

# Applications of density matrix in the fractional quantum mechanics

Jianping Dong\*

Department of Mathematics, College of Science  
Nanjing University of Aeronautics and Astronautics, Nanjing 210016  
P. R. China

## Abstract

The many-body space fractional quantum system is studied using the density matrix method. We give the new results of the Thomas-Fermi model, and obtain the quantum pressure of the free electron gas. We also show the validity of the Hohenberg-Kohn theory in the space fractional quantum mechanics and generalize the density functional theory to the fractional quantum mechanics.

## 1 Introduction

The famous Feynman path integral [1, 2] reveals the relationship between fractals [3] and quantum mechanics. The background of the Feynman approach to quantum mechanics is a path integral over Brownian paths. The Brownian paths are non-differentiable, self-similar curves that have a fractal dimension that is different from its topological dimension. Recently, Laskin [4–8] used Lévy paths instead of the Brownian ones in the path integral and obtained a space fractional Schrödinger equation (FSE) and then developed fractional quantum mechanics. Following him, some other generalizations to the standard Schrödinger equation appeared. Naber [9] showed a time fractional Schrödinger equation, and then Wang and Xu [10] combined the two kinds of fractional Schrödinger equations together to construct a space-time fractional Schrödinger equation. Moreover, the Fractional Heisenberg equation [11–13] is also developed. These generalizations may describe more extensive fractal phenomena in the microcosmic world.

There is a physical reason for the merger of fractional calculus [14, 15] with quantum mechanics. The Feynman path integral formulation of quantum mechanics is based on a path integral over Brownian paths. In diffusion theory, this can also be done to generate the standard diffusion equation; however, there are examples of many phenomena that are only properly described when non-Brownian paths are considered. When this is done, the resulting diffusion equation has fractional derivatives [16–18]. Due to the strong similarity between the Schrödinger equation and the standard diffusion equation one might expect modifications to the Schrödinger equation generated by considering non-Brownian paths in the path integral derivation. This gives the time-fractional, space-fractional, and space-time-fractional Schrödinger equation [9–11].

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\*Email:dongjp.sdu@gmail.com

The space-fractional Schrödinger equation [4] obtained by Laskin reads (in three dimensions)

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = H_\alpha \psi(\mathbf{r}, t), \quad (1.1)$$

where  $\psi(\mathbf{r}, t)$  is the time-dependent wave function, and  $H_\alpha$  ( $1 < \alpha \leq 2$ ) is the fractional Hamiltonian operator given by

$$H_\alpha = -D_\alpha (\hbar \nabla)^\alpha + V(\mathbf{r}, t). \quad (1.2)$$

Here  $D_\alpha$  with physical dimension  $[D_\alpha] = [\text{Energy}]^{1-\alpha} \times [\text{Length}]^\alpha \times [\text{Time}]^{-\alpha}$  is dependent on  $\alpha$  [ $D_\alpha = 1/2m$  for  $\alpha = 2$ ,  $m$  denotes the mass of a particle] and  $(\hbar \nabla)^\alpha$  is the quantum Riesz fractional operator [5, 15] defined by

$$(\hbar \nabla)^\alpha \psi(\mathbf{r}, t) = -\frac{1}{(2\pi\hbar)^3} \int d^3 \mathbf{p} e^{i\mathbf{p} \cdot \mathbf{r}/\hbar} |\mathbf{p}|^\alpha \int e^{-i\mathbf{p} \cdot \mathbf{r}'/\hbar} \psi(\mathbf{r}', t) d^3 \mathbf{r}'. \quad (1.3)$$

So far, the research on the fractional quantum mechanics is based on solving the FSE. In Ref. [4, 19–21], the exact solutions to the FSE with free particle, Dirac delta potential, linear potential, and some other simple potential fields are given. However, because of the double complexity of the fractional calculus and quantum mechanics, it is hard to solve the FSE directly for most cases, especially for the many-body quantum systems. In this paper, we use the density matrix method to study the many-body fractional quantum system. We give the density matrix description of the fractional quantum system, study the Thomas-Fermi model under the framework of the fractional quantum mechanics, and generalize the density functional theory to the fractional quantum mechanics.

