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Study of numerical accuracy of quadratic penalty method in covariant density functional theory

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الملخص

دراسة في الدقه العدديه لطريقة الجزاء التربيعيه في نظرية كثافة الداله

سيتم في هذا البحث دراسة الدقه العدديه لطريقة الجزاء التربيعيه في نظرية كثافة الداله و العوامل التي تعتمد عليها.

Abstrct

The solution of a system of coupled partial differential equations in density functional theory will always provide a solution that corresponds to a minimum. Quadratic penalty method is applied to obtain the solution (excited solution) at any desired point in deformation space. The accuracy of this method will be investigated and its dependence on the number of oscillator shells and number of Gauss-Hermit integration points.

Keywords: Density functional, Lagrangian multipliers, Gauss-Hermit integrationpoints.

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1 Introduction

The study the height of the fission barrier and the fission path in any nuclei requires the calculations of the binding energy as a function of all deformation parameters to be performed. However, when solving a set of partial differential equations in self-consistent theories, the obtained solution will always correspond to either a local or a global minimum. Constraints on the deformation parameter must be applied, in this investigation the method of Lagrange multipliers will be used, to get an excited solution and not to be limited only to the ground state solution. To do so, constraints on the nuclear moment $\hat{Q}$ to have an expectation value q_0 are imposed. The Hamiltonian function must be minimized to the form:

$$H' = H + c\,(\langle \hat{Q} \rangle - q_0)^2 \qquad (1)$$

Where c is stiffness constant, with

$$\frac{\partial H'}{\partial q} = 0 \qquad (2)$$

In general, one can impose as many constraints as needed, but as their numbers increase, the solution becomes unstable and will always diverge. To avoid the numerical instability in this investigation, only the qudrupole constraints will be imposed, i.e. $\hat{Q}_{20}$ and $\hat{Q}_{22}$.

The manuscript is organized as follows. General properties of covariant density functional theory and penalty quadratic constrains methods are discussed in Sec. 2. Finally, in Sec. 3, the results of calculations are discussed.

2 Theoretical framework and the details of numerical calculations

In covariant density functional theory (CDFT), the nucleons are described by the Dirac spinors with mass m and several effective mesons characterized by the quantum numbers of spin, parity and isospin. The

create effective fields in Dirac equation, which corresponds to the Khon-Sham equation[1] in the non-relativistic case. The starting point of Covariant Density Functional Theory (CDFT) is a standard Lagrangian density [2]

$$L = \bar{\Psi}\left(\gamma\left(i\partial - g_\omega\omega - g_\rho\vec{\rho}\vec{\tau} - eA\right) - m - g_\sigma\sigma\right)\Psi + \frac{1}{2}(\partial\sigma)^2 - \frac{1}{2}m_\sigma^2\sigma^2 - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2\omega^2 - \frac{1}{4}\vec{R}_{\mu\nu}\vec{R}^{\mu\nu} + \frac{1}{2}m_\rho^2\vec{\rho}^2 - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} \quad (3)$$

The Lagrangian (3) contains as parameters the meson masses m_σ, m_ω and m_ρ and the coupling constants g_σ, g_ω, and g_ρ. e is the charge of the protons. This model has been first introduced by Walecka [3, 4]. It has turned out that surface properties of finite nuclei cannot be described properly by this model. Therefore, Boguta and Bodmer [5] introduced a density dependence via a non-linear meson coupling replacing the term $\frac{1}{2}m_\sigma^2\sigma^2$ in Eq.(3) by

$$U(\sigma) = \frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{3}g_2\sigma^3 + \frac{1}{4}g_3\sigma^4 \quad (4)$$

The equations of motion obtained from the Lagrangian are solved in the basis of an anisotropic three-dimensional harmonic oscillator in Cartesian coordinates characterized by the deformation parameters β_0 and γ and oscillator frequency $\hbar\omega = 41A^{-1/3}$ MeV, for details see Refs. [6,7]. The truncation of basis is performed in such a way that all states belonging to the shells up to fermionic N_F and bosonic N_B are taken into account.

The calculations are performed with the NL3* parameterization of the RMF Lagrangian [8] shown in Table 1. Apart from the fixed values for the masses m = 939 MeV, m_ω = 782:6 MeV and m_ρ = 763 MeV it contains six phenomenological parameters m_σ, g_σ , g_ω , g_ρ; g_2, and g_3, For details of calculation see Ref. [9].

