An HFB scheme in natural orbitals

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(14 April 1997)

Abstract

We present a formulation of the Hartree-Fock-Bogoliubov (HFB) equations which solves the problem directly in the basis of natural orbitals. This provides a very efficient scheme which is particularly suited for large scale calculations on coordinate-space grids.

The production of new nuclei towards the drip lines and in the super-heavy region (for a review see \cite{1}) has raised a growing interest in the refinement of nuclear mean-field models to accommodate the larger body of experimental data. At the level of precision reached nowadays, a correct treatment of pairing becomes a crucial ingredient \cite{2}. This calls for a full variational optimization of the pairing wave function, what is known as the Hartree-Fock-Bogoliubov (HFB) treatment \cite{3,4}. It is the aim of this short note to present an efficient solution scheme for the HFB equations which relies on a direct variational optimization within the natural orbital basis. The following discussion is formulated for one sort of Fermions. Nuclear applications will use that scheme for neutrons and protons separately. A generalization to proton-neutron pairing is obvious.

Starting point is the BCS ansatz for the wave function of a pairing many-body system

\begin{equation}
|\Phi\rangle = \prod \left( u_{\alpha} + v_{\alpha} a_{\alpha}^{+} a_{\bar{\alpha}}^{+} \right) |\text{Vac}\rangle
\end{equation}
where $a^+_\alpha$ generates a particle in the state $\varphi_\alpha$, $\bar{\alpha}$ is the time reversed partner of $\alpha$, $v_\alpha$ the occupation amplitude for the state, and $u_\alpha = \sqrt{1 - v^2_\alpha}$ the non-occupation amplitude. The ansatz requires that the single-particle states are orthonormalized,

$$\langle \varphi_\alpha | \varphi_\beta \rangle = \delta_{\alpha\beta} \ , \quad (2)$$

and that the occupations add up to the total particle number $\sum v^2_\alpha = N$. These two presuppositions will have to be added as boundary conditions in the variation later on. Note, furthermore, that we have assumed here the case of a time-even state (ground state of even-even nuclei) for which $u_\alpha$ and $v_\alpha$ can be chosen real and for which we can construct the time-reversed wavefunction as $\varphi_{\bar{\alpha}} = -i\hat{\sigma}_y \varphi^*_\alpha$ where $\hat{\sigma}_y$ is a Pauli spin matrix.

The BCS ansatz carries only one-body information which is summarized in the two key densities: the one-body density operator

$$\hat{\rho} = \sum v^2_\alpha \varphi_\alpha \varphi^+_\alpha \ , \quad (3)$$

and the pair-density operator $\hat{\chi} = \sum u_\alpha v_\alpha \varphi_\alpha \varphi^+_\alpha$ from which we are going to use only the local part

$$\chi(r) = \sum u_\alpha v_\alpha \varphi^+_\alpha(r) \varphi_\alpha(r) \ . \quad (4)$$

Thereby, we have employed time-reversal symmetry which also yields the property $\chi^*(r) = \chi(r)$. A discussion of the physical content of the pair density can be found in [5]. Several useful properties are further discussed in [4]. Note that the one-body density matrix (3) is diagonal in the chosen representation which means that we are dealing with the natural orbital basis. It is noteworthy that the pair density is also diagonal in the same basis. This is guaranteed by the relation $[\hat{\rho}, \hat{\chi}] = 0$ which can be derived on general grounds [4].

The standard solution scheme for the HFB problem deals with a four times as large super-density-matrix which encompasses $\hat{\rho}$ as well as $\hat{\chi}$, and it proceeds in three subsequent unitary transformations [3]. There is a treatment in terms of wave functions which is particularly suited for coordinate space representations and which uses a double set of single-particle
wavefunctions, one for the occupation part and one for the non-occupation part [4]. Both schemes are plagued by the doubling of the representation which adds substantial overload to the calculations and which becomes very cumbersome in deformed nuclei. The BCS-ansatz (4) can be formulated in terms of a single set of wave functions, the natural orbitals, and a few occupation amplitudes. It is possible to keep the scheme at that level of expense by a direct variational exploitation of the ansatz, as will be shown in the following.

For simplicity, we work here with the case that the energy separates into a mean-field part and a pairing part as

$$E = E_{mf}(\hat{\rho}) + E_{pair}(\hat{\chi}) \quad .$$

(5)

Although the present scheme is applicable under more general conditions, we use now a particular model for the pairing energy, a volume pairing with a zero-range force

$$E_{pair} = \frac{1}{4} V_P \int d^3 r \, \chi(r)^2$$

(6)

which employs only the local pair density (4). The energy functional determines the mean-field Hamiltonian and pair potential as the functional derivatives

$$\hat{h}_{mf} = \frac{\partial E}{\partial \hat{\rho}} \quad , \quad \Delta(r) = \frac{\partial E}{\partial \chi(r)} = \frac{1}{2} V_P \chi(r) \quad .$$

(7)

Note that we obtain a local pair potential for the particular pairing functional (8).