## 2 Density matrix description of the fractional quantum system

We are interested in systems of  $N$  identical particles (electrons, say) moving in a given external field and interacting with each other with pair forces. In most cases, one is concerned with atoms and molecules without time-dependent interactions, so we may focus on the time-independent FSE [19]. For an isolated  $N$ -electron atomic or molecular system in the Born-Oppenheimer non-relativistic approximation [22, 23], the FSE is given by

$$\hat{H}_\alpha \psi = E \psi, \quad (2.4)$$

where  $E$  is the electronic energy,  $\psi = \psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$  is the time-dependent wave function (the coordinates  $\mathbf{x}_i$  of electron  $i$  comprise space coordinates  $\mathbf{r}_i$  and spin coordinates  $s_i$ ), and  $\hat{H}_\alpha$  is the fractional Hamiltonian operator,

$$\hat{H}_\alpha = \hat{T} + \hat{V}_{ne} + \hat{V}_{ee}, \quad (2.5)$$

where  $\hat{T} = \sum_{i=1}^N D_\alpha (-\hbar^2 \Delta_i)^{\alpha/2}$  is the kinetic energy operator,  $\hat{V}_{ne} = \sum_{i=1}^N v(\mathbf{r}_i)$  is the electron-nucleus attraction energy operator, in which  $v(\mathbf{r}_i) = -\sum_{\theta} \frac{Z_\theta e^2}{r_{\theta i}}$  is the external potential acting on electron  $i$ , the potential due to nuclei of charges  $Z_\theta$ , and  $\hat{V}_{ee} = \sum_{i < j}^N \frac{e^2}{r_{ij}}$  is the electron-electron repulsion energy operator. The total energy  $W$  of this

system is the electronic energy  $E$  plus the nucleus-nucleus repulsion energy,  $\hat{V}_{nn} = \sum_{\theta < \varrho} \frac{Z_\theta Z_\varrho e^2}{R_{\theta\varrho}}$ . That is,  $W = E + \hat{V}_{nn}$ .

Now we introduce the density matrix [22, 23] to describe this quantum system. Considering the  $N$  electrons system in a pure state  $\psi_N(\mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_N)$ , then we can define the density matrix as

$$\gamma_N(\mathbf{x}'_1 \mathbf{x}'_2 \cdots \mathbf{x}'_N, \mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_N) = \psi_N(\mathbf{x}'_1 \mathbf{x}'_2 \cdots \mathbf{x}'_N) \psi_N^*(\mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_N), \quad (2.6)$$

which can be viewed as the coordinate representation of the density operator,

$$\hat{\gamma}_N = |\psi_N\rangle\langle\psi_N|, \quad (2.7)$$

where the Dirac notation is used. Note that  $\hat{\gamma}_N$  is a projection operator, and for normalized  $\psi_N$ ,

$$\text{tr}(\hat{\gamma}_N) = \int \psi_N(\mathbf{x}^N) \psi_N^*(\mathbf{x}^N) d\mathbf{x}^N = 1, \quad (2.8)$$

in which  $\text{tr}(\hat{\gamma}_N)$ , the trace of the operator  $\hat{\gamma}_N$ , is defined as the sum of diagonal elements of the matrix representing  $\hat{\gamma}_N$ , or the integral if the representation is continuous. In the state  $\psi_N$ , the expectation values of any observable  $A$  can be calculated by [22]

$$\langle \hat{A} \rangle = \text{tr}(\hat{A} \hat{\gamma}_N) = \text{tr}(\hat{\gamma}_N \hat{A}), \quad (2.9)$$

where  $\hat{A}$  is the Hermitian linear operator for the observable  $A$ . In view of Eq. (2.9), the density operator  $\hat{\gamma}_N$  carries the same information as the  $N$ -electron wave function  $|\psi\rangle$ .  $\hat{\gamma}_N$  is an operator in the same space as the vector. Note that while  $|\psi_N\rangle$  is defined only up to an arbitrary phase factor,  $\hat{\gamma}_N$  for a state is unique.  $\hat{\gamma}_N$  also is Hermitian. Further more, we can define the reduced density matrices for fermion systems [22],

$$\begin{aligned} \gamma_p(\mathbf{x}'_1 \mathbf{x}'_2 \cdots \mathbf{x}'_p, \mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_N) &= \binom{N}{p} \int \cdots \int \gamma_N(\mathbf{x}'_1 \mathbf{x}'_2 \cdots \mathbf{x}'_p \\ &\quad \mathbf{x}_{p+1} \cdots \mathbf{x}_N, \mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_p \cdots \mathbf{x}_N) d\mathbf{x}_{p+1} \cdots d\mathbf{x}_N, \end{aligned} \quad (2.10)$$

