DENSITY FUNCTIONAL METHOD IN NUCLEAR THEORY

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I. INTRODUCTION

The theory of many-body systems is based on the many-particle Schrodinger equation. During more than eight decades enormous progress $r(\vec{\mathrm{r}})$ has been made in finding approximate solutions of Schrodinger’s equation for systems with several particles, decisively aided by modern electronic computers. However, already one year later after publishing first E.Schrodinger paper making a beginning of the wave mechanics (1926) Thomas and Fermi suggested another approach which can be considered as the simplest variant of the Density Functional theory.

This variant is an alternative approach to the many particle systems in which the particle density distribution

$$\rho(\vec{r})$$

rather than many-particle wave function , plays a central role. Density functional theory is applied now in atomic physics, chemistry, nuclear physics.

Density functional theory makes two kinds of contributions to the theory of many-particle systems.

The first is that following the path of the Schrodinger equation we are thinking in terms of a truncated Hilbert space. However, when sufficiently high accuracy is required the huge basis is needed for a diagonalization of the Hamiltonian. Many components of a total wave function obtained in this way have very small weights and we do not know is there any physics in these values.

Density functional theory provides a complementary perspective. It focuses on quantities in the real 3-dimensional coordinate space, principally on the particle density. Other quantities of great interest are: the exchange correlation density

$$r_{exc}(\overset{\mathbf{r}}{r},\overset{\mathbf{r}}{r}')$$

which describes how the presence of a particle at point “r” depletes the total density of the other particles at the point “ r’ ”; the linear response function,

$$c(\overset{\mathbf{r}}{r},\overset{\mathbf{r}}{r}';w)$$

which describes a change of total density at point “r” due to a perturbing potential at the point “ r’ ” with frequency

$$w$$

Construction of an accurate approximation to the many-particle wave function $\Psi(\vec{r}_1,\ldots,\vec{r}_n)$

Let us assume that an approximate wave function $\tilde{\Psi}$ is sufficiently accurate if

$$|\langle\tilde{\Psi}\,|\,\Psi\rangle\,|^2 \rangle\rangle\, 0.5$$

Consider a system of N particles.

Let we have a very accurate single particle wave function

$$y_{sp}$$

$$|\langle\tilde{y}_{sp}|y_{sp}\rangle| = 1 - e$$

where $e \approx 0.01$

Then for N=200-300

$$|\langle\tilde{\Psi}|\Psi\rangle| = \left(1 - e\right)^{N} \approx e^{-Ne} = e^{2\div 3}$$

For the fully interacting system the situation is much worse.

Recording of the total wave function

$$\Psi(\vec{r}_1, \ldots\ldots, \vec{r}_N)$$

Let us take ‘q’ bits for variable. The total number of bits for N-particle system is

$$B = q^{3N}$$

For N=200 and q=3 (very rough fit)

$$B = 3^{600} \approx 10^{300}$$

The total number of baryons in the accessible universe is estimated as 10^{80}

THOMAS–FERMI METHOD

In heavy atoms the main part of the electrons is in the states with large quantum numbers, i.e. in the states with an electron wave length much smaller than a dimension of atom. In this case aquasiclassical approximation can be applied, i.e. we can talk about a particle momentum as a function of coordinate.

Let $-e\varphi(\vec{r})$ is a potential energy of an electron at the point $\vec{r}$ (e¿0). In the stationary state the maximum total energy must be the same at all points of an atom. Denote this value as $-eA$. Let $p_m(\vec{r})$ is the maximum value of the electron momentum at a point $\vec{r}$. We have

$$\frac{1}{2\mu}p_m^2(\vec{r}) - e\varphi(\vec{r}) = -eA \qquad (1)$$

At the same time in the ground state the maximum momentum of an electron in some volume v is determined by an electron density $\rho(\vec{r})$ in this volume

$$\rho(\vec{r}) = 2\frac{4\pi/3p_m^3(\vec{r})v}{(2\pi\hbar)^3} \tag{2}$$

or

$$\rho(\vec{r}) = \frac{p_m^3(\vec{r})v}{3\pi^2\hbar^3} \tag{3}$$

Substituting $p_m(\vec{r})$ we obtain

$$\rho(\vec{r}) = \frac{(2\mu e(\varphi(\vec{r}) - A))^{3/2}}{3\pi^2\hbar^3} \tag{4}$$

On a boundary of an atom of a radius R $\rho(R) = 0$, i.e.

$$\varphi(R) = A \tag{5}$$

For neutral atom $A = 0$. For partly ionized atom with N electrons

$$A = \frac{e(Z - N)}{R} \tag{6}$$

If $r \to 0$ potential φ should coincide with a potential of a nucleus

$$\varphi \to \frac{eZ}{r} \tag{7}$$

and

$$\lim r\varphi(r) = eZ \tag{8}$$

Electrostatic potential φ is connected with density ρ by the equation

$$\triangle\varphi = 4\pi e\rho \tag{9}$$

Substituting an expression for φ we obtain an equation for a density ρ.

THE HOHENBERG–KOHN FORMULATION OF DENSITY–FUNCTIONAL THEORY

The basic lemma of HK

The ground–state density $\rho(r)$ of a bound system of interacting particles in some external potential $V(r)$ determines this potential uniquely (Hohenberg and Kohn, 1964).

Let $\rho(r)$ be the nondegenerate ground state density of N particles in the potential $V_1(r)$, corresponding to the ground state Ψ_1 , and the energy E_1. Then

$$E_1 = (\Psi_1, H_1\Psi_1)$$
$$= \int V_1(r)\rho(r)dr + (\Psi_1, (T+U)\Psi_1), \quad (1)$$

where H_1 is the total Hamiltonian corresponding to V_1, and T and U are the kinetic and interacting energy operators.

