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Energy Density Functional Gradient Optimization for the Description of Ground States in Deformed Nuclei

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Abstract. In the present work a method is discussed for an explicit multivariate gradient descent minimization of the energy density functional, which is suitable for the description of ground states in atomic nuclei. The suggested formalism ensures a fast convergence of the minimization process with a strict criterion for arriving at the energy density functional's minimum.

1 Introduction

Although simplistic, the treatment of the many-body problem by the mean field ansatz has proven to be very successful. The mean field theory simplifies the task of accounting for all nucleon interactions separately by introducing an average potential, but it still does not provide a reasonable method for extracting physical information apart from solving the Schrdinger equation explicitly. This defficiency can be resolved by using the Hartree-Fock method, which provides an approach to finding an approximation for the quantum system wave function and the corresponding energy simultaneously from a given two-body interaction [1, 2].

It is well known that solving the exact Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle \tag{1}$$

is equivalent to solving the variational equation for the energy functional:

$$\delta E[\Psi] = 0\,. \tag{2}$$

However $|\Psi\rangle$ is not known explicitly, and instead an approximation is made such that $|\Psi\rangle$ is restricted to a set of simple trial wave functions. In the Hartree-Fock anzatz the solution of the Schrödinger equation is searched in terms of a Slater determinant.

Ignoring relativistic effects, the Hamiltonian in some complete orthonormal basis of single particle states can be written as

$$H = \sum_{i,j} T_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k\,, \tag{3}$$

where $a_i^\dagger$ and a_i are the creation and anihilation operators respectively for some single particle state $|i\rangle$, T is the kinetic energy and V is a two body force.

Or rewriting the energy density functional in terms of the single particle density matrix ρ:

$$E[\rho] = \mathrm{tr}(\rho T) + \mathrm{Tr}\,\mathrm{Tr}(\rho V \rho)\,, \tag{4}$$

where ρ is defined as:

$$\rho_{ij} = \langle \Psi | a_i^\dagger a_j | \Psi \rangle\,. \tag{5}$$

Then solving for

$$\delta E[\rho] = 0 \tag{6}$$

would yield the desired solution.

2 Energy Density Functional Gradient Optimization

The gradient descent approach for solving the Hartree-Fock equations is known and well described in the literature [3]. However it is cast in the context of applying the variational principle for the Hartree-Fock Hamiltonian by taking the respective Gateaux derivatives of the energy density functional and requiring the variation of the total energy to vanish [2]. This approach, albeit perfectly valid, requires the chosen single particle basis to be fixed in some known form before proceeding with minimizing the total energy. In the current work an attempt is made to show that this need not be the case.

2.1 The gradient descent

The gradient descent is an iterative algorithm for finding the minimum of a function. It is based on the observation that to reach a local minimum of a function it is possible to take successive steps contrary to the direction and proportional to its gradient or approximation thereof. The starting point for the method is generally unimportant as long as it is in proximity of the searched extremum.

Given a multivariate function $F(\vec{r})$ that is defined and differentiable in the neighborhood of the point $\vec{r}$, then $F(\vec{r})$ decreases fastest in the direction of the negative gradient at that point, namely $\nabla F(\vec{r})$. So introducing a sufficiently small scaling scalar parameter γ a sequence of points $\vec{r}_0, \vec{r}_1, \vec{r}_3 \ldots$ can be constructed in such a way that each successive approximation is closer to the minimum of the function:

$$\vec{r}_{n+1} = \vec{r}_n - \gamma_n \nabla F(\vec{r})\,, \tag{7}$$

where the parameter γ_n is to be determined at each step, so that

$$F(\vec{r}_0) \geq F(\vec{r}_1) \geq F(\vec{r}_3) \geq \ldots \tag{8}$$

2.2 The energy density functional as a multivariate function

In the usual treatment of the Hartree-Fock method the Hamiltonian is represented as a sum of the kinetic energy and a density dependent one-body operator Γ, the self-consistent field [2]:

$$H = T + \Gamma \,, \tag{9}$$

where Γ is defined as the contraction of the antisymmetrized two-body tensor $\tilde{V}$ with the single particle density matrix ρ:

$$\Gamma_{ik} = \sum_{jl} \tilde{V}_{ijkl} \rho_{lj} \,. \tag{10}$$

Whence the variational equation for the total energy is to be solved:

$$\delta E = E[\rho + \delta\rho] - E[\rho] = \sum_{ij} H_{ij} \delta\rho_{ji} = 0 \,. \tag{11}$$

It is possible, however, instead of proceeding to calculate the density matrix variation, to consider the matrix elements ρ_{ij} as free variables and minimize the total energy with respect to them.

