

Quantum hydrodynamic model of density functional theory

Zhenning Cai · Yuwei Fan · Ruo Li · Tiao Lu ·
Wenqi Yao

Received: 24 September 2012 / Accepted: 27 March 2013 / Published online: 7 April 2013
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Abstract In this paper, we extend the method in Cai et al. (J Math Phys 53:103503, 2012) to derive a class of quantum hydrodynamic models for the density-functional theory (DFT). The most popular implement of DFT is the Kohn–Sham equation, which transforms a many-particle interacting system into a fictitious non-interacting one-particle system. The Kohn–Sham equation is a non-linear Schrödinger equation, and the corresponding Wigner equation can be derived as an alternative implementation of DFT. We derive quantum hydrodynamic models of the Wigner equation by moment closure following Cai et al. (J Math Phys 53:103503, 2012). The derived quantum hydrodynamic models are globally hyperbolic thus locally wellposed. The contribution of the Kohn–Sham potential is turned into a nonlinear source term of the hyperbolic moment system. This work provides a new possible way to solve DFT problems.

Keywords Density functional theory · Wigner equation · Moment closure · Quantum hydrodynamics

Z. Cai · Y. Fan · W. Yao
School of Mathematical Sciences, Peking University, Beijing, China
e-mail: caizn@pku.edu.cn

Y. Fan
e-mail: ywfan@pku.edu.cn

W. Yao
e-mail: albee0926@sina.com

R. Li · T. Lu (✉)
HEDPS & CAPT, LMAM & School of Mathematical Sciences, Peking University,
Beijing, China
e-mail: tlu@math.pku.edu.cn

R. Li
e-mail: rli@math.pku.edu.cn

1 Introduction

The simulation of the N -particle system is a very important topic and has a lot of application in many fields such as combustion, chemistry, and nuclear physics. As the exact N -body dynamics cannot realistically be solved except for very small systems, it is necessary to construct reduced models to capture the principle physical features of the system while discarding some effects. The simplest reduced model is the Hartree approximation [18], which regards an N -particle system as N one-particle systems where each particle moves independently within its own orbital and is affected only by the average field generated by all the other particles. The Hartree–Fock equations includes exchange but neglects correlations [13]. The density-functional theory (DFT) deals with both exchange and correlations in an approximate way. It has been proven to be an exceedingly powerful tool in quantum mechanical modeling method used in physics and chemistry to investigate and predict material properties quantitatively such as atoms and molecules. It is centered around a variational principle that states that the ground-state energy of a many-body system is a functional of the spatially dependent density [20]. DFT for the ground state was put on a firm theoretical footing in [20] and was extended to the time-dependent domain to develop time-dependent density functional theory (TDDFT) in [31], which may be applied to describe excited states.

All these approaches are rather costly from the point of view of computation. The Hartree–Fock equations are nonlocal in space. The Kohn–Sham equations [21] are a widely used implementation method of DFT, especially for the ground state problems. It involves finding N -eigenfunctions of the nonlinear Schrödinger equations. And the wavefunction may change abruptly in the real space, so it makes the computation work formidable for systems with large number of particles. The Wigner–Vlasov approach requires meshing of a six-dimensional phase space.

Therefore it would be useful to develop a reduced model that allows more straightforward investigation of the collective electron dynamics. Researchers have been working to derive more efficient implementations of DFT such as the quantum hydrodynamic models. Before the turn up of DFT, Bloch introduced a hydrodynamic model describing an electron gas heuristically [3] as an extension of the Thomas–Fermi model. Only macroscopic variables (electron density, velocity, pressure and electron static potential) appear in the theory. The closure of the Euler equations and the Poisson equation is done by adding some equation of state. In the original paper [3], Bloch identified P with the kinetic pressure of a degenerate Fermi gas. Bloch’s hydrodynamic theory has been applied to a variety of kinetic problems with minor improvements (inclusion of exchange, correlation, and quantum gradient corrections). Ghosh, Berkowitz and Parr gave a thermodynamical interpretation of the density functional theory in the 1984 paper [16]. The GBP approach nicely takes the form of a thermodynamics with a local temperature. Recently in [10], a quantum hydrodynamic model, derived from the Wigner–Poisson equations, is used to investigate the ultrafast electron dynamics in thin metal films. A quantum hydrodynamic model was recently developed in [22] by taking moments of the Wigner phase-space distribution. The moment closure is done by constructing a relation between the pressure and the density under the assumption that metallic nano-structures can be regarded as operating effectively at zero electron

temperature. There are many other jobs studying the quantum hydrodynamics models based on DFT, e.g., [14, 23, 24, 33].

These quantum hydrodynamic models in the literatures are derived by proposing some additional equations of state. These equations of state may be derived by constructing the appropriate distribution function [10, 11]. The derived moment system may suffer from the lack of the well-posedness, which make the calculation unreliable and formidable. Recently, a globally hyperbolic closure method has been derived from the Wigner equation in our previous paper [4, 5]. The method in [5] can be regarded as a series of extended quantum hydrodynamic models. In this paper, we extend this method to the corresponding Wigner equation of the Kohn–Sham equation. As the result, a globally hyperbolic moment system is obtained. The contribution of the Kohn–Sham potential is turned into a nonlinear source term of the hyperbolic moment system. We study the moment system for quantum harmonic oscillator with one and two particles. It is found that for the one-particle system, the solution of the Kohn–Sham equation is exactly the solution of the moment system. For the two-particle system, the residual of the moment system is going to zero with the increasing of the moment expansion order. These two examples indicate that the quantum hydrodynamic model is possible to provide an approximation to the Kohn–Sham equation with satisfied quality.

The rest of this paper is arranged as follows: in Sect. 2 we introduce the Wigner equation of DFT briefly. The globally hyperbolic regularized moment system of the corresponding Wigner equation is derived in Sect. 3. In Sect. 4, we extend the procedure to the time dependent case in the trivial style. In Sect. 5, we study quantum harmonic oscillators. The concluding remarks are in the last section.

For convenience, we only consider the Hartree atomic units, that is, the assumption $\hbar = m = e = 1$ holds, where \hbar is the Planck constant, m is the effective mass of electron and e is the positive electron charge.

2 Wigner equation of density functional theory

The DFT [20] declares that the total energy of the many-electron system is a functional of the electron density and the correct ground state electron density minimizes this energy functional. It lays the groundwork for reducing many-body problem of N electrons with $3N$ spatial coordinates to 3 spatial coordinates, through the use of the functionals of the electron density. One of the key assumptions to realize the calculation of DFT is that an auxiliary noninteracting one-particle system may have the same density as the real interacting many-body system. Thus the density can be written as the sum of the norm squares of a collection of single-particle orbitals

$$\rho(\mathbf{x}) = \sum_{n=1}^N |\psi_n(\mathbf{x})|^2, \quad (1)$$

where the orbitals $\psi_n(\mathbf{x})$, $n = 1 \dots, N$, are called Kohn–Sham (KS) orbitals [21] and $\mathbf{x} \in \mathbb{R}^3$. The KS orbitals are the eigenfunctions of the following Kohn–Sham equations

$$E_j \psi_j(\mathbf{x}) = \left[-\frac{\nabla^2}{2} + V_{\text{KS}}[\rho](\mathbf{x}) \right] \psi_j(\mathbf{x}), \quad (2)$$

where the Kohn–Sham potential is the sum of three terms,

$$V_{\text{KS}}[\rho](\mathbf{x}) = V_{\text{ext}}(\mathbf{x}) + V_{\text{H}}[\rho](\mathbf{x}) + V_{\text{xc}}[\rho](\mathbf{x}). \quad (3)$$

The first term $V_{\text{ext}}(\mathbf{x})$ is the external potential, the second term is the Hartree potential

$$V_{\text{H}}[\rho](\mathbf{x}) = \int \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d\mathbf{x}', \quad (4)$$

and the third term $V_{\text{xc}}[\rho](\mathbf{x})$ is the exchange-correlation potential, which plays a crucial role in the DFT. The quality of the solution of DFT essentially depends on the exchange-correlation term. The origin of this term is the difference between a system of N interacting many-body system and a noninteracting one-body system. Some approximations to this term were well-developed [8,9,26–28,34]. Since our focus is other than this term, here we only consider the local density approximation (LDA) given by

$$V_{\text{xc}}[\rho](\mathbf{x}) = \frac{\delta E_{\text{xc}}}{\delta \rho(\mathbf{x})} = \varepsilon_{\text{xc}}(\rho(\mathbf{x})) + \rho(\mathbf{x}) \frac{\partial \varepsilon_{\text{xc}}(\rho(\mathbf{x}))}{\partial \rho(\mathbf{x})}. \quad (5)$$

where the LDA exchange-correlation energy is

$$E_{\text{xc}} = E_{\text{x}} + E_{\text{c}} = \int \rho(\mathbf{x}) \varepsilon_{\text{xc}}(\rho(\mathbf{x})) d\mathbf{x}. \quad (6)$$

