THE LAGRANGIAN OF THE THOMAS–FERMI MODEL

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Introduction

The Thomas–Fermi model is one of the quasiclassical approximations of the quantum mechanics which in good approximation describes the ground states of central symmetric atoms, molecules, ions, and in general those systems which consist of a number of particles obeying the Fermi–Dirac statistics (electrons, neutrons, protons, etc.).

Within the frames of this model the systems consisting of electrons may be characterized either by the density function $n(x, y, z)$ which gives the number of electrons in unit volume, i.e.,

$$n = \mathrm{d}N/\mathrm{d}V\,, \tag{1}$$

or by the electric potential $U(x, y, z)$, whose source is the electric charge density $\varrho = Zen$, where e is the elementary electric charge and in the case of electrons $Z = -1$.

The basic equations of the model are the relation between n and U, i.e.,

$$U - U_0 = (5K/2e)\, n^{2/3}\,, \tag{2}$$

where U_0 and K are two constants, as well as the potential equation

$$\varepsilon_0 \operatorname{div} \operatorname{grad} (U - U_0) = en\,, \tag{3}$$

where ε_0 is the dielectricity of the vacuum.

Eqs (2) and (3) may be amalgamated into the single Thomas–Fermi equation

$$\varepsilon_0 \operatorname{div} \operatorname{grad} (U - U_0) = e \cdot (3e/5K)^{3/2} \cdot (U - U_0)^{3/2}. \tag{4}$$

This equation is ultimately the basic equation of the model.

In the case where external electric fields are present, their potential U_{ext} may be amalgamated into U because

$$\operatorname{div} \operatorname{grad} U_{\mathrm{ext}} = 0\,. \tag{5}$$

The equations (2), (3), and (4) are not altered by this procedure.

2. The Lagrangian

In the present note we show that both Eqs (2) and (3) may be derived as Eulerian equations from the following Lagrangian

$$L_1 = K\, n^{5/3} - e\, n\, U - \frac{\varepsilon_0}{2} \operatorname{grad} U \cdot \operatorname{grad} U\,, \tag{6}$$

i.e., from the following variational principle

$$\delta \iiint L_1\, dx\, dy\, dz = 0\,, \tag{7}$$

which is supplemented by the restriction

$$N = \iiint n\, dx\, dy\, dz = \text{const}\,, \tag{8}$$

i.e.,

$$\delta N = 0\,, \tag{9}$$

where N is the number of electrons of the system in question.

Proof. By the Lagrangian multiplier U_0 Eqs (7) and (9) may be contracted into one equation. This single equation reads

$$\delta \iiint L\, dx\, dy\, dz = 0\,, \tag{10}$$

where

$$L = L_1 + e\, n\, U_0 = K n^{5/3} - e n (U - U_0) - \frac{\varepsilon_0}{2} \operatorname{grad}(U - U_0)\,.\ \operatorname{grad}(U - U_0)\,. \tag{11}$$

Varying n and U as independent field variables one gets from (10) the following two Eulerian equations

$$\frac{\partial L}{\partial n} \equiv \frac{5}{3} K n^{2/3} - e(U - U_0) = 0\,, \tag{12}$$

and

$$\frac{\partial L}{\partial U} - \frac{\partial}{\partial x} \frac{\partial L}{\partial \frac{\partial U}{\partial x}} - \frac{\partial}{\partial y} \frac{\partial L}{\partial \frac{\partial U}{\partial y}} - \frac{\partial}{\partial z} \frac{\partial L}{\partial \frac{\partial U}{\partial z}} \equiv -e n + \varepsilon_0 \operatorname{div} \operatorname{grad}(U - U_0) \equiv 0\,, \tag{13}$$

coincident with (2) and (3), by which our statement is proved.

3. The physical meaning of the Lagrangian

Now we show that the Lagrangian (6) is equivalent to the total energy density of the system

$$\varepsilon(x, y, z) = Kn^{5/3} + \frac{1}{2} \bar{E}\,\bar{D}, \tag{14}$$

where $Kn^{5/3}$ is the kinetic energy density of the electron gas and $\frac{1}{2}\bar{E}\bar{D}$ is the energy density of the electric field produced by the electron gas as source.

The Lagrangian of Eqs (2) and (3) is

$$L = L_1 + en\,U_0 = Kn^{5/3} - e\,n(U - U_0) - \frac{\varepsilon_0}{2} \operatorname{grad}(U - U_0) \,.\, \operatorname{grad}(U - U_0)\,. \tag{15}$$

According to Eq. (3)

$$en = \varepsilon_0 \operatorname{div} \operatorname{grad}(U - U_0), \tag{3}$$

and so (15) becomes

$$L = Kn^{5/3} - \varepsilon_0(U - U_0) \operatorname{div} \operatorname{grad}(U - U_0) - \frac{\varepsilon_0}{2} \operatorname{grad}(U - U_0) \operatorname{grad}(U - U_0), \tag{16}$$

i.e.,

$$L = Kn^{5/3} - \varepsilon_0 \operatorname{div}\left[(U - U_0) \operatorname{grad}(U - U_0)\right] + \frac{\varepsilon_0}{2} \operatorname{grad}(U - U_0) \operatorname{grad}(U - U_0). \tag{17}$$

Since the Eulerian of $\operatorname{div}(f \operatorname{grad} f)$ vanishes, the Lagrangian (17) is equivalent to:

$$L' = Kn^{5/3} + \frac{\varepsilon_0}{2} \operatorname{grad}(U - U_0) \operatorname{grad}(U - U_0)\,. \tag{18}$$

Taking into account that

$$\bar{E} = -\operatorname{grad}(U - U_0) \tag{19}$$

and

$$\bar{D} = -\varepsilon_0 \operatorname{grad}(U - U_0)$$

one sees that (18) and (14) are identical. Thus we see that the Lagrangian (11) is equivalent to the energy density of system (14).

If the potential $U - U_0$ or grad $(U - U_0)$ vanishes either in the spatial infinity, or at the edge of the system, the Lagrangian and the energy density are not only equivalent but identical.

4. The second Lagrangian

The unified Thomas—Fermi equation (4) also may be derived from a Lagrangian. It reads

$$L_2 = \frac{2e}{5}\left(\frac{3e}{5K}\right)^{3/2}(U - U_0)^{5/2} + \frac{\varepsilon_0}{2}\,\mathrm{grad}\,(U - U_0)\;\mathrm{grad}\,(U - U_0)\,. \tag{20}$$

L_2 is also equivalent to (14).

Summary

It is shown that the Thomas—Fermi equation of the statistical theory of atoms and molecules may be derived from a Lagrangian. The concrete form of the Lagrangian is given.

References

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