Table 1.Parameters of the effective interaction NL3* in the RMF Lagrangian

Parameters of NL3*
m = 939 (MeV)
m_σ = 502.5742 (MeV) g_σ = 10.0944
m_ω= 782.600 (MeV) g_ω = 12.8065
m_ρ= 763.000 (MeV) g_ρ = 4.5748
g_2 = -10.8093 (fm^{-1})
g_3 = -30.1486

2.1 Constraints methods: Penalty Quadratic constraints

The calculations are performed imposing constraints on the axial and triaxial mass quadrupole moments. The method of quadratic constraints uses a variation of the function:

$$< H > + \sum_{\mu=0,2} C_{2\mu}(< \hat{Q}_{2\mu} > - q_{2\mu})^2 \quad (5)$$

Where $< H >$ is the total energy, and $< \hat{Q}_{2\mu} >$ denotes the expectation values of the mass quadrupole operators

$$\hat{Q}_{20} = 2Z^2 - X^2 - Y^2 \quad (6)$$

$$\hat{Q}_{22} = X^2 - Y^2 \quad (7)$$

In these equations, $q_{2\mu}$ is the constrained value of the multipole moment, and $C_{2\mu}$the corresponding stiffness constants [10].

The quadratic constraints add a parabola to the energy curve, so it's creating a local minimum that corresponds to the excited energy. By repeating this method of calculation, the deformation space (Q_{20};Q_{22}), can be mapped and the total binding energy for each point in that space is obtained. The accuracy of this method will be investigated, and its dependence on the number of fermionic shells N_F and number of Gauss-Hermit integration points will be discussed in Sec.3.

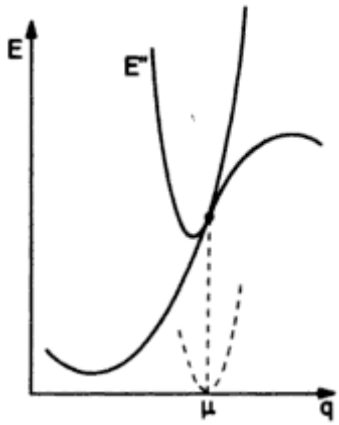

Figure 1: Schematic representation of the quadratic constrains [10]

3 Results and Discussion

The dependence of the accuracy of the penalty quadratic method on the number of fermionic shells N_F and number of Gauss-Hermit integration points is investigated by performing calculations on ^{240}Pu using the NL3*. Fig. 2 shows that near axial symmetric shapes the obtained point in deformation space made of (Q_{20}; 0) is equal to the desired point. However, as we go intro regions with non-zero -deformation, i.e. $Q_{20} \neq 0$, deviation from desired points starts to show up, and as the value of Q_{20} increases the deviation become larger and clearer. As the number of shells increases from 10 to 18, this difference decreases, although it still present. For example, the black circles (which represent the points calculate with N_F=10) at Fig. 2, deviate the most from the desired points (represented by the yellow circles), specially near the points (0.8,0.9) and (0.9,0.9). The points obtained using larger number of shells is clustered on top of each other, and are very close to the desired points. It can be noted that the accuracy of the quadratic penalty method is also dependent on the range of deformation at which the calculations are performed.

When plotting potential energy surfaces, the deviation between the desired and obtained points will make some information about the nucleus to be lost. Calculations has been performed for ^{240}Pu using N_F=20 and two

different values of Gauss-Hermit points 12 and 24, as shown in Figs. 3 and 4.When comparing the two potential energy surfaces, for ^{240}Pu, one can notice that the general topography is very similar, both have an axial symmetric minimum with qudrupole deformation β_2=0.2 and β_2= 0.85. However, there are two major differences between both figures, the first one is the minimum that appears near β_2=1.0 and γ=15^o in Fig. 3, and not showing up in Fig. 4. Thus, increasing the number of integration points will increase the accuracy of the constrained calculations.

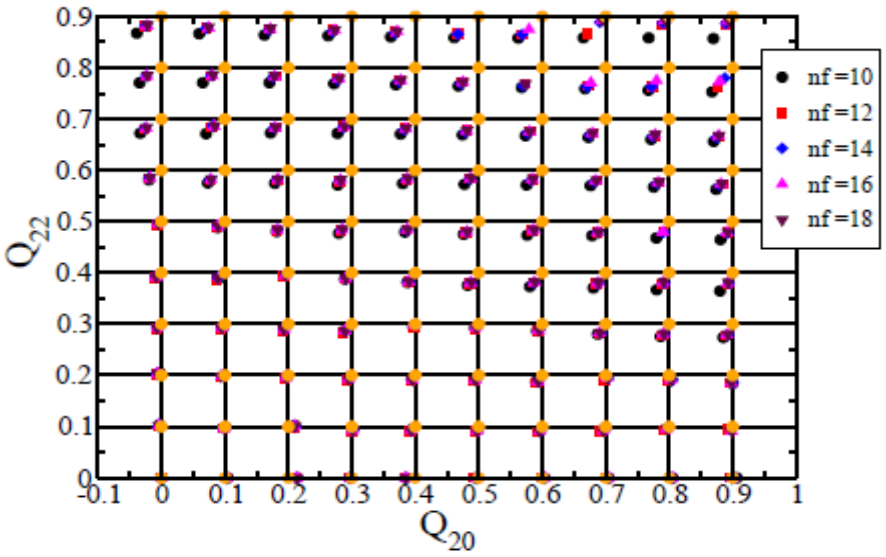

Figure 2: The difference between the desired points and obtained points for 24 Gauss-Hermit points and several values of N_F. Yellow circles shows the desired points

The second difference is that near $\beta_2$2=1.0 and γ =0, when done with 24 points, all the surfaces are concave. However, when it is done at 12 points, one can notice that one of the surfaces isn't concave, but a straight line instead.