The expression of $\varepsilon_{\text{xc}} = \varepsilon_{\text{x}} + \varepsilon_{\text{c}}$ differs from problems to problems. Taking a homogeneous electronic gas (HEG) as an example, the exchange energy is [12,26]

$$E_{\text{x}} = -\frac{3}{4} \left(\frac{3}{\pi} \right)^{1/3} \int \rho(\mathbf{x})^{4/3} d\mathbf{x}. \quad (7)$$

The correlation energy of the HEG in the high density limit is given by [15]

$$\varepsilon_{\text{c}} = 0.0622 \ln(r_s) - 0.096 + \mathcal{O}(r_s), \quad (8)$$

where the Wigner-Seitz radius r_s is related to the density as

$$\frac{4}{3} \pi r_s^3 = \frac{1}{\rho}. \quad (9)$$

Virtually almost all of the concrete application of density functional theory of the ground state of many-electron systems are based on the well-known Kohn–Sham scheme [21]. We are interested in an equivalent form of the Kohn–Sham equations, since our aim is to derive a moment system from the Wigner equation, which is a

counterpart in quantum mechanics of the Boltzmann equation. Firstly, we define the density matrix in terms of the Kohn–Sham orbitals $\{\psi_i\}$ as

$$\rho(\mathbf{x}, \mathbf{x}') = \sum_i P_i \psi_i^*(\mathbf{x}') \psi_i(\mathbf{x}), \tag{10}$$

where $P_i = 1, i = 1, \dots, N$ and $P_i = 0, i = N + 1, \dots$ for ground states. The Wigner function is then defined as the Wigner transform of the density matrix

$$f(\mathbf{x}, \mathbf{p}) = \frac{1}{(2\pi)^3} \int \rho\left(\mathbf{x} + \frac{\mathbf{y}}{2}, \mathbf{x} - \frac{\mathbf{y}}{2}\right) \exp(i\mathbf{p} \cdot \mathbf{y}) \, d\mathbf{y}. \tag{11}$$

Following the method in [19], we can obtain the dynamic equation for $f(\mathbf{x}, \mathbf{p})$ based on (2). By replacing \mathbf{x} in (2) by $\mathbf{x} + \mathbf{y}/2$ and then multiplying both sides with $\psi_j^*(\mathbf{x} - \mathbf{y}/2)$, we obtain

$$E_j \psi_j^*\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) \psi_j\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) = -\frac{1}{2} \psi_j^*\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) \nabla_{\mathbf{x}}^2 \psi_j\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) + V_{KS}\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) \psi_j^*\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) \psi_j\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right). \tag{12}$$

Then by taking the conjugate of (2), replacing \mathbf{x} by $\mathbf{x} - \mathbf{y}/2$, and multiplying both sides with $\psi_j(\mathbf{x} + \mathbf{y}/2)$, we obtain

$$E_j \psi_j\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) \psi_j^*\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) = -\frac{1}{2} \psi_j\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) \nabla_{\mathbf{x}}^2 \psi_j^*\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) + V_{KS}\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) \psi_j\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) \psi_j^*\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right). \tag{13}$$

Multiplying (12)–(13) by $\frac{\mathbf{i}}{(2\pi)^3}$, integrating with respect to \mathbf{y} over \mathbb{R}^3 and making exactly the same argument as in [19], one deduces that the Wigner function defined in (11) is governed by the stationary Wigner equation

$$\mathbf{p} \cdot \nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{p}) + (\Theta[V_{KS}]f)(\mathbf{x}, \mathbf{p}) = 0, \tag{14}$$

where the nonlocal Wigner potential term $\Theta[V_{KS}]f$ is a pseudo-differential operator. It is defined by

$$(\Theta[V_{KS}]f)(t, \mathbf{x}, \mathbf{p}) = \int V_w(t, \mathbf{x}, \mathbf{p}') f(t, \mathbf{x}, \mathbf{p} - \mathbf{p}') \, d\mathbf{p}', \tag{15}$$

where the Wigner potential reads

$$V_w(t, \mathbf{x}, \mathbf{p}) = -\frac{\mathbf{i}}{(2\pi)^3} \int \left[V_{KS}\left(t, \mathbf{x} + \frac{\mathbf{y}}{2}\right) - V_{KS}\left(t, \mathbf{x} - \frac{\mathbf{y}}{2}\right) \right] e^{i\mathbf{y} \cdot \mathbf{p}} \, d\mathbf{y}.$$

It has been shown in [19] that

$$(\Theta[V_{\text{KS}}]f)(\mathbf{x}, \mathbf{p}) = - \sum_{\boldsymbol{\lambda}} \frac{1}{\boldsymbol{\lambda}!(2\mathbf{i})^{|\boldsymbol{\lambda}|-1}} \frac{\partial^{\boldsymbol{\lambda}} V_{\text{KS}}}{\partial \mathbf{x}^{\boldsymbol{\lambda}}} \frac{\partial^{\boldsymbol{\lambda}} f}{\partial \mathbf{p}^{\boldsymbol{\lambda}}}, \quad (16)$$

where $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \lambda_3)$ is a 3-dimensional multi-index, $|\boldsymbol{\lambda}| = \sum_{i=1}^3 \lambda_i$, $\boldsymbol{\lambda}! = \prod_{i=1}^3 \lambda_i!$, $\mathbf{x}^{\boldsymbol{\lambda}} = \prod_{i=1}^3 x_i^{\lambda_i}$,

$$\frac{\partial^{\boldsymbol{\lambda}}}{\partial \mathbf{x}^{\boldsymbol{\lambda}}} = \prod_{i=1}^3 \frac{\partial^{\lambda_i}}{\partial x_i^{\lambda_i}}, \quad \frac{\partial^{\boldsymbol{\lambda}}}{\partial \mathbf{p}^{\boldsymbol{\lambda}}} = \prod_{i=1}^3 \frac{\partial^{\lambda_i}}{\partial p_i^{\lambda_i}},$$

and the summation over $\boldsymbol{\lambda}$ has to be extended over all $\boldsymbol{\lambda} \in \mathbb{N}^3$ for which $|\boldsymbol{\lambda}|$ is odd.

Different from the linear Wigner equation, the potential in (16) takes the same form of the Kohn–Sham potential (3), which consists all the three terms: the external potential, the Hartree potential and the exchange–correlation potential. The latter two terms are dependent on the electron density, and this makes the Wigner equation (14) a nonlinear equation.

It is obvious that $\rho(\mathbf{x}) = \rho(\mathbf{x}, \mathbf{x})$ by the definitions (1) and (10). Noticing that

$$\rho(\mathbf{x}) = \int f(\mathbf{x}, \mathbf{p}) \, d\mathbf{p}, \quad (17)$$

the potential energy, including the external potential energy, the Hartree energy and the exchange–correlation energy, is

$$\int \rho(\mathbf{x}) V_{\text{KS}} \, d\mathbf{x} = \int \int f(\mathbf{x}, \mathbf{p}) V_{\text{KS}} \, d\mathbf{p} \, d\mathbf{x}. \quad (18)$$

One can express the total energy in terms of $f(\mathbf{x}, \mathbf{p})$ as

$$E_{\text{tot}} = \int \int \left\{ \frac{|\mathbf{p}|^2}{2} + V_{\text{KS}} \right\} f(\mathbf{x}, \mathbf{p}) \, d\mathbf{p} \, d\mathbf{x}, \quad (19)$$

where both the kinetic energy and the potential energy are included.

3 Regularized moment system of the Wigner equation

In this section, we follow the method in [5] to derive the regularized moment system for the Wigner equation (14) based on DFT. Comparing the stationary Wigner (14) with the Wigner equation in [5], it is clear that the only difference is that the external electric potential V appears in [5] is substituted by the Kohn–Sham potential V_{KS} , besides that the time derivative vanishes. It is worth mentioning that the moment expansion we adopt is of the Grad type [17].