Now assume that there exists a second potential $V_2(r)$ not equal to $V_1(r)+const$, with ground state Ψ_2, necessarily not equal to $e^{\imath\theta}\Psi_1$, which give rise to the same $\rho(r)$. Then

$$E_2 = \int V_2(r)\rho(r)dr + (\Psi_2, (T+U)\Psi_2) \quad (2)$$

Since Ψ_1 is assumed to be nondegenerate, the Rayleigh–Ritz minimal principle for Ψ_1 gives the inequality

$$
\begin{aligned}
E_1 &< (\Psi_2, H_1\Psi_2) \\
&= \int V_1(r)\rho(r)dr + (\Psi_2, (T+U)\Psi_2) \\
&= E_2 + \int (V_1(r) - V_2(r))\,\rho(r)dr. \qquad (3)
\end{aligned}
$$

Similarly

$$
\begin{aligned}
E_2 &< (\Psi_1, H_2\Psi_1) \\
&= E_1 + \int (V_2(r) - V_1(r))\,\rho(r)dr \qquad (4)
\end{aligned}
$$

Adding equations (3) and (4) leads to the contradiction

$$E_1 + E_2 < E_1 + E_2 \qquad (5)$$

We conclude that the assumption of the existance of a second potential $V_2(r)$, which is unequal to $V_1(r) + constant$ and gives the same $\rho(r)$, must be wrong.

Since $\rho(r)$ determines both N and $V(r)$ it gives us the full H and N for the system. Hence $\rho(r)$ determines implicitly all properties derived from H through the solution of the time–dependent or time–independent Schrödinger equation (even in the presence of additional perturbations).

THE HOHENBERG–KOHN VARIATIONAL PRINCIPLE

The important property of the ground state is its energy E. By wave–function methods E could be calculated either by direct approximate solution of the Schrödinger equation $H\Psi = E\Psi$ or from the Rayleigh–Ritz minimal principle,

$$E = min_{\tilde{\Psi}} \left(\tilde{\Psi}, H\tilde{\Psi}\right), \tag{1}$$

where $\tilde{\Psi}$ is a normalized trial function for the given number of particles N.

The formulation of the minimal principle in terms of trial densities $\tilde{\rho}(r)$, rather than trial wave functions $\tilde{\Psi}$ was first presented in Hohenberg and Kohn (1964). Every trial function $\tilde{\Psi}$ corresponds to a trial density $\tilde{\rho}(r)$ obtained by integrating $\tilde{\Psi} \times \tilde{\Psi}$ over all variables except the first and multiplying by N.

One may carry out the minimization in two stages. First fix a trial $\tilde{\rho}(r)$ and denote by $\tilde{\Psi}^{\alpha}_{\tilde{\rho}}$ the class of trial functions with this $\tilde{\rho}(r)$. We defined the constrained energy minimum, with $\tilde{\rho}(r)$ fixed, as

$$\begin{aligned} E_v[\tilde{\rho}(r)] &\equiv min_{\alpha}\left(\tilde{\Psi}^{\alpha}_{\tilde{\rho}}, H\tilde{\Psi}^{\alpha}_{\tilde{\rho}}\right) \\ &= \int V(r)\tilde{\rho}(r)dr + F[\tilde{\rho}(r)], \end{aligned} \qquad (2)$$

where

$$F[\tilde{\rho}(r)] \equiv min_{\alpha}\left(\tilde{\Psi}^{\alpha}_{\tilde{\rho}}, (T+U)\tilde{\Psi}^{\alpha}_{\tilde{\rho}}\right). \qquad (3)$$

$F[\tilde{\rho}(r)]$ is a universal function of the density $\tilde{\rho}(r)$. In the second step minimize (2) over all $\tilde{\rho}(r)$,

$$E = min_{\tilde{\rho}(r)} E_v[\tilde{\rho}(r)]$$
$$= min_{\tilde{\rho}(r)} \left(\int V(r)\tilde{\rho}(r)dr + F[\tilde{\rho}(r)] \right). \quad (4)$$

For a nondegenerate ground state, the minimum is attained when $\tilde{\rho}(r)$ is the ground state density.

The Hohenberg–Kohn minimum principle may be considered as the formal exactification of Thomas–Fermi theory.

The formidable problem of finding the minimum of $\left(\tilde{\Psi}, H\tilde{\Psi}\right)$ with respect to the $3N$–dimensional trial function Ψ has been transformed into the *seemingly* trivial problem of finding the minimum of $E_v[\tilde{\rho}(r)]$ with respect to the trial function $\tilde{\rho}(r)$.

Actually the definition of $F[\tilde{\rho}(r)]$ leads right back to minimization with respect to $3N-$ dimensional trial wave functions. Nevertheless significant *formal* progress has been made: the strict formulation of the problem of the ground state densities and energies entirely in terms of the density distribution $\tilde{\rho}(r)$ and of a well defined but not explicitly known functional of the density, $F[\tilde{\rho}(r)]$, which represents the sum of kinetic energy and interaction energy $(T+U)$, associated with $\tilde{\rho}(r)$.

One could now easily rederive the Thomas–Fermi theory by making the approximations

$$T = \int \rho(r) \frac{3}{10} k_F^2[\rho(r)] dr,$$
$$U = \frac{1}{2} \int \frac{\rho(r)\rho(r')}{|r - r'|} dr\, dr', \tag{5}$$

where $k_F(\rho)$ is the Fermi wave vector of a uniform electron gas of density ρ and $\frac{3}{10}k_F^2(\rho)$ is the mean kinetic energy per electron of such a gas.

The expression for U is the classical (or mean field) approximation. Various previously known corrections of Thomas–Fermi theory could also be rederived.

The main remaining error is due to the seriously inadequate representation of the kinetic energy T by equation (5) or its gradient–corrected forms. This deficiency is largly remedied by the self–consistent, so–called Kohn–Sham equations.

The self—consistent Kohn—Sham equations

Soon after the publication of the Thomas-Fermi theory, Hartree (1928) proposed a set of self-consistent single-particle equations for the approximate description of the electronic structure of atoms. The concept was physically very simple. Every electron was regarded as moving in an effective single-particle potential

$$V_H(r) = -\frac{Z}{r} + \int \frac{\rho(r')}{|r - r'|} dr' \qquad (1)$$

where the first term represents the potential due to a nucleus of atomic number Z and the second the potential due to the average electronic density distribution (the negative charge of the electron has been used for). Thus each electron obeys the single particle Schrodinger equation

$$\left(-\frac{1}{2}\nabla^2 + V_H(r)\right)\varphi_j(r) = \epsilon_j\varphi_j(r) \tag{2}$$

where “j” denotes both spatial as well as spin quantum numbers. The mean density is given by

$$\rho(r) = \sum_{j=1}^{N} \left|\varphi_j(r)\right|^2 \tag{3}$$

where, in the ground state, the sum runs over the N lowest eigenvalues, to respect the Pauli principle. Equations (1—3) are called the self—consistent Hartree equations.

