On Kinetic Flux Vector Splitting Schemes for Quantum Euler Equations*

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Abstract

The kinetic flux vector splitting (KFVS) scheme, when used for quantum Euler equations, as was done by Yang *et al* [22], requires the integration of the quantum Maxwellians (Bose-Einstein and Fermi-Dirac distributions), giving a numerical flux much more complicated than the classical counterpart. As a result, a nonlinear 2 by 2 system that connects the macroscopic quantities temperature and fugacity with density and internal energy needs to be inverted by iterative methods at every spatial point and every time step. In this paper, we propose to use a simple classical KFVS scheme for the quantum hydrodynamics based on the key observation that the quantum and classical Euler equations share the same form if the (quantum) internal energy rather than temperature is used in the flux. This motivates us to use a classical Maxwellian – that depends on the internal energy rather than temperature – instead of the quantum one in the construction of KFVS, yielding a KFVS which is purely classical. This greatly simplifies the numerical algorithm and reduces the computational cost. The proposed schemes are tested on the 1-D shock tube problem for the Bose and Fermi gases in both classical and nearly degenerate regimes.

1 Introduction

The quantum Euler equations describe the hydrodynamics of a quantum gas. It can be derived via the Chapman-Enskog expansion [2] as the leading order approximation of the quantum Boltzmann equation. Here we mainly consider two kinds of gases: the Bose gas and the Fermi gas. The Bose gas is composed of Bosons, which have an integer value of spin, and obey the Bose-Einstein statistics. The Fermi gas is composed of Fermions, which have half-integer spins and obey the Fermi-Dirac statistics. Many physicists have studied the transport processes in quantum gases, e.g. [11, 18, 21, 20]. In [21] Uehling and Uhlenbeck formulated the quantum Boltzmann equation by heuristic arguments from the classical Boltzmann equation and, using the Chapman-Enskog expansion, gave the corresponding quantum hydrodynamical equations in first (quantum Euler) and second (quantum Navier-Stokes) order approximations, and formal expressions for the viscosity and heat conductivity coefficients.

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Kinetic schemes (or Boltzmann schemes) is a general numerical procedure for solving hyperbolic systems (see for example [7]). For the classical compressible Euler equations, Deshpande and Raul [5] proposed the kinetic theory based fluid-in-cell method and subsequently Deshpande [4] improved it by adding antidiffusive terms. Finally, this work led to the development of kinetic flux vector splitting (KFVS) scheme by Deshpande [4]. Variants of this scheme have also been studied by many other people in the 1980's, such as Pullin's flux equilibrium method (FEM) [16], Reitz's kinetic numerical method (KNM) [17], Aristov and Tcheremissine's method using the discrete velocities of particles [1], Elizarova and Chetverushkin's kinetic-consistent finite difference scheme [6]. Later in early 90's, Perthame considered yet another line of development by replacing the real Maxwellian with the characteristic function [13] [14], where he also proved the entropy and positivity properties of the scheme.

A direct generalization of the KFVS scheme to the quantum Euler equations was done by Yang *et al* in [22, 23]. They adopted the KFVS of Deshpande with the classical Maxwellian replaced by the quantum ones (the Bose-Einstein or the Fermi-Dirac distribution). There are a few difficulties in this formulation. First, due to the complexity of the quantum functions, the numerical fluxes are not as easy to evaluate as the classical ones. Second, to obtain the macroscopic quantities, in particular, temperature and fugacity, one has to invert a nonlinear 2 by 2 system at every spatial point and every time step, which is very computationally intensive. Furthermore, finding a good initial guess for the iterative method is not an easy task.

In this work we propose a much simpler KFVS scheme for the quantum Euler equations. Our formulation is based on the observation that the quantum and classical Euler equations share the same form if the macroscopic variables are properly chosen. Specifically, we still use the classical Maxwellian, except that *the temperature which usually appears in the classical Maxwellian is replaced by the (quantum) internal energy*. This Maxwellian has the same first five moments and, when the Knudsen number approaches zero, yields the same quantum Euler equations as the quantum Maxwellian. As a result, the quantum Euler system can be evolved by a classical KFVS (with the quantum internal energy instead of temperature computed), except at the final output time, if so desired, one needs to compute the temperature or fugacity.

The paper is organized as follows. In the next section, we give a brief introduction to the quantum Boltzmann equation, its basic properties, the corresponding quantum Maxwellians and the quantum Euler equations. In section 3, after a description of the classical KFVS, we discuss some numerical difficulties in previous quantum KFVS schemes, and then give our new KFVS method. A higher order extension is also included. In section 4, the proposed schemes are tested on the 1-D shock tube problem for the Bose and the Fermi gases in both classical and nearly degenerate regimes. Finally some concluding remarks are given in section 5.

2 Quantum Euler Equations

In this section we review some basic facts about the quantum Boltzmann and quantum Euler equations. These will be helpful to introduce the KFVS scheme.