3.1 Hermite expansion of the Wigner function

The Grad type moment expansion proposed by Grad [17] approximates the distribution function by a series of Hermite polynomials. To achieve this, we expand the Wigner function in the following form as in [5–7],

$$f(\mathbf{x}, \mathbf{p}) = \sum_{\alpha \in \mathbb{N}^3} f_\alpha(\mathbf{x}) \mathcal{H}_{\mathcal{T}, \alpha} \left(\frac{\mathbf{p} - \mathbf{u}(\mathbf{x})}{\sqrt{\mathcal{T}(\mathbf{x})}} \right), \tag{20}$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ is a 3-dimensional multi-index. The basis function $\mathcal{H}_{\mathcal{T}, \alpha}$ is defined as

$$\mathcal{H}_{\mathcal{T}, \alpha}(\boldsymbol{\xi}) = \prod_{d=1}^3 \frac{1}{\sqrt{2\pi}} T^{-\frac{\alpha_d+1}{2}} He_{\alpha_d}(\xi_d) \exp\left(-\frac{\xi_d^2}{2}\right), \tag{21}$$

where $He_n(\xi)$ is the n -degree Hermite polynomial

$$He_n(\xi) = (-1)^n \exp\left(\frac{\xi^2}{2}\right) \frac{d^n}{d\xi^n} \exp\left(-\frac{\xi^2}{2}\right). \tag{22}$$

For convenience, $He_n(\xi)$ is taken as zero if $n < 0$, thus $\mathcal{H}_{\mathcal{T}, \alpha}(\boldsymbol{\xi})$ is zero when any component of α is negative. Then we give the relation of the primitive variables $\rho(\mathbf{x}), \mathbf{u}(\mathbf{x}), \mathcal{T}(\mathbf{x}) = k_B T$, which stand for the charge density, local macroscopic momentum and scaled local temperature, respectively, to the Wigner function as

$$\rho(\mathbf{x}) = \int f(\mathbf{x}, \mathbf{p}) \, d\mathbf{p}, \tag{23a}$$

$$\rho(\mathbf{x})\mathbf{u}(\mathbf{x}) = \int \mathbf{p} f(\mathbf{x}, \mathbf{p}) \, d\mathbf{p}, \tag{23b}$$

$$\rho(\mathbf{x})|\mathbf{u}(\mathbf{x})|^2 + 3\rho(\mathbf{x})\mathcal{T}(\mathbf{x}) = \int |\mathbf{p}|^2 f(\mathbf{x}, \mathbf{p}) \, d\mathbf{p}. \tag{23c}$$

The scaled local temperature here means the local temperature defined in [16] multiplied by a Boltzmann constant k_B .

Based on the expansion (20) and the equations above, some simple properties of f_α can be deduced:

$$f_0 = \rho, \quad f_{e_i} = 0, \quad \sum_{d=1}^3 f_{2e_d} = 0, \quad i = 1, 2, 3. \tag{24}$$

where e_d is the 3-dimensional unit multi-index with its d th entry to be 1. Moreover, if we define the pressure tensor $P = \{P_{ij}\}$, $i, j = 1, 2, 3$, by

$$P_{ij} = \int (p_i - u_i)(p_j - u_j) f \, d\mathbf{p}, \tag{25}$$

then direct calculations give us the relations between them and the coefficients f_α as

$$P_{ij} - \frac{1}{3}\delta_{ij} \sum_{d=1}^3 P_{dd} = (1 + \delta_{ij})f_{e_i+e_j}. \quad (26)$$

By the definition of the temperature (23c) and the tensor pressure (25), the scaled temperature \mathcal{T} is a linear combination of P_{ij} as

$$\rho\mathcal{T} = \frac{1}{3} \sum_{d=1}^3 P_{dd}. \quad (27)$$

With the relation (26), we then have

$$P_{ij} = \delta_{ij}\rho\mathcal{T} + (1 + \delta_{ij})f_{e_i+e_j}. \quad (28)$$

It is worth mentioning that in (20) both the expansion center $\mathbf{u}(\mathbf{x})$ and the expansion dilation factor $\sqrt{\mathcal{T}(\mathbf{x})}$ are local parameters, so the expansion (20) will approximate the Wigner function more efficiently than that with an expansion center and dilation factor, both or one of them, being globally fixed, especially when a finite cut-off is introduced.

3.2 Moment expansion of the Wigner equation

We use the same method as in [5] to get the moment equations from the stationary Wigner equation. For completeness, we give a brief description.

We substitute the Hermite expansion (20) into the Wigner equation (14), and collect the coefficients of basis functions with the same order on both sides, and then equate the coefficients of the basis functions of the same order on both sides to yield the derived moment system. Before that, we list some useful properties of Hermite polynomials as below [1]:

1. Orthogonality: $\int_{\mathbb{R}} He_m(x)He_n(x) \exp(-x^2/2) dx = m!\sqrt{2\pi}\delta_{m,n}$;
2. Recursion relation: $He_{n+1}(x) = xHe_n(x) - nHe_{n-1}(x)$;
3. Differential relation: $He'_n(x) = nHe_{n-1}(x)$.

And from the last two relations, we can derive

$$[He_n(x) \exp(-x^2/2)]' = -He_{n+1}(x) \exp(-x^2/2). \quad (29)$$

Especially, we have

$$\frac{\partial}{\partial p_j} \mathcal{H}_{\mathcal{T},\alpha} \left(\frac{\mathbf{p} - \mathbf{u}}{\sqrt{\mathcal{T}}} \right) = -\mathcal{H}_{\mathcal{T},\alpha+e_j} \left(\frac{\mathbf{p} - \mathbf{u}}{\sqrt{\mathcal{T}}} \right). \quad (30)$$

With these relations, the part

$$\mathbf{p} \cdot \nabla_x f$$

of (14) is expanded as

$$\begin{aligned} & \sum_{\alpha \in \mathbb{N}^3} \sum_{j=1}^3 \left[\left(\mathcal{T} \frac{\partial f_{\alpha-e_j}}{\partial x_j} + u_j \frac{\partial f_{\alpha}}{\partial x_j} + (\alpha_j + 1) \frac{\partial f_{\alpha+e_j}}{\partial x_j} \right) \right. \\ & + \sum_{d=1}^3 \frac{\partial u_d}{\partial x_j} (\mathcal{T} f_{\alpha-e_d-e_j} + u_j f_{\alpha-e_d} + (\alpha_j + 1) f_{\alpha-e_d+e_j}) \\ & \left. + \frac{1}{2} \frac{\partial \mathcal{T}}{\partial x_j} \sum_{d=1}^3 (\mathcal{T} f_{\alpha-2e_d-e_j} + u_j f_{\alpha-2e_d} + (\alpha_j + 1) f_{\alpha-2e_d+e_j}) \right] \mathcal{H}_{\mathcal{T},\alpha} \left(\frac{\mathbf{p}-\mathbf{u}}{\sqrt{\mathcal{T}}} \right). \end{aligned} \tag{31}$$

Then using (30), we calculate the pseudo-operator term $\Theta[V_{KS}]f$ expressed in (16), and obtain

$$(\Theta[V_{KS}]f)(x, \mathbf{p}) = \sum_{\alpha, \lambda} \frac{1}{\lambda!(2\mathbf{i})^{|\lambda|-1}} \frac{\partial^\lambda V_{KS}}{\partial \mathbf{x}^\lambda} f_{\alpha-\lambda} \mathcal{H}_{\mathcal{T},\alpha} \left(\frac{\mathbf{p}-\mathbf{u}}{\sqrt{\mathcal{T}}} \right), \tag{32}$$

where the summation over λ means the same as that in (16), and $f_{\alpha-\lambda}$ is taken as zero when any component of $\alpha - \lambda$ is negative.

Collecting the two terms (31) and (32) yielded after the substitution of the Hermite expansion (20) into the Wigner equation (14), we can get the following general moment equations with a slight rearrangement by matching the coefficients of the same basis functions:

$$\begin{aligned} & \sum_{j=1}^3 \left[\left(\mathcal{T} \frac{\partial f_{\alpha-e_j}}{\partial x_j} + u_j \frac{\partial f_{\alpha}}{\partial x_j} + (\alpha_j + 1) \frac{\partial f_{\alpha+e_j}}{\partial x_j} \right) \right. \\ & + \sum_{d=1}^3 \frac{\partial u_d}{\partial x_j} (\mathcal{T} f_{\alpha-e_d-e_j} + u_j f_{\alpha-e_d} + (\alpha_j + 1) f_{\alpha-e_d+e_j}) \\ & \left. + \frac{1}{2} \frac{\partial \mathcal{T}}{\partial x_j} \sum_{d=1}^3 (\mathcal{T} f_{\alpha-2e_d-e_j} + u_j f_{\alpha-2e_d} + (\alpha_j + 1) f_{\alpha-2e_d+e_j}) \right] \\ & = - \sum_{\lambda} \frac{1}{\lambda!(2\mathbf{i})^{|\lambda|-1}} \frac{\partial^\lambda V_{KS}}{\partial \mathbf{x}^\lambda} f_{\alpha-\lambda}. \end{aligned} \tag{33}$$

By setting $\alpha = 0$ in (33), we deduce the mass conservation equation as

$$\sum_{j=1}^3 \left(u_j \frac{\partial \rho}{\partial x_j} + \rho \frac{\partial u_j}{\partial x_j} \right) = \sum_{j=1}^3 \frac{\partial \rho u_j}{\partial x_j} = 0. \tag{34}$$