One may start from the first approximation for

$$\rho(r)$$

(e.g., from Thomas—Fermi theory), construct $V_H(r)$, solve Eq. (2) for the single—particle wave functions and recalculate

$$\rho(r)$$

f

from Eq. (3). Then iterates until a density distribution will be the same as the initial one. The Hartree equations described atomic ground state much better than Thomas—Fermi theory. The difference between them lay in a different treatment of the kinetic energy.

The Hartree differential equation (2) has the form of the Schrodinger equation for noninteracting electrons moving in the external potential V_H .

For a system of noninteracting electrons the Hohenberg—Kohn variational principle takes the form

$$E_{V(r)}[\tilde{\rho}] \equiv \int V(r)\tilde{\rho}(r)dr + T_s[\tilde{\rho}(r)] \geq E$$

where $T_s[\tilde{\rho}(r)]$ Is the kinetic energy of the

ground state of noninteracting electrons with density distribution $\tilde{\rho}(r)$

The Euler—Lagrange equations embodying the fact that the last expression is stationary with respect to variations of $\tilde{\rho}(r)$ which leave the total number of electrons unchanged is

$$\delta E_V[\tilde{\rho}(r)] \equiv \int \delta\tilde{\rho}(r)]\left(V(r) + \frac{\delta}{\delta\tilde{\rho}(r)} T_s[\tilde{\rho}(r)]\big|_{\tilde{\rho}\equiv\rho} - \epsilon\right) dr = 0 \qquad (5)$$

where $\tilde{\rho}(r)$ is the exact ground state density for V(r). Here ϵ is a Lagrange multiplyer to assure particle conservation.

In this soluble, noninteracting case we know that the ground state energy and density can be obtained by calculating the eigenfunctions φ_j and eigenvalues ϵ_j of noninteracting, single particle equations

$$\left(-\frac{1}{2}\nabla^2 + V(r) - \epsilon_j\right)\varphi_j(r) = 0 \qquad (6)$$

yielding

$$E = \sum_{j=1}^{N} \epsilon_j$$

$$\rho(r) = \sum_{j=1}^{N} |\varphi_j(r)|^2 \qquad (7)$$

Returning now to the problem of interacting electrons, which had previously been addressed approximately by the single particle like Hartree equation, we deliberately wrote the functional $F[\tilde{\rho}(r)]$ in the form

$$F[\tilde{\rho}(r)] \equiv T_s[\tilde{\rho}(r)] + \frac{1}{2}\int \frac{\tilde{\rho}(r)\tilde{\rho}(r')}{|r-r'|} dr dr' + E_{xc}[\tilde{\rho}(r)] \quad (8)$$

where $T_s[\tilde{\rho}(r)]$ is the kinetic energy functional for noninteracting electrons. The last term $E_{xc}[\tilde{\rho}(r)]$,

the so called exchange—correlation energy functional is defined by Eq. (8).

Exchange effect

Compare to Hartree approximation the Hartree-Fock approximation leads to an additional, nonlocal exchange term in the Schrodinger equation but does not change the single particle picture, with the wave function described in terms of orbitals with particular spin and occupation numbers.

Shortly after Dirac proposed that exchange effects be included by incorporating a term derived from the exchange energy density in a homogeneous system

$$e_{exc}^{Dirac} = 0.458/r_s (a.u.)$$

where r_s is a measure of the interelectronic distance. The use of the approximate exchange potential in addition to the Hartree term was suggested by Slater. The exchange interaction means that an electron of a given spin will be surrounded by a region where the density of electrons with the same spin is reduced. An introduction of a local exchange potential reproduced HF eigenfunctions and eigenvalues very well showing that an approximation based on the results for a homogeneous system could give a satisfactory description.

The above work has been essential to the development of modern Density Functional theory. As an approximation to the nonlocal exchange potential, the simple local approximation provided the basis for much of the work on the electronic structure of solids. In poractice, total energy calculations require approximations to be made for the exchange correlation energy, E_{xc}, and Kohn and Sham showed that the local density approximation could be applied to the cases of a slowly varying density and very high density.

The Hohenberg—Kohn variational principle for interacting electrons now takes the form

$$E_V[\tilde{\rho}(r)] \equiv \int V(r)\tilde{\rho}(r)dr + T_s[\tilde{\rho}(r)] + \frac{1}{2}\int \frac{\tilde{\rho}(r)\tilde{\rho}(r')}{|r-r'|}dr\,dr' + E_{xc}[\tilde{\rho}(r)] \quad (9)$$

The corresponding Euler-Lagrange equations for a given total number of electrons has the form

$$\delta E_V[\tilde{\rho}(r)] = \int \delta\tilde{\rho}(r) \left(V_{eff}(r) + \frac{\delta}{\delta\tilde{\rho}(r)} T_s[\tilde{\rho}(r)]\Big|_{\tilde{\rho}(r)=\rho(r)} - \epsilon \right) dr = 0 \quad (10)$$

where

$$V_{eff}(r) \equiv V(r) + \int \frac{\rho(r')}{|r-r'|} dr' + V_{xc}(r) \quad (11)$$

and

$$V_{xc}(r) \equiv \frac{\delta}{\delta\tilde{\rho}(r)} E_{xc}[\tilde{\rho}(r)]\Big|_{\tilde{\rho}(r)=\rho(r)} \quad (12)$$

Now the form of Eq. (10) is identical to that of Eq. (5) for noninteracting particles moving in the effective external potential V_{eff} instead of V(r), and

so we conclude that the minimizing density distribution

$\rho(r)$ is given by solving the single particle equation

$$\left(-\frac{1}{2}\nabla^2 + V_{eff}(r) - \epsilon_j\right)\varphi_j(r) = 0 \quad (13)$$

with

$$\rho(r) = \sum_{j=1}^{N} |\varphi_j(r)|^2,$$

$$V_{eff}(r) = V(r) + \int \frac{\rho(r')}{|r - r'|} dr' + V_{xc}(r) \quad (14)$$

where $V_{xc}(r)$ Is the local exchange--correlation potential, depending functionally on the entire density distribution $\tilde{\rho}(r)$ as given by Eq. (12).

These self-consistent equations are now called the Kohn—Sham equations.