The variation with respect to the occupation amplitudes $v_\alpha$ yields

$$0 = \frac{\partial (E - \epsilon_F N)}{\partial v_\alpha} = 4v_\alpha (h_{\alpha\alpha} - \epsilon_F) + 2 \left( \frac{v_\alpha^2}{u_\alpha} - u_\alpha \right) \Delta_{\alpha\alpha}$$

where $\epsilon_F$ is the Lagrange multiplier for the particle number constraint. This equation can be resolved in the standard manner and yields

$$\begin{cases} v_\alpha \\ u_\alpha \end{cases} = \frac{1}{\sqrt{\frac{1}{2} + \frac{1}{2} \frac{h_{\alpha\alpha} - \epsilon_F}{\sqrt{(h_{\alpha\alpha} - \epsilon_F)^2 + \Delta_{\alpha\alpha}^2}}}}$$

(8)

Note that the gap potential $\Delta$ does not necessarily commute with the mean-field Hamiltonian $\hat{h}$. Only the diagonal elements in the natural orbital basis enter and no information about the non-diagonal elements is needed.
The variation with respect to the single particle wavefunctions needs to take care of the orthonormality which is done by adding $-\sum_{\alpha\beta} \lambda_{\alpha\beta} (\varphi_\alpha | \varphi_\beta)$. The thus constrained variation yields

$$\hat{\mathcal{H}}_\alpha \varphi_\alpha = \sum_\beta \lambda_{\alpha\beta} \varphi_\beta \quad (9)$$

with a generalized mean-field Hamiltonian

$$\hat{\mathcal{H}}_\alpha \varphi_\alpha = \frac{\partial E}{\partial \varphi_\alpha^*} = \left[ v_\alpha^2 \hat{h}_{mf} + u_\alpha \Delta(r) \right] \varphi_\alpha.$$ \quad (10)

This $\hat{\mathcal{H}}_\alpha$ is a state dependent Hamiltonian and the full matrix of Lagrangian multipliers needs to be taken into account. Thereby it is crucial that they constitute a symmetric matrix $\lambda_{\alpha\beta} = \lambda_{\beta\alpha}$. This allows to symmetrize explicitly

$$\lambda_{\alpha\beta} = \frac{1}{2} \left( \varphi_\beta | \hat{\mathcal{H}}_\alpha + \hat{\mathcal{H}}_\beta | \varphi_\alpha \right) \quad (11)$$

which links pairwise all $\alpha$ with $\beta$ and thus eq. (9) delivers a decisive problem.

Altogether, the equations (8), (10), (9), and (11) constitute the HFB equations formulated directly in the natural orbital basis. This nonlinear problem is best solved iteratively. We propose an interlaced iteration employing the efficient damped gradient step which is best suited for coordinate space techniques:

1. Start from a given set $\{\varphi_\alpha, v_\alpha\}$.
2. Compute the densities $\hat{\rho}$ and $\chi(r)$, and subsequently the corresponding Hamiltonians $\hat{h}_{mf}$ and $\Delta(r)$.
3. Compute the new $v_\alpha$ and $u_\alpha$ according to Eq. (8).
4. Compute the action of the state-dependent mean field $\hat{\mathcal{H}}_\alpha$ and store the resulting set $\{\hat{\mathcal{H}}_\alpha \varphi_\alpha\}$.
5. Compute the matrix of constraints $\lambda_{\alpha\beta}$, Eq. (11).
6. Perform the damped gradient step with

$$\varphi_\alpha \leftarrow \mathcal{O}\{\varphi_\alpha - D_\alpha[\hat{H}_\alpha \varphi_\alpha - \Sigma_\beta \lambda_{\alpha\beta} \varphi_\beta]\}\}$$  \hspace{1cm} (12)

where $\mathcal{O}$ means orthonormalization and $D_\alpha$ is an appropriate damping operator. This completes the scheme and returns to the starting point, step 1.

The state-dependent Hamiltonian (10) requires a state-dependent damping for which we generalize the form of [6] to

$$D_\alpha = \frac{x_0}{v_\alpha^2 (50 \text{ MeV} + \hat{T}) + u_\alpha v_\alpha \frac{1}{2} \max \{\Delta(r)\}}$$  \hspace{1cm} (13)

where $\hat{T}$ is the kinetic energy operator and $x_0 \approx 0.2$ a numerical parameter. With that choice, we have implemented this scheme successfully into a spherical Skyrme-Hartree-Fock code and tested it extensively for a variety of Skyrme forces and nuclei from $^{16}\text{O}$ to the isotopes of Pb, including proton rich as well as neutron rich exotic nuclei. The scheme proves to be reliable and very efficient. It allows a fast computation of the HFB ground state, costing only 20% more iterations than the much simpler BCS approximation, and each iteration as such is as fast as in the BCS case because only one set of single particle wavefunctions is handled. We thus have a promising alternative HFB scheme which can simplify large scale calculations of deformed nuclei.
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