By setting $\alpha = e_d$, with $d = 1, 2, 3$ and noting that $f_{e_d} = 0$ in (33), we obtain

$$\rho \sum_{j=1}^3 u_j \frac{\partial u_d}{\partial x_j} + \rho \frac{\partial \mathcal{T}}{\partial x_d} + \mathcal{T} \frac{\partial \rho}{\partial x_d} + \sum_{j=1}^3 (\delta_{jd} + 1) \frac{\partial f_{e_d+e_j}}{\partial x_j} = -\rho \frac{\partial V_{KS}}{\partial x_d},$$

which can be simplified into

$$\sum_{j=1}^3 u_j \frac{\partial u_d}{\partial x_j} + \frac{1}{\rho} \sum_{j=1}^3 \frac{\partial P_{jd}}{\partial x_j} = -\frac{\partial V_{KS}}{\partial x_d}. \quad (35)$$

By setting $\alpha = 2e_d$, with $d = 1, 2, 3$ and noting that $f_{e_d} = 0$, we get

$$\begin{aligned} \frac{\rho}{2} \sum_{j=1}^3 u_j \frac{\partial \mathcal{T}}{\partial x_j} + \rho \mathcal{T} \frac{\partial u_d}{\partial x_d} + \sum_{j=1}^3 \sum_{l=1}^3 (1 + \alpha_j) f_{2e_d-e_l+e_j} \frac{\partial u_l}{\partial x_j} \\ + \sum_{j=1}^3 \left(u_j \frac{\partial f_{2e_d}}{\partial x_j} + (1 + 2\delta_{jd}) \frac{\partial f_{2e_d+e_j}}{\partial x_j} \right) = 0. \end{aligned} \quad (36)$$

Noting that $\sum_{d=1}^3 f_{2e_d} = 0$, we sum the equations above over $d = 1, 2, 3$ to get

$$\sum_{j=1}^3 u_j \frac{\partial \mathcal{T}}{\partial x_j} + \frac{2}{3\rho} \sum_{j=1}^3 \sum_{d=1}^3 \left(P_{jd} \frac{\partial u_d}{\partial x_j} + (1 + 2\delta_{jd}) \frac{\partial f_{2e_d+e_j}}{\partial x_j} \right) = 0. \quad (37)$$

In fluid dynamics, $\sum_{j=1}^3 u_j \frac{\partial}{\partial x_j}$ is called the *convective rate of change* [32], which makes up the substantial derivative with the time derivative. For the stationary Wigner equation, though the time derivative vanishes, the convective rate of change plays a special role in the moment equations. Next we will derive equations satisfied by the convective rate of change of f_α and P_{ij} . Since (27) holds, we have

$$\frac{\partial \mathcal{T}}{\partial x_j} = \frac{1}{3\rho} \sum_{d=1}^3 \frac{\partial P_{dd}}{\partial x_j} - \frac{\mathcal{T}}{\rho} \frac{\partial \rho}{\partial x_j}, \quad j = 1, 2, 3. \quad (38)$$

Substituting (35), (37) and (38) into (33), we eliminate the convective rate of change of \mathbf{u} and \mathcal{T} and the spatial derivatives of \mathcal{T} . Then the quasi-linear form of the moment system reads:

$$\begin{aligned} \sum_{j=1}^3 \left(\mathcal{T} \frac{\partial f_{\alpha-e_j}}{\partial x_j} + u_j \frac{\partial f_\alpha}{\partial x_j} + (\alpha_j + 1) \frac{\partial f_{\alpha+e_j}}{\partial x_j} \right) \\ + \sum_{j=1}^3 \sum_{d=1}^3 \frac{\partial u_d}{\partial x_j} \left(\mathcal{T} f_{\alpha-e_d-e_j} + (\alpha_j + 1) f_{\alpha-e_d+e_j} - \frac{P_{jd}}{3\rho} \sum_{k=1}^3 f_{\alpha-2e_k} \right) \end{aligned}$$

$$\begin{aligned}
 & - \sum_{j=1}^3 \sum_{d=1}^3 \frac{f_{\alpha-e_d}}{\rho} \frac{\partial P_{jd}}{\partial x_j} - \frac{1}{3\rho} \left(\sum_{k=1}^3 f_{\alpha-2e_k} \right) \sum_{j=1}^3 \sum_{d=1}^3 (1+2\delta_{jd}) \frac{\partial f_{2e_d+e_j}}{\partial x_j} \\
 & + \sum_{j=1}^3 \left(\left(-\frac{\mathcal{T}}{2\rho} \frac{\partial \rho}{\partial x_j} + \frac{1}{6\rho} \sum_{d=1}^3 \frac{\partial P_{dd}}{\partial x_j} \right) \sum_{k=1}^3 (\mathcal{T} f_{\alpha-2e_k-e_j} + (\alpha_j + 1) f_{\alpha-2e_k+e_j}) \right) \\
 & = - \sum_{\lambda} \frac{1}{\lambda!(2i)^{|\lambda|-1}} \frac{\partial^\lambda V_{KS}}{\partial \mathbf{x}^\lambda} f_{\alpha-\lambda}, \quad \forall |\alpha| \geq 2. \tag{39}
 \end{aligned}$$

We should point out again the summation over λ is extended over all the non-negative integers λ_d , $d = 1, 2, 3$ for which $|\lambda|$ is odd and greater than or equal to 1.

With (28), we can have the equations for P_{ij} by (38) and (39). Precisely, we have the equations for $P_{ii}/2$, $i = 1, 2, 3$, as

$$\begin{aligned}
 & \sum_{j=1}^3 u_j \frac{\partial P_{ii}/2}{\partial x_j} + \sum_{j=1}^3 \left(\frac{1}{2} + \delta_{ij} \right) \rho \mathcal{T} \frac{\partial u_j}{\partial x_j} + \sum_{j=1}^3 \sum_{d=1}^3 (2\delta_{ij} + 1) f_{2e_i-e_d+e_j} \frac{\partial u_d}{\partial x_j} \\
 & + \sum_{j=1}^3 (2\delta_{ij} + 1) \frac{\partial f_{2e_i+e_j}}{\partial x_j} = 0. \tag{40}
 \end{aligned}$$

If $i \neq j$, we have $P_{ij} = f_{e_i+e_j}$, thus these equations are already in (39).

We collect the equations (34), (35), (40) and (39) together to obtain a moment system with an infinite number of equations. Noting that the relations given in (24) and the relation between P_{ij} and f_α given in (26), we can see that what we obtain is a quasi-linear system for $\{\mathbf{u}, P_{ij}, f_\alpha\}$. We would like to point out that there are two main differences between the system derived here base on DFT for the ground state and that derived from time-dependent Wigner equation in [5]. One is the time derivative term in the later system vanishes, and the other is the potential $V(\mathbf{x})$ is replaced by $V_{KS}(\mathbf{x})$, which is a nonlinear source term of the quasi-linear system of f_α .

3.3 Moment closure by globally hyperbolic regularization

The moment system derived from the stationary Wigner equation consists of (34), (35), (40) and (39). It is clear that this is a system with an infinite number of equations taking ρ, u_d, P_{ij} and $f_\alpha, |\alpha| \geq 3$, as unknowns. To obtain a system with finite unknowns, we will truncate the expansion (20) and close the system following the method in [4].

Precisely, we let $M \geq 3$ be a positive integer, $\mathcal{M} = \{f_\alpha\}_{|\alpha| \leq M}$ be a finite set, and $F_M(\mathbf{u}, \mathcal{T})$ denote the linear space spanned by all $\mathcal{H}_{\mathcal{T},\alpha} \left(\frac{\mathbf{p}-\mathbf{u}(\mathbf{x})}{\sqrt{\mathcal{T}(\mathbf{x})}} \right)$'s with $|\alpha| \leq M$, and we truncate the expansion by taking $f_\alpha \notin \mathcal{M}$ as zero, then the expansion (20) becomes

$$f(\mathbf{x}, \mathbf{p}) = \sum_{|\alpha| \leq M} f_\alpha(\mathbf{x}) \mathcal{H}_{\mathcal{T},\alpha} \left(\frac{\mathbf{p} - \mathbf{u}(\mathbf{x})}{\sqrt{\mathcal{T}(\mathbf{x})}} \right), \tag{41}$$

with $f(\mathbf{x}, \mathbf{p}) \in F_M(\mathbf{u}, T)$ and $f_\alpha \in \mathcal{M}$. The moment equations which contain the convective rate of change of $f_\alpha \notin \mathcal{M}$ are disregarded in (39) and the spatial derivative of $f_\alpha \notin \mathcal{S}_M$ is taken as zero. Then, (34), (35), (40) and (39) with $2 \leq |\alpha| \leq M$ lead to a system with a finite number of equations. This is thus an M -order truncation.