The ground state energy is given by

$$E = \sum_j \epsilon_j + E_{xc}[\rho(r)] - \int V_{xc}(r)\rho(r)dr$$

$$-\frac{1}{2}\int \frac{\rho(r)\rho(r')}{|r-r'|}dr\,dr' \quad (15)$$

If one neglects E_{xc} and V_{xc}

the Kohn-Sham equations (13-15) reduce to the self-consistent Hartree equations.

The Kohn—Sham theory may be regarded as the formal exactification of Hartree theory. With the exact E_{xc} and V_{xc} all many body effects are in principle included. Clearly this directs attention to the functional $E_{xc}[\tilde{\rho}(r)]$ The practical usefulness of the ground state Density Functional Theory depends entirely on whether approximations for the functional

$$E_{xc}[\tilde{\rho}(r)]$$

could be found which are at the same time sufficiently simple and sufficiently accurate.

REMARKS

1. The exact effective single particle potential $V_{eff}(r)$ of the Kohn—Sham theory, Eq. (14), can be regarded as that unique, fictitious external potential which leads, for noninteracting particles, to the same physical density $\rho(r)$ as that of the interacting particles in the physical external potential V(r). Thus if the physical density distribution is independently known (from experiment or accurate calculations) V_{eff} and hence V_{xc} can be directly obtained from $\rho(r)$

2. Because of their linkage to the exact physical density $\rho(r)$ the Kohn—Sham single particle wave functions $\varphi_j(r)$ may be considered as “density optimal”, while, of course the Hartree—Fock wave functions are “totally-energy-optimal’ in the sense that their normalized determinant leads to the lowest ground state energy attainable with a single determinant.

KINETIC ENERGY FUNCTIONAL

So far Density Functional Theory has been presented as a formal *mathematical framework* for viewing a structure of some many body system from the perspective of the partical density. This mathematical framework has been motivated by physical consideration, but to make concrete use of it we are needed in an effective approximation for $F[\rho(r)]$.

These approximations reflect the physics of the structure of a system and come from outside of Density Functional Theory. Below we restrict ourselves by a consideration of the kinetic energy functional.

One–particle density matrix

$$\gamma(\vec{r},\vec{r}') = \sum_{j \le F} \varphi_j^*(\vec{r})\varphi_j(\vec{r}')$$

$$\rho(\vec{r}) = \gamma(\vec{r},\vec{r}) \qquad (1)$$

$$
\begin{aligned}
T &= -\frac{\hbar^2}{2m}\int d^3\vec{r} \sum_{j \leq F} \varphi_j^*(\vec{r})\nabla^2\varphi_j(\vec{r}') \\
&= \frac{\hbar^2}{2m}\int d^3\vec{r} \sum_{j \leq F} \nabla\varphi_j^*(\vec{r})\nabla\varphi_j(\vec{r}') \\
&= \frac{\hbar^2}{2m}\int d^3\vec{r}\left[\nabla_r\nabla_{r'}\gamma(\vec{r},\vec{r}')\right]_{\vec{r}'\to\vec{r}} \qquad (2)
\end{aligned}
$$

Kohn–Sham density matrix

$$\gamma_s(\vec{r},\vec{r}') = \sum_{j=1}^{\infty} \theta(\varepsilon_F - \varepsilon_j) < \vec{r}|\varphi_j >< \varphi_j|\vec{r}' >$$
$$= < \vec{r}|\theta(\varepsilon_F - \hat{t} - \hat{V}_s)|\vec{r}' > \quad (4)$$

$$\hat{E}_F(\vec{r}) = \varepsilon_F - \hat{V}_s(\vec{r})$$
$$\gamma_s(\vec{r},\vec{r}') = < \vec{r}|\theta(\hat{E}_F - \hat{t})|\vec{r}' > . \quad (5)$$

We have here a function of two noncommutative operators.

Kirzhnits Method

$$\gamma_s(\vec{r},\vec{r}') = \int \frac{d^3k}{(2\pi\hbar)^3} < \vec{r}|\theta(\hat{E}_F - \hat{t})|\vec{k} >< \vec{k}|\vec{r}' > \quad (6)$$

This expression leads us to the following mathematical problem:

there is an eigen function $|a>$ of an operator $\hat{a}$

$$\hat{a}|a> = a|a> . \quad (7)$$

How can we compute the quantity?

$$f(\hat{a}+\hat{b})|a> \tag{8}$$

if the operator $\hat{b}$ does not commute with $\hat{a}$

$$[\hat{a},\hat{b}]\neq 0. \tag{9}$$

Above $f=\theta$, $\hat{a}=-\hat{t}$, $\hat{b}=\hat{E}_F$.

Laplace transformation

$$f(\hat{a}+\hat{b})|a> = \frac{1}{2\pi\imath}\int_{c-\imath\infty}^{c+\imath\infty} d\beta F(\beta) e^{\beta(\hat{a}+\hat{b})}|a> \qquad (10)$$

Next one introduce operator

$$\hat{K}(\beta) = e^{-\beta\hat{b}} e^{\beta(\hat{a}+\hat{b})} e^{-\beta\hat{a}} \qquad (11)$$

$$e^{\beta(\hat{a}+\hat{b})} = e^{\beta\hat{b}}\hat{K}(\beta)e^{\beta\hat{a}} \tag{12}$$

Using this result we obtain

$$f(\hat{a}+\hat{b})|a> = \frac{1}{2\pi\imath}\int_{c-\imath\infty}^{c+\imath\infty} d\beta F(\beta) e^{\beta(a+\hat{b})}$$
$$\times \hat{K}(\beta)|a> \qquad (13)$$

A crucial advantage of the last result as opposed to Eq. (10) is the fact that the eigenvalue a has now replaced the operator $\hat{a}$ in the argument of the exponential function.

Operational calculations

$$e^{\beta(\hat{a}+\hat{b})} = ? \tag{14}$$

If $[\hat{a}, \hat{b}] = 0$ then $e^{\beta(\hat{a}+\hat{b})} = e^{\beta\hat{b}}e^{\beta\hat{a}}$.
Consider a case when $[\hat{a}, \hat{b}] \neq 0$.

$$e^{\beta(\hat{a}+\hat{b})} = e^{\beta\hat{b}}\hat{K}(\beta)e^{\beta\hat{a}} \qquad (15)$$

Such a form of this expression is convenient if an exponential operator acts on an eigenfunction of the operator $\hat{a}$.