where  $\binom{N}{p}$  is a binomial coefficient. In particular,

$$\gamma_2(\mathbf{x}'_1 \mathbf{x}'_2, \mathbf{x}_1 \mathbf{x}_2) = \frac{N(N-1)}{2} \int \cdots \int \gamma_N(\mathbf{x}'_1 \mathbf{x}'_2 \mathbf{x}_3 \cdots \mathbf{x}_N, \mathbf{x}_1 \mathbf{x}_2 \mathbf{x}_3 \cdots \mathbf{x}_N) d\mathbf{x}_3 \cdots d\mathbf{x}_N, \quad (2.11)$$

and

$$\gamma_1(\mathbf{x}'_1, \mathbf{x}_1) = N \int \cdots \int \gamma_N(\mathbf{x}'_1 \mathbf{x}_2 \cdots \mathbf{x}_N, \mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_N) d\mathbf{x}_2 \cdots d\mathbf{x}_N. \quad (2.12)$$

Many operators of interest do not involve spin coordinates, for instance the Hamiltonian operators for atoms or molecules. This makes desirable further reduction of the density matrices of the first and the second orders. We define the first-order and second-order spinless density matrices by

$$\rho_1(\mathbf{r}'_1, \mathbf{r}_1) = \int \gamma_1(\mathbf{r}'_1 \mathbf{s}_1, \mathbf{r}_1 \mathbf{s}_1) d\mathbf{s}_1. \quad (2.13)$$

and

$$\rho_2(\mathbf{r}'_1 \mathbf{r}'_2, \mathbf{r}_1 \mathbf{r}_2) = \iint \gamma_2(\mathbf{r}'_1 \mathbf{s}_1 \mathbf{r}'_2 \mathbf{s}_2, \mathbf{r}_1 \mathbf{s}_1 \mathbf{r}_2 \mathbf{s}_2) d\mathbf{s}_1 d\mathbf{s}_2. \quad (2.14)$$

We also introduce a shorthand notation for the diagonal element of  $\rho_1$  and  $\rho_2$ :

$$\rho(\mathbf{r}_1) = \rho_1(\mathbf{r}_1, \mathbf{r}_1), \rho_2(\mathbf{r}_1, \mathbf{r}_2) = \rho_2(\mathbf{r}_1 \mathbf{r}_2, \mathbf{r}_1 \mathbf{r}_2). \quad (2.15)$$

Note that the diagonal element of  $\rho_1$  is just the electron density, because that

$$\rho(\mathbf{r}_1) = \rho_1(\mathbf{r}_1, \mathbf{r}_1) = N \int \cdots \int |\psi|^2 d\mathbf{s}_1 d\mathbf{x}_2 \cdots d\mathbf{x}_N. \quad (2.16)$$

A useful relationship between the first and the second order spinless density matrices is given as follows,

$$\rho_1(\mathbf{r}'_1, \mathbf{r}_1) = \frac{2}{N-1} \int \rho_2(\mathbf{r}'_1 \mathbf{r}_2, \mathbf{r}_1 \mathbf{r}_2) d\mathbf{r}_2. \quad (2.17)$$

In particular,

$$\rho(\mathbf{r}_1) = \frac{2}{N-1} \int \rho_2(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_2. \quad (2.18)$$

After these definitions, the expectation value, for an antisymmetric N-body wave function, of a local one-electron operator  $\hat{O}_1 = \sum_{i=1}^N O_1(r_i)$ , can be expressed as

$$\langle \hat{O}_1 \rangle = \text{tr}(\hat{O}_1 \hat{\gamma}_N) = \int [O_1(\mathbf{r}_1) \rho_1(\mathbf{r}'_1, \mathbf{r}_1)]_{\mathbf{r}'_1=\mathbf{r}_1} d\mathbf{r}_1. \quad (2.19)$$

Similarly, the expectation value of a two-electron operator  $\hat{O}_2 = \sum_{i<j}^N O_2(r_i, r_j)$  is

$$\langle \hat{O}_2 \rangle = \text{tr}(\hat{O}_2 \hat{\gamma}_N) = \int [O_2(\mathbf{r}_1 \mathbf{r}_2) \rho_2(\mathbf{r}'_1 \mathbf{r}_2, \mathbf{r}_1 \mathbf{r}_2)]_{\mathbf{r}'_1=\mathbf{r}_1, \mathbf{r}'_2=\mathbf{r}_2} d\mathbf{r}_1 d\mathbf{r}_2. \quad (2.20)$$