Following [4], we let

$$\mathcal{S}_M = \{\alpha \in \mathbb{N}^3 \mid |\alpha| \leq M\},$$

and permute the element of \mathcal{S}_M by lexicographic order, then for any $\alpha \in \mathcal{S}_M$,

$$\mathcal{N}(\alpha) = \sum_{i=1}^3 \binom{\sum_{k=4-i}^3 \alpha_k + i - 1}{i} + 1 \tag{42}$$

stands for the ordinal number of α in \mathcal{S}_M , and the cardinal number of set \mathcal{S}_M is

$$N = |\mathcal{S}_M| = \mathcal{N}(Me_3) = \binom{M+3}{3},$$

where $|\cdot|$ denotes the cardinal number of a set, which is also total number of moments if an M -order truncation is applied.

Let $\mathbf{w} = (w_1, \dots, w_N)^T \in \mathbb{R}^N$ and for each $i, j \in \{1, 2, 3\}$ and $i \neq j$,

$$w_1 = \rho, \quad w_{\mathcal{N}(e_i)} = u_i, \tag{43a}$$

$$w_{\mathcal{N}(2e_i)} = \frac{P_{ii}}{2}, \quad w_{\mathcal{N}(e_i+e_j)} = P_{ij}, \tag{43b}$$

$$w_{\mathcal{N}(\alpha)} = f_\alpha, \quad 3 \leq |\alpha| \leq M. \tag{43c}$$

The moment system (34), (35), (40) and (39) is collected into a quasi-linear form

$$\sum_{j=1}^3 \mathbf{M}_j(\mathbf{w}) \frac{\partial \mathbf{w}}{\partial x_j} = \mathbf{G}(\mathbf{w})\mathbf{w}, \tag{44}$$

by taking the derivatives of $f_\alpha \notin \mathcal{S}_M$ to be zero, where \mathbf{M}_j and \mathbf{G} are $N \times N$ matrices and the diagonal entries of \mathbf{M}_j are all u_j . The entries of \mathbf{M}_j are given as the coefficients of the terms in (34), (35), (40) and (39) with spatial derivatives of \mathbf{w} . Readers can observe that $\mathbf{M}_j - u_j \mathbf{I}$ is independent of u_j , and $u_j \mathbf{I}$ corresponds to the convective rate of change part, which is same as that in [4]. The entries of \mathbf{G} arise from the nonlocal Wigner potential term. (35) shows

$$\mathbf{G}_{\mathcal{N}(e_i),1} = -\frac{1}{\rho} \frac{\partial V_{KS}}{\partial x_i}, \quad i = 1, 2, 3. \tag{45}$$

And (39) indicates that other nonzero entries are

$$\mathbf{G}_{\mathcal{N}(\alpha),\mathcal{N}(\alpha-\lambda)} = -\frac{1}{\lambda!(2i)^{|\lambda|-1}} \frac{\partial^\lambda V_{KS}}{\partial \mathbf{x}^\lambda}, \tag{46}$$

where $|\lambda|$ is odd and $|\lambda|$ is greater than 1 and $|\alpha - \lambda| \neq 1$ or 2. In case of $|\alpha - \lambda| = 1$, we have $\mathbf{G}_{\mathcal{N}(\alpha), \mathcal{N}(\alpha-\lambda)} = 0$ since $f_{e_i} = 0, i = 1, 2, 3$. In case of $|\alpha - \lambda| = 2$, (46) is valid if $\alpha - \lambda = e_i + e_j, i \neq j$, since $w_{\mathcal{N}(e_i+e_j)} = P_{ij} = f_{e_i+e_j}$. The difference is in case of $\alpha - \lambda = 2e_i, i = 1, 2, 3$. Precisely by (28), we have

$$\mathbf{G}_{\mathcal{N}(\alpha), \mathcal{N}(2e_j)} = - \sum_i \left(\delta_{ij} - \frac{1}{3} \right) \frac{1}{(\alpha - 2e_i)!(2i)^{|\alpha|-3}} \frac{\partial^{\alpha-2e_i} V_{KS}}{\partial \mathbf{x}^{\alpha-2e_i}}, \quad j = 1, 2, 3, \tag{47}$$

where $i = 1, 2, 3$ satisfies that there exists a λ , satisfying $|\lambda|$ odd and $\alpha - \lambda = 2e_j$.

All other entries of \mathbf{G} vanishes except for the ones specified above. It is clear that the matrix \mathbf{G} is strictly lower triangular, thus it is nilpotent. As a result, the effect of \mathbf{G} to the high order moments is essentially slower than exponential growth rate.

In M -order truncation, as done in [17], we take $f_\alpha, \partial f_\alpha / \partial x_j$ and $f_\alpha \notin \mathcal{S}_M$ as zeroes to close the system. It has been pointed out in [4] that it is not appropriate to set $\partial f_{\alpha+e_j} / \partial x_j = 0, |\alpha| = M$, as the closure proposed in [17] since the system is lack of hyperbolicity if $f_\alpha(\mathbf{x}), |\alpha| = M - 1$ or M is not small enough. To obtain a system with global hyperbolicity, we adopt the regularization given in [4]. For any α with $|\alpha| = M$, we define

$$\mathcal{R}_M^j(\alpha) = (\alpha_j + 1) \left[\sum_{d=1}^3 f_{\alpha-e_d+e_j} \frac{\partial u_d}{\partial x_j} + \frac{1}{2} \left(\sum_{d=1}^3 f_{\alpha-2e_d+e_j} \right) \frac{\partial \mathcal{T}}{\partial x_j} \right], \tag{48}$$

and

$$\hat{\mathbf{M}}_j \frac{\partial \mathbf{w}}{\partial x_j} = \mathbf{M}_j \frac{\partial \mathbf{w}}{\partial x_j} - \sum_{|\alpha|=M} \mathcal{R}_M^j(\alpha) I_{\mathcal{N}(\alpha)}, \quad \text{for any admissible } \mathbf{w}, \tag{49}$$

where I_k is the k th column of the $N \times N$ identity matrix. We regularize the system (44) as

$$\sum_{j=1}^3 \hat{\mathbf{M}}_j(\mathbf{w}) \frac{\partial \mathbf{w}}{\partial x_j} = \mathbf{G} \mathbf{w}, \tag{50}$$

which is the quantum hydrodynamics model based on DFT we derived. It has been proved in [4] that

Theorem 1 *The regularized moment system (50) is hyperbolic for any \mathbf{w} with $\mathcal{T} > 0$. Precisely, for a given unit vector $\mathbf{n} = (n_1, n_2, n_3)$, the matrix*

$$\sum_{j=1}^3 n_j \hat{\mathbf{M}}_j(\mathbf{w}) \tag{51}$$

is real diagonalizable with real eigenvalues as

$$\mathbf{u} \cdot \mathbf{n} + C_{k,m} \sqrt{\mathcal{T}}, \quad 1 \leq k \leq m \leq M + 1, \quad (52)$$

where $C_{k,m}$ is a root of m -order Hermite polynomial, and satisfies $C_{1,m} < \dots < C_{m,m}$. The structure of the N eigenvectors can be fully clarified.

Based on this theorem, the regularized moment system (50) is locally well-posed due to the hyperbolicity. We would like to mention here that the regularization here actually does not add any new terms to the system (44). On the contrary, it has erased the terms in (39) with a factor $\alpha_j + 1$ in its coefficient for the equations of f_α with $|\alpha| = M$ only.

3.4 Kohn–Sham potential

In the moment system (50), entries of \mathbf{G} rely on the various order derivatives of V_{KS} . Next, we will investigate precise formation of the various order derivatives of V_{KS} .