Differentiating Eq. (15) over β we obtain

$$(\hat{a}+\hat{b})e^{\beta(\hat{a}+\hat{b})} = \hat{b}e^{\beta(\hat{a}+\hat{b})} + e^{\beta\hat{b}}\frac{d\hat{K}(\beta)}{d\beta}e^{\beta\hat{a}} + e^{\beta\hat{b}}\hat{K}(\beta)e^{\beta\hat{a}}\hat{a} \tag{16}$$

$$\frac{d\hat{K}(\beta)}{d\beta} = e^{-\beta\hat{b}}\hat{a}e^{\beta\hat{b}}\hat{K} - \hat{K}\hat{a} \tag{17}$$

$$\frac{d\hat{K}(\beta)}{d\beta} = e^{-\beta\hat{b}}\hat{a}e^{\beta\hat{b}}\hat{K} - \hat{K}\hat{a} \tag{17}$$

There is known the following very useful expression

$$e^{-\beta\hat{b}}\hat{a}e^{\beta\hat{b}} = \sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}[\hat{b}[\hat{b}...[\hat{b},\hat{a}]...]] \tag{18}$$

It is seen that

$$\hat{K}(0) = 1 \tag{19}$$

In general case all commutators of $\hat{a}$ and $\hat{b}$ are not equal to zero. In this case a problem becomes very complicated. The situation is simplified if there is a small parameter in the problem. Let us, for instance, the meaning of the commutators of the high order decrease with the increase of their complexity.

Let us denotes as $\hat{Q}_n^m$ a commutator of the $(n+m)$ order

$$\hat{Q}_n^m = [\hat{a}[\hat{a}...[\hat{a}[\hat{b}...[\hat{b}, \hat{a}]...]]...]], \qquad (20)$$

and through $\hat{K}_n$ the set of all terms of n-th order in the operator $\hat{K}$. Then we obtain from Eq. (17)

$$\frac{d\hat{K}_n(\beta)}{d\beta} = [\hat{a}, \hat{K}_{n-1}]$$

$$+ \sum_{k=1}^{n} \frac{(-\beta)^k}{k!} \hat{Q}_k^0 \hat{K}_{n-k}. \qquad (21)$$

Taking into account that $\hat{K}_0 = 1$ we obtain

$$\hat{K}_1 = -\frac{\beta^2}{2}\hat{Q}_1^0, \tag{22}$$

$$\hat{K}_2 = \frac{\beta^3}{6}\left(\hat{Q}_2^0 - \hat{Q}_1^1\right) + \frac{\beta^4}{8}\left(\hat{Q}_1^0\right)^2, \tag{23}$$

$$\begin{multline}\hat{K}_3 = -\frac{\beta^4}{24}\left(\hat{Q}_3^0 - \hat{Q}_2^1 + \hat{Q}_1^2\right) \\ +\frac{\beta^5}{120}\left(3\hat{Q}_1^1\hat{Q}_1^0 + 7\hat{Q}_1^0\hat{Q}_1^1 - 4\hat{Q}_1^0\hat{Q}_2^0 - 6\hat{Q}_2^0\hat{Q}_1^0\right) \\ -\frac{\beta^6}{48}\left(\hat{Q}_1^0\right)^3, \tag{24}\end{multline}$$

Let us consider the following expansion

$$\hat{K}(\beta) = \sum_{n=0}^{\infty} \beta^n \hat{O}_n \tag{25}$$

$$\hat{O}_0 = \hat{K}(0), \tag{26}$$

$$\hat{O}_1 = \frac{d\hat{K}(\beta)}{d\beta}\Big|_{\beta=0} \tag{27}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \tag{28}$$

$$\hat{O}_n$$

$$= \frac{1}{n!}\frac{d^n\hat{K}(\beta)}{d\beta^n}\Big|_{\beta=0} \tag{29}$$

The following recurrence relation has been derived for $\hat{O}_n$

$$\hat{O}_n = \frac{1}{n}[\hat{a}, \hat{O}_{n-1}] + \sum_{k=1}^{n-1} \frac{(-1)^k}{k!} \hat{Q}_k^0 \hat{O}_{n-1-k} \tag{30}$$

Substituting this result into Eq. (12) we obtain

$$f(\hat{a}+\hat{b})|a> = \sum_{n=0}^{\infty}\left(\frac{1}{2\pi\imath}\int_{c-\imath\infty}^{c+\imath\infty} d\beta F(\beta)\beta^{n}e^{\beta(a+\hat{b})}\right)$$
$$\times\hat{O}_{n}|a> . \qquad (31)$$

Since the inverse Laplace transform in brackets formally represents the n–th derivative $f^{(n)}$ of the function f one is eventually led to the expansion

$$f(\hat{a}+\hat{b})|a> = \sum_{n=0}^{\infty} f^{(n)}(a+\hat{b})\hat{O}_n|a> \quad (32)$$

This is a central equation of a Kirzhnits formalism.

For the matrix element $< \vec{r}|\theta(\hat{E}_F - \hat{t})|\vec{k} >$ the last expansion leads to the series

$$\begin{aligned} &< \vec{r}|\theta(\hat{E}_F - \hat{t})|\vec{k} > = \\ &\theta\left(E_F(\vec{r}) - \frac{\hbar^2 k^2}{2m}\right) < \vec{r}|\vec{k} > \\ &+ \sum_{n=0}^{\infty} \delta^{(n)}\left(E_F(\vec{r}) - \frac{\hbar^2 k^2}{2m}\right) \\ &\times < \vec{r}|\hat{O}_{n+1}|\vec{k} > . \end{aligned} \tag{33}$$

$$\gamma_s(\vec{r},\vec{r}') = \gamma_s^{(0)}(\vec{r},\vec{r}') + \gamma_s^{(2)}(\vec{r},\vec{r}'), \qquad (34)$$

$$\gamma_s^{(0)}(\vec{r},\vec{r}') = \frac{1}{\pi^2} k_F^3 j_1(z)/z, \qquad (35)$$

$$\begin{aligned}\gamma_s^{(2)}(\vec{r},\vec{r}') = \frac{1}{\pi^2}\left(\frac{1}{24}[j_0(z) - zj_1(z)]\frac{\nabla^2 k_F^2}{k_F}\right. \\ -\frac{1}{4}[zj_0(z)](\nabla k_F^2)\cdot\frac{\vec{y}}{y} \\ +\frac{1}{12}[z^2 j_0(z)]\frac{1}{k_F}\nabla\left((\nabla k_F^2)\cdot\frac{\vec{y}}{y}\right)\cdot\frac{\vec{y}}{y} \\ \frac{1}{96}[j_0(z)(1+z^2) - zj_1(z)]\frac{(\nabla k_F^2)^2}{k_F^3} \\ \left. +\frac{1}{32}[z^2 j_0(z) - z^3 j_1(z)]\frac{1}{k_F^3}\left((\nabla k_F^2)\cdot\frac{\vec{y}}{y}\right)^2\right)\end{aligned} \tag{36}$$

Above $z = k_F|\vec{y}|$, $\vec{y} = \vec{r} - \vec{r}'$.