Using the above results, combining all the parts, the expectation value of the Hamiltonian (2.5), is obtained,

$$\begin{aligned} E &= \text{tr}(\hat{H}_\alpha \hat{\gamma}_N) = E(\rho_1(\mathbf{r}'_1, \mathbf{r}_1), \rho_2(\mathbf{r}_1, \mathbf{r}_2)) \\ &= \int [D_\alpha (-\hbar^2 \Delta_r)^{\alpha/2} \rho_1(\mathbf{r}', \mathbf{r})]_{\mathbf{r}'=\mathbf{r}} d\mathbf{r} + \int v(\mathbf{r}) \rho(\mathbf{r}) d\mathbf{r} + \iint \frac{e^2}{r_{12}} \rho_2(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2. \end{aligned} \quad (2.21)$$

The three terms in this formula represent respectively the electronic kinetic energy, the nuclear-electron potential energy, and the electron-electron potential energy. If we write

$$\rho_2(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{2} \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) [1 + h(\mathbf{r}_1, \mathbf{r}_2)]. \quad (2.22)$$

Then the third term in Eq. (2.21) can be rewritten as

$$\iint \frac{e^2}{r_{12}} \rho_2(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_2 d\mathbf{r}_1 = J[\rho] + \frac{1}{2} \iint \frac{e^2}{r_{12}} \rho(\mathbf{r}_1) \rho_{xc}(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2, \quad (2.23)$$

where

$$J[\rho] = \frac{1}{2} \iint \frac{e^2}{r_{12}} \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2, \quad (2.24)$$

and  $\rho_{xc}(\mathbf{r}_1, \mathbf{r}_2) = \rho(\mathbf{r}_2) h(\mathbf{r}_1, \mathbf{r}_2)$ . Here,  $\rho_{xc}(\mathbf{r}_1, \mathbf{r}_2)$  is called the exchange-correlation hole [22, 23], and

$$\int \rho_{xc}(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_2 = -1. \quad (2.25)$$

So far, the density matrix description of the fractional quantum mechanics has been made. Now we begin to study the fractional quantum mechanics by use of these results.

### 3 The Thomas-Fermi model

In the standard quantum mechanics, the first attempt to study the density functional theory of electron structure is the works of Thomas and Fermi in the 1920s. Here, under the framework of the fractional quantum mechanics, we also start from the Thomas-Fermi Model [22–24]. We divide the space into many small cells, each of side  $l$  and volume  $\Delta V = l^3$ , each containing some fixed number of electrons  $\Delta N$ , and we assume that the electron in each cell behave like independent fermions at the temperature 0K, with the cells independent of one another. Then we first study the energy levels of a particle in each cell. The particle is like in a three-dimensional infinite well,

$$V(x, y, z) = \begin{cases} 0, & \text{if } x, y, z \in (0, l); \\ \infty, & \text{otherwise.} \end{cases} \quad (3.26)$$

So we have the following FSE,

$$D_\alpha(-\hbar^2\Delta)^{\alpha/2}\psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad (3.27)$$

with the boundary conditions

$$\psi(\mathbf{r}) = 0, \text{ when } x = l, \text{ or } y = l, \text{ or } z = l, \text{ or } x = y = z = 0. \quad (3.28)$$

It is easy to prove that  $\psi(\mathbf{r}) = Ce^{i\mathbf{k}\cdot\mathbf{r}}$  is a basic solution to Eq. (3.27). Here,  $\mathbf{k} = (k_x, k_y, k_z)$ , satisfying

$$E = D_\alpha\hbar^\alpha|\mathbf{k}|^\alpha. \quad (3.29)$$

The general solution to Eq. (3.27) can be expressed by

$$\psi(\mathbf{r}) = A \sin(\mathbf{k} \cdot \mathbf{r}) + B \cos(\mathbf{k} \cdot \mathbf{r}). \quad (3.30)$$

