear physics. See Ref. [4,5] for more details.

Time-dependent density functional theory and canonical-basis formulation

The basic theorems for the ground state can be generalized to systems under a time-dependent external field [6, 5]. This leads to time-dependent equations:

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}U_\mu^q\\ V_\mu^q\end{pmatrix}=\begin{pmatrix}h_q-\mu_q & \Delta_q\\ -\Delta_q^* & -(h_q-\mu_q)^*\end{pmatrix}\begin{pmatrix}U_\mu^q\\ V_\mu^q\end{pmatrix}, \tag{3}$$

where all the fields and wave functions now depend on time. The time-dependent external fields are included either in $h_q(\boldsymbol{r},\sigma;t)$ or $\Delta_q(\boldsymbol{r},\sigma;t)$. The self-consistent solutions of Eq. (3) describe the time evolution of the densities of a nucleus. The chemical potential μ_q is arbitrary here. In fact, the dynamics does not depend on the value of μ_q. The theory is called "Time-dependent Hartree-Fock-Bogoliubov" (TDHFB) theory in nuclear physics.

Solution of Eq. (3) is still computationally difficult, since we have to calculate the time evolution of all the quasi-particle wave functions. In order to reduce the computational cost, we have developed an approximate method, called "Canonical-basis time-dependent Hartree-Fock-Bogoliubov" (Cb-TDHFB) method [7]. Adopting a diagonal approximation for the pair fields, we end up the equations for a pair of canonical states $(\phi_k^q(t),\phi_{\bar{k}}^q(t))$ with $q=n,p$:

$$i\hbar\frac{\partial}{\partial t}\left|\phi_k^q(t)\right\rangle=\left[h_q(t)-\eta_k^q(t)\right]\left|\phi_k^q(t)\right\rangle, \tag{4}$$

$$i\hbar\frac{\partial}{\partial t}\left|\phi_{\bar{k}}^q(t)\right\rangle=\left[h_q(t)-\eta_{\bar{k}}^q(t)\right]\left|\phi_{\bar{k}}^q(t)\right\rangle, \tag{5}$$

and the equations for their occupation and pair probabilities $(\rho_k^q(t),\kappa_k^q(t))$:

$$i\hbar\frac{d}{dt}\rho_k^q(t)=\kappa_k^q(t)\Delta_k^{q*}(t)-\kappa_k^{q*}(t)\Delta_k^q(t), \tag{6}$$

$$i\hbar\frac{d}{dt}\kappa_k^q(t)=\kappa_k^q(t)\Delta_k^{q*}(t)-\Delta_k^q(t)\left[2\rho_k^q(t)-1\right]. \tag{7}$$

Here, the real parameters $(\eta_k^q(t),\eta_{\bar{k}}^q(t))$ are chosen as the single-particle energies,

$\eta_k^q(t) = \langle \phi_k^q(t) | h_q(t) | \phi_k^q(t) \rangle$. The gap parameters $\Delta_k^q(t)$ are the diagonal part of the pair field, $\Delta_k^q(t) = -\langle \phi_k^q(t) | \Delta_q(t) | \phi_{\bar{k}}^q(t) \rangle$. This diagonal approximation for the pair field leads to the "Hartree-Fock+BCS" (HF+BCS) states for the calculation of ground states. The computational cost of Cb-TDHFB is significantly smaller than the full TDHFB of Eq. (3), roughly speaking, by a few to several orders of magnitude. See Ref. [7,8] for details.

Linear response and finite amplitude method

When the external fields are weak, we may linearize the TDDFT equation (3) and obtain the linear response equation. We have developed a method to facilitate the solutions of the linear response equation, called "finite amplitude method" (FAM) [9,10,11].

Applying a weak time-dependent external field of a given frequency ω, $F(t) = F(\omega)e^{-i\omega t} + \mathrm{h.c.}$, to the ground state,

$$F(\omega) = \sum_{\mu,\nu} \left(\frac{1}{2} F_{\mu\nu}^{20}(\omega) a_\mu^\dagger a_\nu^\dagger + \frac{1}{2} F_{\mu\nu}^{02}(\omega) a_\nu a_\mu + F_{\mu\nu}^{11}(\omega) a_\mu^\dagger a_\nu \right), \tag{8}$$

where $(a_\mu^\dagger, a_\nu)$ are the quasi-particle creation/annihilation operators at the ground state, the linear response equations are given as

$$\left(E_\mu + E_\nu - \hbar\omega\right) X_{\mu\nu}(\omega) + \delta H_{\mu\nu}^{20}(\omega) = -F_{\mu\nu}^{20}(\omega), \tag{9}$$

$$\left(E_\mu + E_\nu + \hbar\omega\right) Y_{\mu\nu}(\omega) + \delta H_{\mu\nu}^{02}(\omega) = -F_{\mu\nu}^{02}(\omega). \tag{10}$$

Here, $(X_{\mu\nu}, Y_{\mu\nu})$ are the forward and backward amplitudes, which we should to determine by solving Eqs. (9) and (10). $\delta H_{\mu\nu}^{20(02)}(\omega)$ are the residual fields which linearly depend on $(X_{\mu\nu}, Y_{\mu\nu})$. The main idea of the FAM is to calculate the residual fields without expansion with respect to $(X_{\mu\nu}, Y_{\mu\nu})$. Instead, we use an iterative solution of the equations with the finite difference method. This will facilitate programing computer codes and reduce the computational cost. See Refs. [9,10] for the detailed formulation and [11] for numerical implementation.