Above $z = k_F|\vec{y}|$, $\vec{y} = \vec{r} - \vec{r}'$.

$$k_F(\vec{r}) = \left(\frac{2m}{\hbar^2}E_F(\vec{r})\right)^{1/2} \qquad (37)$$

$j_0(z)$ and $j_1(z)$ are the spherical Bessel functions.

Once the density matrix is known, expression for the kinetic energy functional $T_s(\rho)$ is readily obtained

$$T_s = \int d^3 r t_s(r). \tag{38}$$

To second order in $\hbar$

$$t_s(\vec{r}) = \frac{\hbar^2}{10m\pi^2}k_F^5 - \frac{\hbar^2}{48m\pi^2}k_F\nabla^2 k_F^2 - \frac{\hbar^2}{64m\pi^2}\frac{(\nabla k_F^2)^2}{k_F}. \tag{39}$$

Results at this level are of use only if the potential $V_s(\vec{r})$ is given. The Fermi energy ε_F can be calculated by specification of the particle number $N = \int d^3r\, \rho(\vec{r})$.

ENERGY DENSITY FORMALISM IN NUCLEI

The theorem of Kohn and coworkers was originally proved for the case of electron gas. However, its extension to more complex fermion systems is straightforward. The statement says that the total energy of a fermion ensemble can be written as a functional of the local density. This is conceptually very attractive, in nuclear physics, since it tends to replace the complicated expressions of the many—body problem by a Lagrangian formalism, simpler in nature.

The difficulty lies, however, in the fact that there is no way of knowing the Lagrangian *a priori.* Thus, although the functional should be universal it can only be approximated according to some recipe.

In the very special case of the nuclear matter the problem is considerably reduced. The functional can be easily constructed by finding a polynomial form in successive powers of k_F *or density whose coefficients are adjusted to fit the binding energy per particle* E/A calculated from realistic nucleon—nucleon interaction. Therefore, a natural way of writing the functional for actual nuclei consists in starting with a volume energy part directly derived from nuclear matter and to add surface and Coulomb effects.

We separate the total energy into a nuclear matter part and inhomogeneity and Coulomb correction. This energy is given by

$$\epsilon(\rho) = \epsilon_{vol}(\rho,\alpha) + \frac{1}{2}e\rho_p\phi_c$$
$$-0.738e^2\rho_p^{4/3} + (\hbar^2/8m)\eta(\nabla\rho)^2 \qquad (1)$$

with $\rho(r) = \rho_p(r) + \rho_n(r)$, these two functions being subject to the conditions

$$\int \rho_n(r)d^3r = N, \quad \int \rho_p(r)d^3r = N \qquad (2)$$

The neutron excess α is defind as

$$\alpha = [\rho_n(r) - \rho_p(r)]/\rho(r) \qquad (3)$$

The volume energy term ϵ_{vol} corresponds to the energy in the infinite homogenous medium. Its potential energy part is expressed as

$$V(\rho,\alpha)\cdot\rho \tag{4}$$

with

$$\begin{aligned} V(\rho,\alpha) = b_1(1+a_1\alpha^2)\cdot\rho \\ +b_2(1+a_2\alpha^2)\cdot\rho^{4/3} \\ +b_3(1+a_3\alpha^2)\cdot\rho^{5/3}. \end{aligned} \tag{5}$$

The coefficients a_i and b_i are derived from a nuclear matter calculation.

The Coulomb potential is given by the Poisson equation

$$\Delta\phi_C = 4\pi e\rho_p \qquad (6)$$

and the exchange part of the Coulomb energy is approximated by a term proportional to $\rho_p^{4/3}$.

The gradient term accounts for the inhomogeneity corrections. The coefficient η is kept as a parameter.

The ground state energy is then obtained by applying a variational principle to

$$E = \int \left(\epsilon(\rho) - E_{op} \cdot \rho_p - E_{on} \cdot \rho_n \right) d^3 r, \quad (7)$$

with respect to ρ_p and ρ_n. The Euler–Lagrange formalism leads to a system of coupled second order differential equations. The solution of the differential equations are unstable in the low density region. To overcome this difficulties, the differential equations are integrated up to the point where the nucleon distribution reaches 0.15 of its central value. Beyond this point exponential tails are fitted tonthe proton and neutron distributions.

Expanding the functional around some equilibrium density

$$E_{vol} \cong E_0(\rho_0, \alpha) + a(\rho_0, \alpha) \cdot x + \frac{1}{2}\mathcal{K}(\rho_0, \alpha) \cdot x^2 \qquad (8)$$

where

$$E_0(\rho_0, \alpha) \cong \epsilon_0[1 - a_r((N - Z)/A)^2] \quad (9)$$

and

$$a(\rho_0, \alpha) = (\partial \epsilon_{vol}/\partial \rho)|_{\rho=\rho_0} \qquad (10)$$

The last term of equation (8) represents the compressibility correction. The Coulomb and surface energies can be also expanded around the equilibrium density.