Considering the boundary condition (3.28), we have

$$B = 0, \sin(k_x L) = \sin(k_y L) = \sin(k_z L) = 0, \quad (3.31)$$

which means

$$k_x L = n_x \pi, k_y L = n_y \pi, k_z L = n_z \pi, \quad (3.32)$$

where  $n_x, n_y, n_z$  can be any integer. So  $\mathbf{k} = (k_x, k_y, k_z) = \frac{\pi}{L}(n_x, n_y, n_z)$ . Then from Eq. (3.29), we get

$$E(n_x, n_y, n_z) = D_\alpha\hbar^\alpha|\mathbf{k}|^\alpha = D_\alpha\left(\frac{\pi\hbar}{L}\right)^\alpha R^\alpha, \quad (3.33)$$

where  $R = \sqrt{n_x^2 + n_y^2 + n_z^2}$ . Considering the spin states of electrons, every space state  $(n_x, n_y, n_z)$  can be occupied by two electrons. For high quantum numbers, that is, for large  $R$ , the number of distinct energy levels with energy smaller than  $E(n_x, n_y, n_z)$  can be approximated by the volume of one octant of a sphere with radius  $R$  in the space  $(n_x, n_y, n_z)$ . That's because that every array of positive integers  $(n_x, n_y, n_z)$  corresponds to one point in the first quadrant of the space  $(n_x, n_y, n_z)$  and there is only one grid point in per volume unit. Therefore, the number of distinct quantum states, in the interval  $(R, R + dR)$ , is given by

$$dN = 2 \cdot \frac{1}{8} \cdot 4\pi R^2 dR = \pi R^2 dR, \quad (3.34)$$

where the factor 2 enters because each energy level is doubly occupied, by one electron with spin  $\alpha$  and another with spin  $\beta$ . By the Pauli exclusion principle, we know that the number of distinct quantum states is also the number of the electrons. When  $N$  is large, the change of  $N$  can be viewed as continuous. Differentiating Eq. (3.33) yields

$$dE = \alpha D_\alpha \left(\frac{\pi\hbar}{L}\right)^\alpha R^{\alpha-1} dR. \quad (3.35)$$

Thus

$$dN = \pi R^2 (\alpha D_\alpha)^{-1} \left(\frac{L}{\pi\hbar}\right)^\alpha R^{1-\alpha} dE, \quad (3.36)$$

That is

$$\frac{dN}{dE} = \pi R^2 (\alpha D_\alpha)^{-1} \left(\frac{L}{\pi\hbar}\right)^\alpha R^{1-\alpha}, \quad (3.37)$$

the right side of which gives the number of electrons with energy in the interval  $(E, E + dE)$ . Thus, the number of electrons with energy smaller than the Fermi energy  $E_f$  is

$$N = \int_0^{E_f} \frac{dN}{dE} dE = \frac{\pi}{3} (D_\alpha)^{-3/\alpha} \left(\frac{L}{\pi\hbar}\right)^3 (E_f)^{3/\alpha}. \quad (3.38)$$

The total energy for the volume cell can now be calculated as

$$E = \int_0^{E_f} E \frac{dN}{dE} dE = \frac{3}{\alpha+3} (D_\alpha)^{-3/\alpha} \left(\frac{L}{\pi\hbar}\right)^3 (E_f)^{(\alpha+3)/\alpha}, \quad (3.39)$$

which can be rewritten as

$$E = \frac{3}{\alpha+3} N E_f = \frac{3}{\alpha+3} D_\alpha \hbar^\alpha (3\pi^2)^{\alpha/3} \left(\frac{N}{L^3}\right)^{\alpha/3+1} L^3. \quad (3.40)$$

When the volume cell  $V \rightarrow 0$ ,  $L^3 = dV = d\mathbf{r}$  and electronic density  $\rho = \frac{N}{L^3} = \frac{N}{V} = \rho(\mathbf{r})$ . From Eq. (3.40), we obtain the total energy  $dE$  for the volume cell  $d\mathbf{r}$  as

$$dE = \frac{3}{\alpha+3} D_\alpha \hbar^\alpha (3\pi^2)^{\alpha/3} (\rho(\mathbf{r}))^{\alpha/3+1} d\mathbf{r}. \quad (3.41)$$

Adding the contributions from all cells, we find the total kinetic energy to be

$$T_{TF}[\rho] = C_F \int (\rho(\mathbf{r}))^{\alpha/3+1} d\mathbf{r}, \quad (3.42)$$

where  $C_F = \frac{3}{\alpha+3} D_\alpha \hbar^\alpha (3\pi^2)^{\alpha/3}$ . This is the kinetic energy functional for the Thomas-Fermi model in the fractional quantum mechanics. When  $\alpha = 2$ , by use of the atom unit, we have  $T_{TF}[\rho] = C_F \int (\rho(\mathbf{r}))^{5/3} d\mathbf{r}$ , and  $C_F = \frac{3}{10} (3\pi^2)^{2/3} \approx 2.871$ , which accords with the standard quantum mechanics [22].