From nuclear structure to nuclear reaction

The results of nuclear structure calculations can be used for nuclear reaction

models. For instance, the nucleon density distribution can be used for calculation of the total reaction cross sections [13]. In the optical limit approximation of the Glauber model, the phase shift function as a function of the impact parameter $\boldsymbol{b}$ is given by

$$e^{i\chi(\boldsymbol{b})} = \exp\left[-\iint d\boldsymbol{r}_P d\boldsymbol{r}_T \rho_P(\boldsymbol{r}_P)\rho_T(\boldsymbol{r}_T)\Gamma_{NN}(\boldsymbol{s}_P - \boldsymbol{s}_T + \boldsymbol{b})\right]$$

where $\boldsymbol{s}_{P(T)}$ are the transverse component of the projectile (target) coordinates, $\Gamma_{NN}(\boldsymbol{s}_P - \boldsymbol{s}_T + \boldsymbol{b})$ are the nucleon-nucleon profile function, and $\rho_{P(T)}(\boldsymbol{r})$ are the projectile (target) density distributions. The total reaction cross section is given as integration over $\boldsymbol{b}$,

$$\sigma_R = \int d\boldsymbol{b} P(\boldsymbol{b})$$

with the reaction probability

$$P(\boldsymbol{b}) = 1 - \left|e^{i\chi(\boldsymbol{b})}\right|^2$$

The density distributions can be also used for calculation of the folding potentials.

$$U(\boldsymbol{r}) = \iint d\boldsymbol{r}_P d\boldsymbol{r}_T \rho_P(\boldsymbol{r}_P)\rho_T(\boldsymbol{r}_T) v_{NN}(\boldsymbol{r} - \boldsymbol{r}_P + \boldsymbol{r}_T)$$

The nucleon-nucleus optical potentials can be calculated in a similar way [14].

Numerical calculations with 3D coordinate-space representation

To perform the numerical calculations with (TD)DFT, we must choose the basis to represent each (quasi-)particle state. The choice of the basis is arbitrary, but depends on the purpose and the adopted energy density functional. We use the Skyrme energy density functional, and it is convenient to adopt the three-dimensional (3D) coordinate space discretized in mesh as the basis. Therefore, the quasi-particle wave functions in Eq. (2) are given by vectors,

$$\begin{pmatrix} U_\mu^q(1) \\ \vdots \\ U_\mu^q(M) \end{pmatrix}, \qquad \begin{pmatrix} V_\mu^q(1) \\ \vdots \\ V_\mu^q(M) \end{pmatrix}, \tag{11}$$

where M is twice of the number of discretized mesh points. The factor of two comes from the spin degrees of freedom. Accordingly, the single-particle

Hamiltonian h_q and the pair fields Δ_q are given by $M \times M$ matrices. However, due to the zero-range nature of the Skyrme energy density functional, the matrix is almost diagonal, except for kinetic terms and a few derivative terms. Therefore, the coordinate-space representation is an effective way to perform the calculations.

The time-dependent simulation can be done with the same coordinate and real-time representation. The time is also discretized with a mesh Δt, and the time-dependent quasi-particle states at $t_i = i \times \Delta t$ are expressed as vectors in Eq. (3):

$$\begin{pmatrix} U_\mu^q(1,t_i) \\ \vdots \\ U_\mu^q(M,t_i) \end{pmatrix}, \qquad \begin{pmatrix} V_\mu^q(1,t_i) \\ \vdots \\ V_\mu^q(M,t_i) \end{pmatrix}. \tag{12}$$

In the canonical-basis TDHFB equations (4) and (5), the same representation in the coordinate space and the real time is adopted for the canonical basis states. See Refs. [7,8] for details.

In the linear response equation, the forward and backward amplitudes are also represented in the mesh space. Instead of time, they are functions of frequency ω. Thus, we also discretize ω and solve the FAM equations (9) and (10). For the iterative solver, we use either the generalized conjugate residual method or the modified Broyden method. See Refs. [9,10,11] for details.

The calculations of properties provided in InPACS and Dens have been performed as follows:

(1) Ground-state deformation and other properties shown [8,12] (InPACS)
  Method: HF+BCS
  Adopted energy density functional: SkM*+monopole pairing
  Representation: 3D coordinate mesh representation
  Symmetry restriction: None

(2) Proton and neutron density distributions [14] (InPACS)
  Method: HFB
  Adopted energy density functional: Sly4+mixed pairing
  Representation: 1D coordinate mesh representation

Symmetry restriction: Spherical shape

(3) Photoabsorption cross sections [8,12]

Method: Cb-TDHFB

Adopted energy density functional: SkM*+monopole pairing

Representation: 3D coordinate mesh representation

Symmetry restriction: None

(4) Proton and neutron density distributions [8,12] (Dens)

Method: HF+BCS

Adopted energy density functional: SkM*+monopole pairing

Representation: 3D coordinate mesh representation

Symmetry restriction: None

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