Collecting the different contributions we get at equilibrium (x=0) the semiempirical mass formula of Bethe and Weizsaecker

$$E = \epsilon_0 \left(1 - a_r \left(\frac{N-Z}{A} \right)^2 \right) \cdot A$$

$$+ a_s(\alpha) \cdot A^{2/3} + \frac{3}{5} (Ze)^2 \left(\frac{4\pi\rho_0}{3A} \right)^{1/3} \qquad (11)$$

The energy density formalism provides a good way of deriving an average potential to be used in shell model calculations

$$E[\rho] = \int \mathcal{E}(\rho) d^3r - \lambda \int \rho d^3r \tag{12}$$

$$\rho(r) = \sum_j \varphi_j^*(r) \varphi_j(r) \tag{13}$$

$$\mathcal{E}(\rho) = T(\rho) + U(\rho),$$

$$T(\rho) = \frac{\hbar^2}{2m} \sum_j \nabla \varphi_j^*(r) \nabla \varphi_j(r), \tag{14}$$

$$\frac{\delta E}{\delta \varphi_j^*(r)} = \left(-\frac{\hbar^2}{2m} \Delta \right. \\ \left. + \frac{\delta U}{\delta \rho(r)} - \lambda \right) \varphi_j(r) \tag{15}$$

Thus $\frac{\delta U}{\delta \rho(r)}$ is a single particle potential.

Current and density algebra approach

$$\hat{H} = \frac{\hbar^2}{2m}\int d^3x \; \nabla\psi^+(x)\cdot\nabla\psi(x)$$

$$+\iint d^3x\, d^3y \; \psi^+(x)\,\psi(x)\, U(x-y)\, \psi^+(y)\,\psi(y)$$

$$\hat{\rho}(x) = \psi^+(x)\,\psi(x)$$

$$\hat{\vec{j}}(x) = \frac{\hbar}{2mi}\left(\psi^+(x)\cdot\nabla\psi(x) - \nabla\psi^+(x)\cdot\psi(x)\right)$$

$$\hat{T}_{nk}(x) = \frac{\partial\psi^+(x)}{\partial x_n}\,\frac{\partial\psi(x)}{\partial x_k} + \frac{\partial\psi^+(x)}{\partial x_k}\,\frac{\partial\psi(x)}{\partial x_n}$$

$$[\hat{\rho}(x), \hat{\vec{j}}(y)] = -i\,\frac{\hbar}{m}\,\nabla_x\left[\delta(x-y)\,\hat{\rho}(x)\right]$$

$\frac{\hbar^2}{4m}\int d^3x \sum_n \hat{T}_{nn}(x)$ is a kinetic energy

$$\left[\int d^3x\ \hat{T}_{nk}(x),\ \hat{\rho}(y)\right] = \frac{2mi}{\hbar}\left(\frac{\partial}{\partial y_n}\hat{j}_k(y) + \frac{\partial}{\partial y_k}\hat{j}_n(y)\right)$$

$$\left[\int d^3x\ \hat{T}_{nk}(x),\ \hat{j}_l(y)\right] = \frac{i\hbar}{m}\left(\frac{\partial}{\partial y_n}\hat{T}_{kl}(y) + \frac{\partial}{\partial y_k}\hat{T}_{nl}(y) - \frac{\partial^2\hat{\rho}(y)}{\partial y_k\,\partial y_n\,\partial y_l}\right)$$

$$\left[\hat{H}, \hat{\rho}(x)\right] = i\hbar\ \mathrm{div}\,\hat{\vec{j}}(x)$$

$$\left[\hat{H}, \hat{j}_k(x)\right] = i\hbar\cdot\frac{\hbar^2}{2m^2}\sum_{n=1}^{3}\frac{\partial}{\partial x_n}\left(\hat{T}_{nk}(x) - \frac{1}{2}\frac{\partial^2\hat{\rho}(x)}{\partial x_n\,\partial x_k} - \frac{2}{m}\hat{\rho}(x)\int d^3y\,\frac{\partial U(x-y)}{\partial x_k}\hat{\rho}(y)\right)$$

$$\hat{T}_{nk}(x) = \frac{m^2}{\hbar^2}\left\{ \left(\hat{j}_k(x)\,\frac{1}{\hat{\rho}(x)}\,\hat{j}_n(x) + \hat{j}_n(x)\,\frac{1}{\hat{\rho}(x)}\,\hat{j}_k(x) \right) + \frac{1}{2\hat{\rho}(x)}\,\frac{\partial}{\partial x_k}\hat{\rho}(x)\cdot\frac{\partial}{\partial x_n}\hat{\rho}(x) + \mathrm{const}\cdot\delta_{kn} \right\}$$

$$\hat{H} = \frac{\hbar^2}{4m}\int d^3x \sum_n \hat{T}_{nn}(x) + \int d^3x\, d^3y\, \hat{\rho}(x)\, U(x-y)\, \hat{\rho}(y)$$

Vibrational excitations

$$\bar{j}(x) = \frac{1}{2}\rho(x)\nabla\varphi(x) + \frac{1}{2}\nabla\varphi(x)\cdot\rho(x)$$

- irrotational motion

$$[\rho(x), \varphi(y)] = \frac{i\hbar}{m}\delta(x-y)$$

$$\hat{H} = \frac{m}{8}\int d^3x \{\hat{\rho}(x), \nabla\hat{\varphi}(x)\}_+ \frac{1}{\hat{\rho}(x)}\{\hat{\rho}(x), \nabla\hat{\varphi}(x)\}$$

$$+ \frac{\hbar^2}{8m}\int d^3x \frac{\left(\nabla\hat{\rho}(x)\right)^2}{\hat{\rho}(x)}$$

← Weizsäcker term

$$+ \int d^3x\, d^3y\, \hat{\rho}(x)\, U(x-y)\, \hat{\rho}(y)$$

$$U(x-y) \rightarrow \sim\delta(x-y)$$

$$\rightarrow \mathcal{E}[\hat{\rho}(x)]\,\delta(x-y)$$

$$8 \longrightarrow \wr$$

$$H = H(\rho_0) + \hat{H}_2$$

$$\hat{H}_2 = \frac{m}{2}\int d^3x\, \rho_0(x)\left[\nabla\varphi(x)\right]^2$$

$$+ \frac{\hbar^2}{3m}\int d^3x \left(\frac{\Delta\rho_0}{\rho_0^2} - \frac{(\nabla\rho_0)^2}{\rho_0^3}\right)\left[\delta\rho(x)\right]^2$$

$$+ \frac{\hbar^2}{3m}\int d^3x\, \frac{\left[\nabla\delta\rho(x)\right]^2}{\rho_0(x)}$$

$$+ \frac{1}{2}\int d^3x\, \frac{\delta^2\mathcal{E}[\rho_0(x)]}{\delta\rho_0^2(x)}\left[\delta\rho(x)\right]^2$$