Recalling Eq. (2.21), we can get an energy formula for an atom in terms of electron density alone,

$$E_{TF}[\rho(\mathbf{r})] = C_F \int (\rho(\mathbf{r}))^{\alpha/3+1} d\mathbf{r} - Ze^2 \int \frac{\rho(\mathbf{r})}{r} d\mathbf{r} + \iint \frac{e^2}{r_{12}} \rho_2(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2. \quad (3.43)$$

For the ground state of an atom of interest the electron density minimizes the energy functional  $E_{TF}[\rho(\mathbf{r})]$ , under the constraint

$$N = N[\rho(\mathbf{r})] = \int \rho(\mathbf{r}) d\mathbf{r}, \quad (3.44)$$

where  $N$  is the total number of electrons in the atom. By the method of Lagrange multipliers, the ground-state electron density must satisfy the variational principle

$$\delta \left\{ E_{TF}[\rho(\mathbf{r})] - \mu_{TF} \left( \int \rho(\mathbf{r}) d\mathbf{r} - N \right) \right\} = 0, \quad (3.45)$$

where  $\mu_{TF}$  is the Lagrange multiplier. After executing the variation, we can get

$$\mu_{TF} = \frac{\alpha + 3}{\alpha} C_F \rho^{\alpha/3}(\mathbf{r}) - \varphi(\mathbf{r}), \quad (3.46)$$

where  $\varphi(\mathbf{r})$  is the electrostatic potential at point  $\mathbf{r}$  due to the nucleus and the entire electron distribution:

$$\varphi(\mathbf{r}) = \frac{Ze^2}{r} - \int \frac{e^2 \rho(\mathbf{r}_2)}{|\mathbf{r} - \mathbf{r}_2|} d\mathbf{r}_2. \quad (3.47)$$

Eq. (3.46) can be solved in conjunction with the constraint (3.44), and the resulting electron density then inserted in (3.43) to give the total energy. There are the results of the Thomas-Fermi model for the atom in the fractional quantum mechanics. Just as in the standard quantum mechanics, it is a simple model, without considering the exchange and correlation energy terms. But in all the results, the parameter  $\alpha$  is contained. Proper choose of  $\alpha$  may provide better results than the standard quantum mechanics.

Now we turn to solve the equations (3.46) and (3.47). For neutral atoms, when  $r \rightarrow \infty$ ,  $\varphi(\mathbf{r}) \rightarrow 0$  and  $\rho(\mathbf{r}) \rightarrow 0$ , so from Eq. (3.46), we have  $\mu_{TF} = 0$ , which means

$$\rho(\mathbf{r}) = C^{-3/\alpha} \varphi^{3/\alpha}(\mathbf{r}), \quad (3.48)$$

where  $C = C_F(\alpha + 3)/\alpha$ . Then using the results of the Poisson equation [25], the expression of  $\varphi(\mathbf{r})$  in Eq. (3.47) satisfies the following equation

$$\nabla^2 \varphi(\mathbf{r}) = 4\pi e^2 \rho(\mathbf{r}) - 4\pi e^2 Z \delta(\mathbf{r}), \quad (3.49)$$

Substituting Eq. (3.48) for  $\rho(\mathbf{r})$  gives

$$\nabla^2 \varphi(\mathbf{r}) = 4\pi e^2 C^{-3/\alpha} \varphi^{3/\alpha}(\mathbf{r}) - 4\pi e^2 Z \delta(\mathbf{r}). \quad (3.50)$$

Additionally, by the spherically symmetric of the atom, we can write

$$\varphi(\mathbf{r}) = \varphi(r) = \frac{Ze^2}{r} \omega(r). \quad (3.51)$$

Then we have

$$\nabla^2 \varphi(\mathbf{r}) = \frac{Ze^2}{r} \frac{d^2 \omega(r)}{dr^2} - 4\pi e^2 Z \omega(0) \delta(\mathbf{r}). \quad (3.52)$$

Eq. (3.50) minus Eq. (3.52) side by side gives

$$\frac{d^2 \omega(r)}{dr^2} = M r^{1-\frac{3}{\alpha}} [\omega(r)]^{\frac{3}{\alpha}}, \quad (3.53)$$

where

$$M = 4\pi C^{-3/\alpha} Z^{3/\alpha-1} e^{6/\alpha},$$

and the boundary condition  $\omega(0) = 1$  is introduced. Letting  $x = ar$  and  $a = M^{\alpha/[3(\alpha-1)]}$ , we obtain a differential equation for  $\omega(x)$ ,

$$\frac{d^2 \omega(x)}{dx^2} = x^{1-\frac{3}{\alpha}} [\omega(x)]^{\frac{3}{\alpha}}, \quad (3.54)$$