The energy density functional for a general density dependent one-body hamiltonian $H[\rho]$ is writen as:

$$E[\rho] = \mathrm{tr}(\rho H[\rho]) \,. \tag{12}$$

Then to minimize the total energy the gradient descent method for the denisty matrix can be applied:

$$\rho_{n+1} = \rho_n - \gamma_n \varepsilon_n \,, \tag{13}$$

where n is the iteration step number and ε_n is the matrix representing the gradient of the energy functional with respect to the density matrix elements at that step, or written as a matrix derivative:

$$\varepsilon_n = \frac{\partial}{\partial\rho} E[\rho_n] = H^T[\rho_n] + \mathrm{tr}\left(\rho \frac{\partial}{\partial\rho} H[\rho_n]\right) . \tag{14}$$

The derivative of the Hamiltonian that appears in (14) can be evaluated numerically if analytical expression is not available.

2.3 Idempotency and number of particles

Asumming the iterations start from a density matrix which is idempotent and the intial state has an exact, well defined, number of particles the iterative procedure should keep those properties. To ensure this the idempotency condition can be imposed explicitly:

$$\rho_{n+1}^2 = \rho_{n+1} \,, \tag{15}$$

or after substituting ρ_{n+1} from (13):

$$\rho_n^2 - \gamma_n \{\rho_n, \varepsilon_n\} + \gamma_n^2 \varepsilon_n^2 = \rho_n - \gamma_n \varepsilon_n \,. \tag{16}$$

Taking into account that $\rho_n^2 = \rho_n$ it follows that:

$$-\gamma_n \varepsilon_n = -\gamma_n \{\rho_n, \varepsilon_n\} + \gamma_n^2 \varepsilon_n^2 \,, \tag{17}$$

substituting (17) back into (13) yields for the iteration step:

$$\rho_{n+1} = \rho_n - \gamma_n \{\rho_n, \varepsilon_n\} + \gamma_n^2 \varepsilon_n^2 \,. \tag{18}$$

Knowing the number of particles is given by the trace of the denisty matrix and should be invariant through the process, that is $\mathrm{tr}\,(\rho_{n+1}) = \mathrm{tr}\,(\rho_n)$

$$\mathrm{tr}\,(\rho_{n+1}) = \mathrm{tr}\,(\rho_n) - \gamma_n \,\mathrm{tr}\,(\{\rho_n, \varepsilon_n\}) + \gamma_n^2 \,\mathrm{tr}\left(\varepsilon_n^2\right), \tag{19}$$

an explicit expression for the scalar parameter γ_n can be obtained, dropping the trivial case $\gamma_n = 0$:

$$\gamma_n = \frac{\mathrm{tr}\,(\{\rho_n, \varepsilon_n\})}{\mathrm{tr}\,(\varepsilon_n^2)} \,. \tag{20}$$

2.4 Convergence and properties

As with all variants of the gradient descent method convergence is guaranteed for convex surfaces, whereas saddle points and nonconvex energy surfaces pose a significant difficulty. It is slower to converge than higher order iterative approaches like Newton or quasi-Newton methods, bit tends to be more reliable when the initial point is far from the searched extremum. The presented approach is expected, however, to be faster and more stable than searching for an energy minimum by successive diagonalizations of the Hamiltonian.

3 Conclusion

The presented method is an alternative to the usual variational treatment of the Hartree-Fock problem and shows a consideration of the minimization of the energy density functional by treating it as a multivariate function optimization. In addition the actual minimization procedure is separated cleanly from the chosen basis, as the only reagents for realizing the approach are the matrix elements of the respective operators in said basis. Furthermore, no assumptions are made about the structure of the Hamiltonian, thus there are no requirements about specific symmetries being present. As this is a work in progress a complete benchmark for speed and accuracy against established Hartree-Fock codes, like HFODD and HFBTHO, is still needed.

Further development could include applying the same principles for problems with more basis functions, as it should be possible, in principle, to employ the same anzatz for minimization of the energy density functional in more complex bases, for example such that are needed as with the self-consistent Highly truncated diagonalization approach. This would lift the need for dealing with large-scale many-body Hamiltonian diagonalization [4].

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