$$\left[\delta\rho(x), \varphi(y)\right] = \frac{i\hbar}{m}\delta(x-y)$$

$$\left[\hat{H}_2, b_j^+\right] = \hbar\omega_j b_j^+$$

$$b_j^+ = \int d^3x\, f_j(x)\,\delta\hat{\rho}(x) + i\int d^3x\, g_j(x)\,\hat{\varphi}(x)$$

$$\nabla\left(\rho_0(x)\,\nabla f_j(x)\right) = \omega_j\, g_j(x)$$

$$\int d^3y\, \frac{\delta^2 E}{\delta\rho_0(x)\,\delta\rho_0(y)}\, g_j(y) = -\,\omega_j f_j(x)$$

$$E = \int d^3x\, \mathcal{E}[\rho_0(x)]$$

$$+\frac{\hbar^2}{\xi m}\int d^3x\, \frac{\left[\nabla\rho_0(x)\right]^2}{\rho_0(x)}$$

$$\frac{2\hbar^2}{\xi m^2}\left\{\nabla\left(\frac{1}{\rho_0(x)}\,\nabla g_j(x)\right) - \left(\frac{\Delta\rho_0(x)}{\rho_0^2(x)} - \frac{\left(\nabla\rho_0(x)\right)^2}{\rho_0^3(x)}\right) g_j(x)\right\}$$

$$-\;\frac{\delta^2\mathcal{E}[\rho_0(x)]}{m\,\delta\rho_0(x)^2}\, g_j(x) = +\,\omega_j f_j(x)$$

$$\delta_{jj'} = -\,\frac{2\hbar}{m}\int d^3x\, f_j(x)\, g_{j'}(x)$$

$$[\,b_j,\, b_{j'}^{+}\,] = \delta_{jj'}$$

$$\delta\rho(x) = -\frac{\hbar}{m}\sum_j g_j(x)\left(b_j^+ + b_j\right)$$

$$\varphi(x) = i\frac{\hbar}{m}\sum_j f_j(x)\left(b_j^+ - b_j\right)$$

There are two solutions with

$$\omega_j = 0$$

corresponding to:

Number of particles conservation

$$f_j = 1\ ,\quad g_j = 0\ ,\quad b_j^+ \sim \int d^3x\, \delta\hat{\rho}(x) = \delta\hat{N}$$

Total momentum conservation

$$f_j = 0\ ,\quad g_j = \nabla\rho_0(x)$$

$$b_j^+ \sim \int d^3x\, \nabla\rho_0(x)\cdot\varphi(x) = -\int d^3x\, \rho_0(x)\,\nabla\varphi(x)$$

Large nuclei

$A \sim 200 - 300$

$a \ll R$

Inside nucleus we can neglect

$\nabla \rho_0$

and

$$\rho_0 \frac{\delta^2 \mathcal{E}}{\delta \rho_0^2} = m C_s^2$$

$$\begin{cases} \rho_0(0)\, \Delta f_j(x) = \omega_j\, g_j(x) \\ \frac{1}{\rho_0}\left(\frac{2\hbar^2}{\xi m^2}\Delta - C_s^2\right) g_j(x) = \omega_j f_j(x) \end{cases}$$

f_j, g_j are eigenfunctions of Δ

$$g_j(x) = \frac{\xi m^2 C_s^2}{4\hbar^2 \omega_j}\left(-\sqrt{1 + \frac{8\hbar^2\omega_j^2}{\xi m^2 C_s^4}} + 1\right) \rho_0(0)\, f_j(x)$$

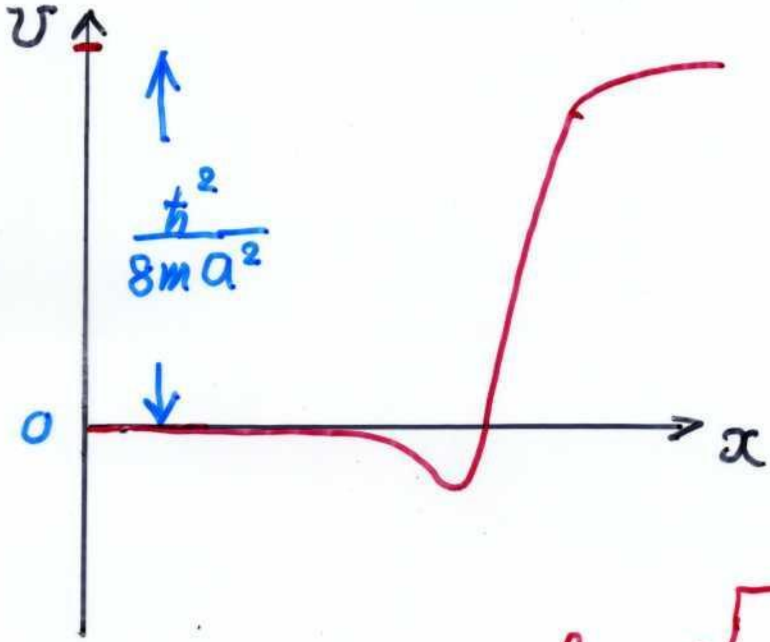
$$-\left(C_s^2 - \frac{2\hbar^2}{\xi m^2}\Delta\right)\Delta f_j(x) = \omega_j^2 f_j(x)$$

$$\omega_j^2 \sim k_j^2 C_s^2 + \dots$$

Boundary conditions

$$U(x) = \frac{\hbar^2}{2m}\left(\frac{\Delta\rho_0(x)}{2\rho_0(x)} - \frac{1}{4}\left(\frac{\nabla\rho_0(x)}{\rho_0(x)}\right)^2\right)$$

1) $\rho_0(x) \sim \left(1+\exp\left(\frac{x-R}{a}\right)\right)^{-1}$



$$\omega_j = k_j c_s\sqrt{1+\frac{2}{3}\frac{\hbar^2 k_j^2}{m^2 c_s^2}}$$

$$f_j \sim j_l(k_{nl}x)\,Y_{lm}(\bar{x})$$

2) $$\rho_0(x) \sim \exp\left(-\frac{x^2}{\bar{R}^2}\right)$$

$$U(x) = -\frac{\hbar^2}{2m\bar{R}^4}\left(x^2 - 3\bar{R}^2\right)$$

Conclusion

- Energy density functional. Ground state energy and density. Many body effects.
- Effective single partical potential
- Residual interaction