In (3), the Kohn–Sham potential is the sum of three terms: the external potential, the Hartree potential and the exchange-correlation potential. The first term will not be discussed in this section for which is not dependent on the electron system. For the Hartree potential, since

$$V_H[\rho](\mathbf{x}) = \int \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d\mathbf{x}' = \int \frac{\rho(\mathbf{x}' + \mathbf{x})}{|\mathbf{x}'|} d\mathbf{x}',$$

we have

$$\frac{\partial^\lambda V_H[\rho](\mathbf{x})}{\partial \mathbf{x}^\lambda} = \int \frac{1}{|\mathbf{x}'|} \frac{\partial^\lambda \rho(\mathbf{x}' + \mathbf{x})}{\partial \mathbf{x}^\lambda} d\mathbf{x}', \quad (53)$$

where λ is a multi-index, defined as (16). For the exchange-correlation potential, since $\varepsilon_{xc} = \varepsilon_x + \varepsilon_c$ differs from problems to problems, we only consider the homogeneous electric gas as an example. (7) indicates that

$$V_x[\rho](\mathbf{x}) = \frac{\delta E_x}{\delta \rho(\mathbf{x})} = - \left(\frac{3}{\pi} \right)^{1/3} \rho(\mathbf{x})^{1/3}, \quad (54)$$

hence, we have

$$\frac{\partial^\lambda V_x[\rho](\mathbf{x})}{\partial \mathbf{x}^\lambda} = - \left(\frac{3}{\pi} \right)^{1/3} \frac{\partial^\lambda \rho(\mathbf{x})^{1/3}}{\partial \mathbf{x}^\lambda}. \quad (55)$$

The correlation energy of HEG in the high density limit is

$$\varepsilon_c(\rho) \approx 0.0622 \ln(r_s) - 0.096, \quad (56)$$

where r_s satisfies

$$\frac{4}{3} \pi r_s^3 = \frac{1}{\rho}.$$

Substituting it into (56) to calculate V_c , we can obtain

$$V_c[\rho](\mathbf{x}) = \varepsilon_c(\rho(\mathbf{x})) + \rho(\mathbf{x}) \frac{\partial \varepsilon_c(\rho(\mathbf{x}))}{\partial \rho(\mathbf{x})} = \frac{0.0622}{3} \left(\ln \left(\frac{3}{4\pi} \right) - \ln(\rho(\mathbf{x})) - 1 \right) - 0.096.$$

Therefore, the derivative of V_c reads

$$\frac{\partial^\lambda V_c[\rho](\mathbf{x})}{\partial \mathbf{x}^\lambda} = -\frac{0.0622}{3} \frac{\partial^\lambda \ln(\rho(\mathbf{x}))}{\partial \mathbf{x}^\lambda}. \tag{57}$$

Collecting (53), (55) and (57), one can observe that the various derivatives of V_{KS} are attributed to the various derivatives of $\rho(\mathbf{x})$. In numerical simulation, we need only to calculate the various derivatives of ρ to describe the effect of the inner potential.

4 Time dependent Wigner equation

For the time-dependent Kohn–Sham equation

$$i \frac{\partial \tilde{\psi}_j(t, \mathbf{x})}{\partial t} = -\frac{1}{2} \nabla_{\mathbf{x}}^2 \tilde{\psi}_j(t, \mathbf{x}) + V_{KS} \tilde{\psi}_j(t, \mathbf{x}), \tag{58}$$

we can obtain the time-dependent equation

$$\frac{\partial f(t, \mathbf{x}, \mathbf{p})}{\partial t} + \mathbf{p} \cdot \nabla_{\mathbf{x}} f(t, \mathbf{x}, \mathbf{p}) + (\Theta[V_{KS}]f)(t, \mathbf{x}, \mathbf{p}) = 0, \tag{59}$$

where

$$f(t, \mathbf{x}, \mathbf{p}) = \frac{1}{(2\pi)^3} \sum_k P_k \int \tilde{\psi}_j^*(t, \mathbf{x} - \mathbf{y}/2) \tilde{\psi}_j(t, \mathbf{x} + \mathbf{y}/2) \exp(i\mathbf{p} \cdot \mathbf{y}) \, d\mathbf{y}. \tag{60}$$

The time-dependent Wigner equation will be of interest for the treatment of excited states and the transient phenomena. For a given initial distribution function which is not very far away from a ground state distribution, this provides a practical way to find the ground state other than the Kohn–Sham equations, if the Wigner function will evolve to its ground state.

Following [5], it is trivial to give the moment system for the time-dependent Wigner equation (59) from (58). Actually, the time-dependent Wigner equation is also similar as the Boltzmann equation, thus the closed moment system can be derived (cf. [4,5]).

With the expansion (20),

$$\frac{\partial f(t, \mathbf{x}, \mathbf{p})}{\partial t}$$

is expanded as

$$\sum_{\alpha \in \mathbb{N}^3} \left(\frac{\partial f_{\alpha}}{\partial t} + \sum_{d=1}^3 \frac{\partial u_d}{\partial t} f_{\alpha - e_d} + \frac{1}{2} \frac{\partial \mathcal{T}}{\partial t} \sum_{d=1}^3 f_{\alpha - 2e_d} \right) H_{\mathcal{T}, \alpha} \left(\frac{\mathbf{p} - \mathbf{u}}{\sqrt{\mathcal{T}}} \right). \quad (61)$$

Collecting the three terms (61), (31) and (32) yielded after the substitution of Hermite expansion (20) into the time-dependent Wigner equation (59), we can get the following general moment equations by matching the coefficients of the same basis functions:

$$\begin{aligned} & \frac{\partial f_{\alpha}}{\partial t} + \sum_{d=1}^3 \frac{\partial u_d}{\partial t} f_{\alpha - e_d} + \frac{1}{2} \frac{\partial \mathcal{T}}{\partial t} \sum_{d=1}^3 f_{\alpha - 2e_d} \\ & + \sum_{j=1}^3 \left[\left(\mathcal{T} \frac{\partial f_{\alpha - e_j}}{\partial x_j} + u_j \frac{\partial f_{\alpha}}{\partial x_j} + (\alpha_j + 1) \frac{\partial f_{\alpha + e_j}}{\partial x_j} \right) \right. \\ & + \sum_{d=1}^3 \frac{\partial u_d}{\partial x_j} (\mathcal{T} f_{\alpha - e_d - e_j} + u_j f_{\alpha - e_d} + (\alpha_j + 1) f_{\alpha - e_d + e_j}) \\ & \left. + \frac{1}{2} \frac{\partial \mathcal{T}}{\partial x_j} \sum_{d=1}^3 (\mathcal{T} f_{\alpha - 2e_d - e_j} + u_j f_{\alpha - 2e_d} + (\alpha_j + 1) f_{\alpha - 2e_d + e_j}) \right] \\ & = - \sum_{\lambda} \frac{1}{\lambda! (2i)^{|\lambda| - 1}} \frac{\partial^{\lambda} V_{KS}}{\partial \mathbf{x}^{\lambda}} f_{\alpha - \lambda}. \end{aligned} \quad (62)$$

In the fluid dynamics, if $\phi(t, \mathbf{x})$ is an arbitrary differentiable function of the Eulerian variables \mathbf{x} and time t , then

$$\begin{array}{ccccccc} \frac{d\phi(t, \mathbf{x})}{dt} & = & \frac{\partial \phi(t, \mathbf{x})}{\partial t} & + & (\mathbf{u} \cdot \nabla) \phi(t, \mathbf{x}) & & \\ \uparrow & & \uparrow & & \uparrow & & \\ \text{substantial derivative} & & \text{time derivative} & & \text{convective rate of change} & & \end{array} \quad (63)$$

where ∇ is the gradient operator with respect to the \mathbf{x} components, and the substitution derivative represents the differentiation “following a fluid particle” [25]. Using this notation, (62) is reformulated as

$$\begin{aligned} & \frac{df_{\alpha}}{dt} + \sum_{d=1}^3 \frac{du_d}{dt} f_{\alpha - e_d} + \frac{1}{2} \frac{d\mathcal{T}}{dt} \sum_{d=1}^3 f_{\alpha - 2e_d} \\ & + \sum_{j=1}^3 \left[\left(\mathcal{T} \frac{\partial f_{\alpha - e_j}}{\partial x_j} + (\alpha_j + 1) \frac{\partial f_{\alpha + e_j}}{\partial x_j} \right) \right. \\ & \left. + \sum_{d=1}^3 \frac{\partial u_d}{\partial x_j} (\mathcal{T} f_{\alpha - e_d - e_j} + (\alpha_j + 1) f_{\alpha - e_d + e_j}) \right] \end{aligned}$$

$$\begin{aligned}
 & \left. + \frac{1}{2} \frac{\partial \mathcal{T}}{\partial x_j} \sum_{d=1}^3 \left(\mathcal{T} f_{\alpha-2e_d-e_j} + (\alpha_j + 1) f_{\alpha-2e_d+e_j} \right) \right] \\
 & = - \sum_{\lambda} \frac{1}{\lambda! (2i)^{|\lambda|-1}} \frac{\partial^\lambda V_{KS}}{\partial \mathbf{x}^\lambda} f_{\alpha-\lambda}.
 \end{aligned} \tag{64}$$

Comparing (64) and (33), the only difference is the convective rate of change in (33) is replaced by the substantial derivative in (64). Since in Sect. 3.3 the moment system (44), derived from (33), can be written into

$$\sum_{j=1}^3 \left((\mathbf{M}_j - u_j \mathbf{I}) \frac{\partial \mathbf{w}}{\partial x_j} + u_j \mathbf{I} \frac{\partial \mathbf{w}}{\partial x_j} \right) = \sum_{j=1}^3 (\mathbf{M}_j - u_j \mathbf{I}) \frac{\partial \mathbf{w}}{\partial x_j} + \mathbf{u} \cdot \nabla \mathbf{w} = \mathbf{G} \mathbf{w}, \tag{65}$$

where $\mathbf{u} \cdot \nabla \mathbf{w}$ represents the convective rate of change, we can get the moment system corresponding to (64) by replacing the convective rate of change in (65) with the substantial derivative as

$$\sum_{j=1}^3 (\mathbf{M}_j - u_j \mathbf{I}) \frac{\partial \mathbf{w}}{\partial x_j} + \frac{d\mathbf{w}}{dt} = \frac{\partial \mathbf{w}}{\partial t} + \sum_{j=1}^3 \mathbf{M}_j \frac{\partial \mathbf{w}}{\partial x_j} = \mathbf{G} \mathbf{w}, \tag{66}$$

where \mathbf{M} and \mathbf{G} are the same as that in (44).