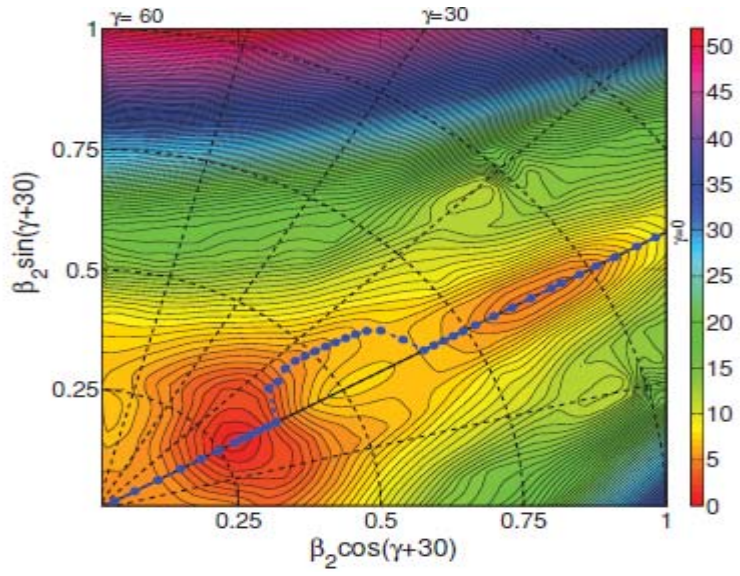

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Figure 3: Potential energy surfaces for 240Pu, using NF =20 and 24 integration points [9].

The concave lines are an indication on the direction of the minimum energy fission path, while the straight lines don't give such an indication. The concavity of the surfaces determines in which direction the fission path must go. The effect of number of integration points has its origin from the fact that as the shape transition from spherical to superdeformed and then into hyperdeformed, then into fission. Due to the increase in the surface area and thus larger contribution to the surface energy, more integration points on the surface will be needed.

Finally, as the deformation increases, the surface area of the nucleus increases, and more integration points will be needed to obtain the needed numerical accuracy. When we performed calculations using 12 Gauss-Hermit integration points we were able only to go up to $\beta_2 = 1.0$, and beyond this deformation the calculations were unstable and often no convergence is obtained.

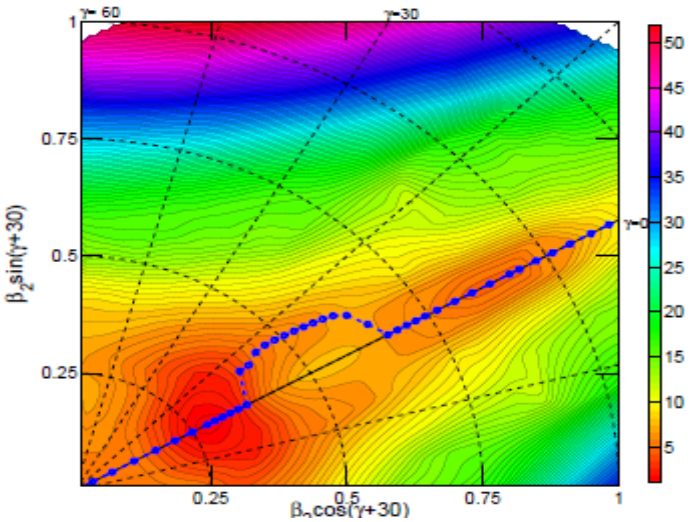

Figure 4: The same as Fig. 3, but using 12 integration points

However, as the number of integration points increased from 12 to 24, we were able to perform calculations up to $\beta_2 = 2.3$, with no problems in stability of the solution, and we were able always to get a convergent solution. Using this result we can start to perform calculations to study the effect of both triaxial and octupole deformation on the height of the outer fission barrier in actinides. These calculations are ongoing and will be discussed in details in a future manuscript.

4 Conclusions

The accuracy of the quadratic penalty method of the Lagrangian multipliers has been investigated. It was found that the dependence on the number of Gauss-Hermit integration points is important. When the calculations were performed for two different numbers of Gauss-Hermit points, mainly 12 and24 points, it was found that one could miss a minimum if the calculations were performed with insufficient number of integration points. It was also found that the accuracy of the quadratic penalty method is dependent on the range of deformation at which the calculations are performed.

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