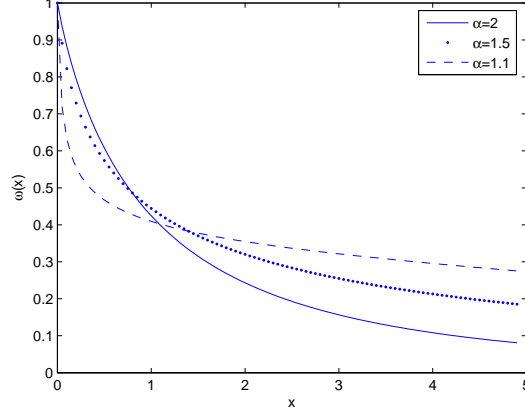


Figure 1: The curves for the numerical solutions of  $\omega(x)$  for  $\alpha = 1.1, 1.5, 2$ .  $\alpha = 2$  corresponds to the standard quantum mechanics (see Ref. [22–24]).

with the boundary conditions  $\omega(0) = 1$ ,  $\omega(\infty) = 0$ . This problem can be solved numerically. The numerical result is given in Fig. 1 for different  $\alpha$ . From the figure, we know that for all  $\alpha$ , the curves decrease monotonously, and for a smaller  $\alpha$ , the curve decreases more rapidly at the beginning, but more slowly as  $x \rightarrow \infty$ . Note that Eq. (3.54) has an exact solution  $\omega(x) = Bx^A$ , where  $A = 3(\alpha - 1)/(\alpha - 3)$ , and  $B = [A(A - 1)]^{\alpha/(3-\alpha)}$ . This solution does not satisfy the boundary condition at  $x = 0$ , but can be a good approximate expression for  $\omega(x)$  when  $x$  is large.

## 4 Quantum pressure of the free electron gas

By use of the results in the previous section, we can study the quantum pressure of the electron gas in the fractional quantum mechanics. Defining the variation of the volume of the electron gas by  $d\Omega$ , the needed energy from outside by  $dA$ , then the pressure  $p$ , of the electron gas, satisfies

$$d\Omega = -pdA, \quad (4.55)$$

Meantime, the internal thermal energy increases by  $dU = dA$ , so

$$p = -\frac{dU}{d\Omega}. \quad (4.56)$$

For degenerate Fermi electron gas, using Eq. (3.39), we have

$$U = N\bar{E} = \frac{3N}{\alpha + 3}E_f. \quad (4.57)$$

Thus

$$dU = \frac{3N}{\alpha + 3}dE_f. \quad (4.58)$$

Remembering Eq. (3.38), we can get

$$E_f^{\frac{3}{\alpha}} = N\frac{3}{\pi}(D_\alpha)^{\frac{3}{\alpha}}\frac{(\pi\hbar)^3}{\Omega}, \quad (4.59)$$



where the volume of the electron gas  $\Omega = L^3$ . The above equation can be converted into

$$\frac{3}{\alpha} \ln E_f = \text{constant} - \ln \Omega. \quad (4.60)$$

Differentiating the both sides gives

$$d\Omega = -\frac{3}{\alpha} \frac{\Omega}{E_f} dE_f. \quad (4.61)$$

Then, with the help of Eqs. (4.58) and (4.61), the pressure  $p$  of the electron gas can be calculated by Eq. (4.56),

$$p = -\frac{dU}{d\Omega} = \frac{\alpha}{\alpha+3} \frac{N}{\Omega} E_f = \frac{\alpha}{\alpha+3} \rho E_f, \quad (4.62)$$

where  $\rho = N/\Omega$  denotes the density of the electron gas. Finally, combing Eq. (4.59) and (4.62), the pressure  $p$  is expressed by the density  $\rho$  as follows,

$$p = \frac{\alpha}{\alpha+3} (3\pi^2)^{\frac{\alpha}{3}} D_\alpha \hbar^\alpha \rho^{\frac{\alpha}{3}+1}. \quad (4.63)$$

This means there is a stabilizing internal pressure in the solid object. But this pressure derives ultimately from the anti-symmetrization requirement for the wave functions of identical fermions, so it can be called the degeneracy pressure [26]. When  $\alpha = 2$ , Eq. (4.63) reduces to the result in the standard quantum mechanics [26].