In Sect. 3.3, we have pointed out that \mathbf{M} may not be real diagonalizable if f_α , $|\alpha| = M - 1$ or M is not small enough, and a globally hyperbolic regularization was proposed. Here we inherit the regularization, and obtain the globally hyperbolic moment system as

$$\frac{\partial \mathbf{w}}{\partial t} + \sum_{j=1}^3 \hat{\mathbf{M}}_j \frac{\partial \mathbf{w}}{\partial x_j} = \mathbf{G} \mathbf{w}, \tag{67}$$

where $\hat{\mathbf{M}}_j$ is the same as that in (50).

Theorem 1 indicates that the moment system (67) is locally well-posed due to the hyperbolicity. According to the derivation in Sect. 3.3, one find that we get a moment system, which is an extended hydrodynamic system and can be truncated up to any order $M \in \mathbb{N}$, $M \geq 3$, to approximate the time-dependent Wigner equation.

5 Quantum harmonic oscillator

Quantum harmonic oscillators are the quantum-mechanical analogue of classical harmonic oscillator, and is one of the most important model systems [29]. In this section, we study the quantum harmonic oscillator for both a one-particle system and a two-particle system with a parabolic potential. For both systems, the wavefunction of the Schrödinger equation and the solution of the corresponding Kohn–Sham equation can be obtained simultaneously. This makes it possible to examine the residual of

the moment system if we substitute the solution of the Kohn–Sham equation into the moment system. The moment system we derived is then partially validated once it is observed that the residual of the system is very small such that the moment system is almost satisfied by the solution of the Kohn–Sham equation.

The one-particle system is fairly simple that its Kohn–Sham equation is the same as the Schrödinger equation. The moments of the Wigner function for this system are all zero expect for the density and the temperature. Therefore, it is trivial to verify that the solution of the Kohn–Sham equation is exactly the solution of the moment system we derived for arbitrary order.

For the two-particle system, the Kohn–Sham equation with the exchange correlation potential given in [30] can provide exactly the same density function for the ground state as the two-particle Schrödinger equation. A few of the low order moments of the Wigner function can be directly calculated and the magnitude of the moments is decaying to zero with the increasing of the order of the moments. The solution of the Kohn–Sham equation is then substituted into the moment system we derived to study the residual of the moment system. Making use of the decay of the moments, it is verified that the residual of the moment system is decaying to zero, too.

5.1 One-particle system

The one-dimensional quantum harmonic oscillator describes a single particle in a parabolic potential

$$V(x) = -\omega^2 x^2 / 2 \quad (68)$$

by using the Schrödinger equation

$$\left(-\frac{1}{2} \nabla^2 + \frac{1}{2} \omega^2 x^2 \right) \Psi(x) = E \Psi(x), \quad (69)$$

where E denotes an eigenvalue or eigen energy. The ground state is given as

$$\Psi(x) = \left(\frac{\omega}{\pi} \right)^{1/4} \exp \left(-\frac{\omega x^2}{2} \right), \quad (70)$$

corresponding to the ground energy

$$E = \frac{1}{2} \omega. \quad (71)$$

The Wigner function corresponding to the wavefunction (70) is

$$f(x, p) = \frac{1}{2\pi} \int \psi^*(x + y/2) \psi(x - y/2) e^{ipy} dy = \frac{1}{\pi} \exp \left(-2\omega x^2 - \frac{p^2}{2\omega} \right). \quad (72)$$

In this case $f(x, p)$ is positive definite and can be straightforwardly interpreted as the probability distribution in the phase space.

The 1D stationary momentum system for truncation order 3 for the parabolic can be written as [5]

$$u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0, \tag{73}$$

$$\rho u \frac{\partial u}{\partial x} + \frac{\partial P}{\partial x} = -\frac{\partial V}{\partial x} \rho, \tag{74}$$

$$u \frac{\partial P/2}{\partial x} + \frac{3}{2} P \frac{\partial u}{\partial x} + 3 \frac{\partial f_3}{\partial x} = 0. \tag{75}$$

$$-\frac{P^2}{2\rho^2} \frac{\partial \rho}{\partial x} + \frac{P}{2\rho} \frac{\partial P}{\partial x} + u \frac{\partial f_3}{\partial x} = 0. \tag{76}$$

Using the expression of $f(x, p)$ in (72), we obtain density $\rho(x)$, mean velocity $u(x)$ and and temperature $T(x)$

$$\rho = \int_{-\infty}^{\infty} f(t, x, p) dp = \sqrt{\frac{2\omega}{\pi}} \exp(-2\omega x^2), \tag{77}$$

$$u = \frac{1}{\rho} \int_{-\infty}^{\infty} p f(t, x, p) dp = 0, \tag{78}$$

$$T = \frac{P}{\rho} = \frac{1}{\rho} \int_{-\infty}^{\infty} (p - u)^2 f(t, x, p) dp = \omega, \tag{79}$$

where P is the pressure and in 1D case

$$P = \rho T. \tag{80}$$

Plugging (77), (78) and (79) into the momentum system (73)–(76), and noting (68), it is clear that the moments up to order 3 of the Wigner function describing a harmonic oscillator are the solution of the derived moment system. Further, it is easy to see this conclusion holds for moments up to any order noting the following trivial fact any moments of order higher than 3 are zero.

5.2 Two-particle system

Now we consider a two-particle system describing two electrons oscillate in the parabolic well (the Hooke’s atom). The two-particle Schrödinger equation is given as

$$\left(-\frac{1}{2} \nabla_{x_1}^2 - \frac{1}{2} \nabla_{x_2}^2 - V_{\text{ext}}(x_1) - V_{\text{ext}}(x_2) + \frac{1}{|x_1 - x_2|} \right) \Psi(x_1, x_2) = E \Psi(x_1, x_2). \tag{81}$$

Here the external potential in the Hooke's atom is given by

$$V_{\text{ext}}(\mathbf{x}) = \frac{1}{2}k_{\text{Hooke}}|\mathbf{x}|^2, \quad k_{\text{Hooke}} = \frac{1}{4}. \quad (82)$$

We introduce the difference vector and the center of mass as new variables

$$\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2, \quad \mathbf{X} = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2). \quad (83)$$

An exact solution of (81) can be obtained (e.g., see [30]). That is, the wave function of the ground state corresponding to the ground state energy $E = 5/2$ can be written as an analytical formula

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = C e^{-X^2/2} e^{-x^2/8} (1 + x/2), \quad (84)$$

where $x = |\mathbf{x}|$ and $C = 1/[2\pi^{5/4}(5\sqrt{\pi} + 8)^{1/2}] = 0.0291122\text{a.u.}$ In [30], this two-particle system (81) is transformed into the Kohn–Sham equation

$$\left(-\frac{1}{2}\nabla^2 + V_{\text{KS}}\right)\psi_i(\mathbf{x}) = \varepsilon_i\psi_i(\mathbf{x}), \quad i = 1, \dots, N, \quad (85)$$

where

$$V_{\text{KS}} = V_{\text{ext}} + V_{\text{H}} + V_{\text{xc}}. \quad (86)$$

The density $\rho(\mathbf{x})$ is defined as

$$\rho(\mathbf{x}) = 2 \int |\Psi(\mathbf{x}, \mathbf{x}_2)|^2 d^3\mathbf{x}_2. \quad (87)$$

Plugging (84) into (87) yields the analytical expression of $\rho(\mathbf{x}) = \rho(x)$ [30],

$$\rho(x) = \pi\sqrt{2\pi}C^2 e^{-x^2/2} \left\{ 7 + x^2 + \frac{8e^{-x^2/2}}{\sqrt{2\pi}} + 4(1 + x^2)\frac{1}{x}\text{erf}\left(\frac{x}{\sqrt{2}}\right) \right\}, \quad (88)$$

where $\text{erf}(x)$ is the error function defined by

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} dy. \quad (89)$$

It is easy to see that $\rho(x)$ is even since

$$\frac{1}{x}\text{erf}\left(\frac{x}{\sqrt{2}}\right) = \frac{\sqrt{2}}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)2^n n!} x^{2n}. \quad (90)$$

