

The nuclear Energy Density Functional formalism

Preliminary document

Lagrange method

T. Duguet*

*Centre de Saclay, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France
National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824, USA and
Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA*

The Lagrange method to minimize a function under a set of constraints is briefly summarized.

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*Electronic address: thomas.duguet@cea.fr

I. INTRODUCTION

Consider a function $E(x_1, x_2, \dots, x_n)$ depending on n variables $\{x_i\}$. One would like to determine the minimum of E in the n dimensional space assuming that the variables $\{x_i\}$ obey $m < n$ constraints. Such constraints manifest through the set of independent equations

$$G_k(x_1, x_2, \dots, x_n) = 0, \quad k = 1, 2, \dots, m . \quad (1)$$

The independence of the m equations means that there is no non-zero constants $\{a_k\}$ such that

$$\sum_{k=1}^m a_k G_k(x_1, x_2, \dots, x_n) = 0 . \quad (2)$$

A variation $\{\delta x_i\}$ of $\{x_i\}$ generates a first-order variation of E of the form

$$\delta E(x) = \sum_{i=1}^n \frac{\partial E}{\partial x_i}(x) \delta x_i . \quad (3)$$

The variation $\delta E(x)$ is null for any variation δx_i around the point $x_0 = \{x_{0i}\}$ where E reaches its minimum. Consequently, the function E satisfies at $x = x_0$ the condition

$$\sum_{i=1}^n \frac{\partial E}{\partial x_i}(x) \delta x_i = 0, \quad \forall \delta x_i, \quad i = 1, 2, \dots, n . \quad (4)$$

– For independent variables $\{x_i\}$, and thus independent variations $\{\delta x_i\}$, the condition (4) is equivalent to fulfilling simultaneously the n independent equations

$$\left. \frac{\partial E}{\partial x_i}(x) \right|_{x=x_0} = 0, \quad \forall i = 1, 2, \dots, n , \quad (5)$$

that eventually provide $\{x_{0i}\}$.

– Taking the constraints (1) into account, the n variations $\{\delta x_i\}$ can no longer be considered as being independent. Their interrelations manifest through the m equations obtained by varying Eq. (1) according to

$$\sum_{i=1}^n \frac{\partial G_k}{\partial x_i}(x) \delta x_i = 0, \quad k = 1, 2, \dots, m . \quad (6)$$

As a consequence, only $n-m$ of the n variations $\{\delta x_i\}$ are independent and Eq. (4) is no longer equivalent to the set of equations (5).

II. LAGRANGE METHOD

The Lagrange method is designed to solve the above difficulty in an elegant and practical manner. The method consists of multiplying each of the m equations (6) by an arbitrary number λ_k , summing over k and subtracting the result from Eq.(4). Such a procedure leads to

$$\sum_{i=1}^n \left[\frac{\partial E}{\partial x_i}(x) - \sum_{k=1}^m \lambda_k \frac{\partial G_k}{\partial x_i}(x) \right] \delta x_i = 0 \quad (7)$$

One can then choose the m parameters λ_k so that the m equations

$$\frac{\partial E}{\partial x_i}(x) - \sum_{k=1}^m \lambda_k \frac{\partial G_k}{\partial x_i}(x) = 0, \quad i = 1, 2, \dots, m \quad (8)$$

are satisfied. This is possible if the square matrix made out of elements $\frac{\partial G_k}{\partial x_i}(x)$ with $k, i = 1, 2, \dots, m$ is invertible. If it is not the case, one has to find a better suited set of m variables $\{x_i\}$ among the n ones. As the constraints (1)

are independent, there is necessarily a choice of m variables $\{x_i\}$ such that the matrix $\frac{\partial G_k}{\partial x_i}(x)$ is invertible. In the present case, Eq. (7) reduces to

$$\sum_{i=m+1}^n \left[\frac{\partial E}{\partial x_i}(x) - \sum_{k=1}^m \lambda_k \frac{\partial G_k}{\partial x_i}(x) \right] \delta x_i = 0 \quad , \quad (9)$$

which now contains $n-m$ independent variations $\{\delta x_i\}$. Equation (9) stands for any such independent variations if one has

$$\frac{\partial E}{\partial x_i}(x) - \sum_{k=1}^m \lambda_k \frac{\partial G_k}{\partial x_i}(x) = 0 \quad , \quad (10)$$

for each $i = m+1, m+2, \dots, n$. Adding Eq. (8), one eventually obtains the set

$$\frac{\partial E}{\partial x_i}(x) - \sum_{k=1}^m \lambda_k \frac{\partial G_k}{\partial x_i}(x) = 0, \quad \forall i = 1, 2, \dots, n \quad , \quad (11)$$

which is eventually equivalent to

$$\frac{\partial}{\partial x_i} \left(E(x) - \sum_{k=1}^m \lambda_k G_k(x) \right) = 0, \quad \forall i = 1, 2, \dots, n \quad . \quad (12)$$

By comparing Eq. (12) with Eq. (5), one notes that the Lagrange method works as if the function E had been replaced by the function $E - \sum_{k=1}^m \lambda_k G_k$, while considering the n variations δx_i as being independent. The quantities $\{\lambda_k\}$ are the so-called Lagrange parameters, or Lagrange multipliers, and are as many as the number of constraints (1) imposed on the variables $\{x_i\}$. Lagrange parameters constitute m unknowns in the minimization procedure and are determined such that the solution of Eq. (12) does fulfill the constraints (1).