## 5 Accurate theory: Hohenberg-Kohn theorems

In the previous sections, we study the many-body fractional quantum system under the Thomas-Fermi model, an exquisitely simple model. To get the accurate results, we recognize the density functional theory [22, 23] just as in the standard quantum mechanics. From the discussion in Ref. [4], we know that the hamiltonian  $H_\alpha$  for the space fractional quantum system is still a hermite operator. Employing the minimum-energy principle for the ground state, we can easily prove that the Hohenberg-Kohn theorems [22, 23] still hold in the space fractional quantum mechanics. We now give the two theorems without proof, and the proof is exactly the same with the standard quantum mechanics:

1. The electron density  $\rho(\mathbf{r})$  determines the ground-state wave function and all the other electronic properties of the system.

2. For a trial density  $\tilde{\rho}(\mathbf{r})$ , such that  $\tilde{\rho}(\mathbf{r}) \geq 0$  and  $\int \tilde{\rho}(\mathbf{r}) d\mathbf{r} = N$ ,

$$E_0 \leq E_v[\tilde{\rho}], \quad (5.64)$$

where  $E_v[\tilde{\rho}]$  is the energy functional of the quantum system with external potential  $v(\mathbf{r})$ . From Eq. (2.21) in Sec. 2, the total energy can be written as

$$E_v[\rho] = T[\rho] + V_{ne}[\rho] + V_{ee}[\rho] = \int v(\mathbf{r})\rho(\mathbf{r})d\mathbf{r} + F_{HK}[\rho], \quad (5.65)$$

where  $F_{HK}[\rho] = T[\rho] + V_{ee}[\rho]$ . We may write  $V_{ee}[\rho] = J[\rho] + \text{nonclassical term}$ , where  $J[\rho]$  is the classical repulsion. The nonclassical term is a very elusive, very important quantity; it is the major part of the "exchange-correlation energy". Assuming

differentiability of  $E_v[\rho]$ , the ground-state electron density must satisfy the variational principle

$$\delta \left\{ E_v[\rho(\mathbf{r})] - \mu \left( \int \rho(\mathbf{r}) d\mathbf{r} - N \right) \right\} = 0, \quad (5.66)$$

which gives the Euler-Lagrange equation

$$\mu = \frac{\delta E_v}{\delta \rho(\mathbf{r})} = v(\mathbf{r}) + \frac{\delta F_{HK}[\rho]}{\delta \rho(\mathbf{r})}. \quad (5.67)$$

The quantity  $\mu$  is the Lagrange multiplier and called the chemical potential. If we knew the exact  $F_{HK}[\rho]$ , Eq. (5.66) would be an exact equation for the ground-state electron density. As in the standard quantum mechanics, accurate calculational implementations of the density functional theory are far from easy to achieve, because of the unfortunate fact that the functional  $F_{HK}[\rho]$  is hard to come by in explicit form. To implement density functional theory, the Kohn-sham method [22, 23] can also be used here and the resulting Kohn-sham equation will contain a fractional operator. Further research on this subject will be done in our future work.

## 6 Conclusions

In this paper, the many-body space fractional quantum system, governing by fractional Schrödinger equation obtained by Laskin, is studied using the density matrix method. We give the results of the Thomas-Fermi model, calculate the quantum pressure of electron gas in the fractional quantum mechanics. We also show the validity of the Hohenberg-Kohn theorems, and generalize the density functional theory (DFT) to fractional quantum mechanics. These results provide the possibility to study the fractional quantum system without solving the FSE directly.

The density functional theory is a popular tool applied to study the electron structure of solids [27–29], but because the exchange-correlation term is unknown and hard to define, there are always modifications needed. The fractional quantum mechanics, which is built in the sense of Lévy flight, is a generalisation to the standard one, which is built in the sense of Brownian motion. The Lévy flight is a natural generalization of the Brownian motion, and the fractal dimension of Brownian paths is two, while that of Lévy paths is  $\alpha$  ( $1 < \alpha \leq 2$ ). The many-body quantum systems can exhibit the characteristic of fractal with the fractal dimension not equal to two, so it is reasonable to believe that the fractional Schrödinger equation can better describe the behavior of the microcosmic particles. The density functional theory in the fractional quantum mechanics may be an alternative way to study the structure of the many-body quantum systems, and without making more modifications to the exchange-correlation terms, by choosing a proper parameter  $\alpha$ , the DFT in the fractional quantum mechanics may provides better results than in the standard quantum mechanics, which needs our further studies.

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