The Kohn–Sham orbitals of (85) are

$$\varphi_i(\mathbf{x}) = \sqrt{\rho(\mathbf{x})/2}, \quad i = 1, 2. \tag{91}$$

The two particles are in the same Kohn–Sham orbitals and have the same Kohn–Sham energy $E_i = 5/4$, $i = 1, 2$ due to spin. With the assumption the functional derivative $V_H + V_{xc}$ vanishes at infinity, the latter two parts of the Kohn–Sham potential (the first part is the external potential) can be written in terms of the density as

$$[V_H + V_{xc}](x) = E_i + \frac{1}{2} \frac{\nabla^2 \sqrt{\rho(x)}}{\rho(x)} - \frac{1}{8} x^2. \tag{92}$$

Let us calculate the moments and plug them into our moment equations and find the residual is going to zero as the order goes to infinity. The Wigner function is defined by

$$f(\mathbf{x}, \mathbf{p}) = \sum_{i=1}^2 \frac{1}{(2\pi)^3} \int \bar{\varphi}_i(\mathbf{x} + \mathbf{y}/2) \varphi_i(\mathbf{x} - \mathbf{y}/2) \exp(i\mathbf{p} \cdot \mathbf{y}) \, d\mathbf{y}. \tag{93}$$

Plugging (91) into the above equation, we obtain the Wigner function as

$$f(\mathbf{x}, \mathbf{p}) = \frac{1}{(2\pi)^3} \int \sqrt{\rho(\mathbf{x} - \mathbf{y}/2)\rho(\mathbf{x} + \mathbf{y}/2)} \exp(i\mathbf{p} \cdot \mathbf{y}) \, d\mathbf{y}. \tag{94}$$

It is easy to verify that

$$\int f(\mathbf{x}, \mathbf{p}) \, d\mathbf{p} = \rho(\mathbf{x}), \tag{95}$$

$$\rho \mathbf{u} = \int f(\mathbf{x}, \mathbf{p}) \mathbf{p} \, d\mathbf{p} = \mathbf{0}. \tag{96}$$

We expand $f(\mathbf{x}, \mathbf{p})$ into the Hermite series

$$f(\mathbf{x}, \mathbf{p}) = \sum_{\alpha} f_{\alpha} \mathcal{H}_{\mathcal{T}, \alpha} \left(\frac{\mathbf{p}}{\sqrt{\mathcal{T}(\mathbf{x})}} \right), \tag{97}$$

where

$$f_{(0,0,0)} = \rho(\mathbf{x}), \quad f_{e_j} = 0, \quad j = 1, 2, 3,$$

$$\mathcal{T}(\mathbf{x}) = \frac{1}{3\rho} \int |\mathbf{p}|^2 f(\mathbf{x}, \mathbf{p}) \, d\mathbf{p}, \tag{98}$$

which can be calculated by

$$\mathcal{T} = \frac{1}{4} \frac{1}{\kappa(x^2)} - \frac{d \ln \kappa(t)}{dt} \Big|_{t=x^2} - \frac{4}{3} t \frac{d^2}{dt^2} \ln \kappa(t) \Big|_{t=x^2}, \tag{99}$$

where

$$\kappa(t) = \rho(\sqrt{t}) \exp(t/2), \quad (100)$$

which is equivalent to applying the change of variables $x^2 \rightarrow t$ to the part of $\rho(x)$ in (88) after dropping the $\exp(-x^2/2)$ factor.

The first moment equation (34) is reduced into an identity when we plug (95) and (96) into (34). Actually all the moment equations which are not modified by closure are satisfied by the moments of $f(x, p)$. We only need to examine the moment equations of order $|\alpha| = M$ in the regularized moment system of order M which has been modified due to the truncation and closure. Substituting the exact moments into the regularized moment system and calculating the residual yields

$$\text{Res}(\alpha) = \sum_{j=1}^3 \mathcal{R}_M^j(\alpha) + \sum_{j=1}^3 (\alpha_j + 1) \frac{\partial f_{\alpha+e_j}}{\partial x_j} \quad (101)$$

where the closure term $\mathcal{R}_M^j(\alpha)$ is defined in (48) and the truncation term $\sum_{j=1}^3 (\alpha_j + 1) \frac{\partial f_{\alpha+e_j}}{\partial x_j}$ is easy to be identified by observing the original moment equation (39). Since in this two-particle system, $u = 0$, the residue (101) is reduced into

$$\text{Res}(\alpha) = \frac{1}{2} (\alpha_j + 1) \left(\sum_{d=1}^3 f_{\alpha-2e_d+e_j} \right) \frac{\partial \mathcal{T}}{\partial x_j} + \sum_{j=1}^3 (\alpha_j + 1) \frac{\partial f_{\alpha+e_j}}{\partial x_j}. \quad (102)$$

We use Theorem 2 in [2] to prove that the residue (102) goes to zero as the truncation order M goes to infinity, i.e.,

$$\lim_{|\alpha| \rightarrow \infty} \text{Res}(\alpha) = 0. \quad (103)$$

A simple outline of the proof is given as follows. A direct inference of Theorem 2 in [2] is that a function $f(x)$ in $L^2(-\infty, \infty)$ can be expanded into a converging series

$$f(x) = \sum_{\alpha} f_{\alpha} \mathcal{H}_{\alpha}(x), \quad (104)$$

and

$$\lim_{\alpha \rightarrow \infty} f_{\alpha} \rightarrow 0. \quad (105)$$

(103) is true if we prove that

$$\lim_{|\alpha| \rightarrow 0} f_{\alpha} = 0, \quad (106)$$

and

$$\lim_{|\alpha| \rightarrow 0} \frac{\partial f_\alpha}{\partial x_j} = 0, \tag{107}$$

since $|\mathcal{T}|$ is uniformly bounded because $\kappa(x^2)$ has a low bound greater than zero.

In order to prove (106), we only need to check where $f(x, p)$ is square integrable. While using the Parseval equality of the Fourier transform, we only need to check whether

$$\sqrt{\rho(x - y/2)\rho(x + y/2)} = \int f(x, p) \exp(-i p \cdot y) dp \tag{108}$$

is square integrable. This is obvious since

$$\sqrt{\rho(x - y/2)\rho(x + y/2)} = \exp(-x^2/2) \exp(-y^2/8) \sqrt{\kappa(|x - y/2|^2)\kappa(|x + y/2|^2)}, \tag{109}$$

where $\sqrt{\kappa(|x - y/2|^2)\kappa(|x + y/2|^2)}$ is of polynomial growth in y as $|y|$ going to infinity. The similar argument applied for $\frac{\partial \sqrt{\rho(x - y/2)\rho(x + y/2)}}{\partial x_j}$ gives (107).

6 Discussion and conclusion remarks

In [5], we extend the moment closure method [4] for the Boltzmann equation to its quantum counterpart, the Wigner equation. Using the same moment closure technique, we in this paper derive a class of hydrodynamic models to implement the density functional theory as an alternative of the Kohn–Sham equations. We study the quantum harmonic oscillators and validate the proposed models by observing that the residual yielded by substituting the moments into the moment system goes to zero as the truncation order goes to infinity. We are now developing numerical method for the derived model to solve DFT problems.

As the starting point of the present paper, the Wigner function is a six-variable function. Here we start from the Wigner equation, then take moments of the Wigner function, and eventually obtain the moment system by taking the moments of the Wigner equation. After taking the moments, every component in the moment system is turned back to a three-variable function.

In the Kohn–Sham equations, the unknown is the density, which is a three-variable function, while to obtain the density, the eigen-system of the Kohn–Sham equations has to be clarified. To get the eigen-system of Kohn–Sham equations, there are some essential difficulties with the increasing of the system size. In the moment system we derived, though the unknowns include a set of three-variable functions instead of a single three-variable function, it is possible to be solved by the techniques developed for solution of steady-state conservation laws. In the typical applications of the steady-state conservation laws nowadays, for example the steady flow around a multi-element

airfoil, the difficulties due to the increasing of the system size seems not so essential as that in solving an eigenvalue problem. This brings us new hope to the DFT problems with large system size.

Acknowledgments We would like thank the anonymous referees for their comments so instructive. This research of R. Li was supported in part by the National Basic Research Program of China (2011CB309704) and Fok Ying Tong Education and NCET in China. T. Lu was supported in part by NSFC (Grant No. 11011130029, 91230107).

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