2.1 Quantum Boltzmann Equation

The Quantum Boltzmann equation (QBE), also known as the Uehling-Uhlenbeck equation [21], describes the time evolution of a dilute Bose or Fermi gas,

$$f_t + v \cdot \nabla_x f = \mathcal{Q}(f) \quad x \in \Omega \subset \mathbb{R}^{d_x},\ v \in \mathbb{R}^{d_v} \tag{2.1}$$

Here $f(t,x,v)$ is the number density depending on time t, position x and particle velocity v. The collision operator $\mathcal{Q}$ is

$$\mathcal{Q}(f)(v) = \int_{\mathbb{R}^{d_v}} \int_{\mathbb{S}^{d_v-1}} B(v_1 - v, \omega) \left[f' f_1' (1 \pm \epsilon_0 f)(1 \pm \epsilon_0 f_1) - f f_1 (1 \pm \epsilon_0 f')(1 \pm \epsilon_0 f_1') \right] d\omega dv_1 \tag{2.2}$$

where $\epsilon_0 = \frac{h^{d_v}}{m^{d_v} g}$, h is the Planck constant, m is the particle mass, and g is the spin degeneracy ($g = 2s+1$, s is the principal spin quantum number of the particle, e.g. $s = \frac{1}{2}$ for electron, $s = 1$ for photon). In this paper, the upper sign will always correspond to the Bose gas while the lower sign to the Fermi gas. Since f is the number density, it has to be nonnegative. For the Fermi gas, $f \leq \frac{1}{\epsilon_0}$ by the Pauli exclusion principle. f, f_1, f' and f_1' are the shorthand notations for $f(t,x,v)$, $f(t,x,v_1)$, $f(t,x,v')$ and $f(t,x,v_1')$ respectively. (v, v_1) and (v', v_1') are the velocities before and after collision. They are related by the following parametrization:

$$v' = v + [(v_1 - v) \cdot \omega]\omega \tag{2.3}$$

$$v_1' = v_1 - [(v_1 - v) \cdot \omega]\omega \tag{2.4}$$

where ω is the unit vector along $v - v'$. The collision kernel B is a nonnegative function which only depends on $|v_1 - v|$ and $|\cos\theta|$,

$$B(v_1 - v, \omega) = 2|v_1 - v||\cos\theta|\sigma(|v_1 - v|, 1 - 2|\cos\theta|) \tag{2.5}$$

where θ is the angle between $v_1 - v$ and ω, while σ is the scattering cross-section. In the hard sphere model, $B(v_1 - v, \omega) = 2r^2|(v_1 - v) \cdot \omega| = 2r^2|v_1 - v||\cos\theta|$, where r is the radius of the particle.

One can derive a few properties of the QBE similar to the classical Boltzmann equation.

- Weak form of the collision operator,

$$\int_{\mathbb{R}^{d_v}} \mathcal{Q}(f)\phi dv = \frac{1}{4} \int_{\mathbb{R}^{d_v}} \int_{\mathbb{R}^{d_v}} \int_{\mathbb{S}^{d_v-1}} (\phi + \phi_1 - \phi' - \phi_1') B(v_1 - v, \omega)$$
$$\cdot [f' f_1' (1 \pm \epsilon_0 f)(1 \pm \epsilon_0 f_1) - f f_1 (1 \pm \epsilon_0 f')(1 \pm \epsilon_0 f_1')] d\omega dv_1 dv \tag{2.6}$$

  for any test function ϕ.

- A collision invariant is a continuous function $\phi(v)$ such that $\phi + \phi_1 = \phi' + \phi_1'$ for all v, v_1 and ω. Any collision invariant is a function of the form $\phi(v) = \alpha + \beta \cdot v + \gamma|v|^2$, where α, β, γ are arbitrary real numbers.

- In particular,

$$\int_{\mathbb{R}^{d_v}} \mathcal{Q}(f) dv = \int_{\mathbb{R}^{d_v}} \mathcal{Q}(f) v dv = \int_{\mathbb{R}^{d_v}} \mathcal{Q}(f)|v|^2 dv = 0 \tag{2.7}$$

and if f is a solution of the QBE, the following local conservation laws hold

$$\begin{aligned}\partial_t \int_{\mathbb{R}^{d_v}} f dv + \nabla_x \cdot \int_{\mathbb{R}^{d_v}} v f dv = 0 \\ \partial_t \int_{\mathbb{R}^{d_v}} v f dv + \nabla_x \cdot \int_{\mathbb{R}^{d_v}} v \otimes v f dv = 0 \\ \partial_t \int_{\mathbb{R}^{d_v}} \frac{1}{2}|v|^2 f dv + \nabla_x \cdot \int_{\mathbb{R}^{d_v}} v \frac{1}{2}|v|^2 f dv = 0\end{aligned} \tag{2.8}$$

Define

$$\text{density} \qquad \rho = \int_{\mathbb{R}^{d_v}} f dv, \tag{2.9}$$

$$\text{macroscopic velocity} \qquad u = \frac{\int_{\mathbb{R}^{d_v}} v f dv}{\rho}, \tag{2.10}$$

$$\text{stress tensor} \qquad \mathbb{P} = \int_{\mathbb{R}^{d_v}} (v-u) \otimes (v-u) f dv, \tag{2.11}$$

$$\text{specific internal energy} \qquad e = \frac{\int_{\mathbb{R}^{d_v}} \frac{1}{2}|v-u|^2 f dv}{\rho}, \tag{2.12}$$

$$\text{heat flux} \qquad q = \int_{\mathbb{R}^{d_v}} \frac{1}{2}(v-u)|v-u|^2 f dv \tag{2.13}$$

the above system can then be recast as

$$\begin{aligned}\partial_t \rho + \nabla_x \cdot (\rho u) = 0 \\ \partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u + \mathbb{P}) = 0 \\ \partial_t \left(\rho e + \frac{1}{2}\rho u^2\right) + \nabla_x \cdot \left(\left(\rho e + \frac{1}{2}\rho u^2\right) u + \mathbb{P} u + q\right) = 0\end{aligned} \tag{2.14}$$

2.1.1 Boltzmann's H-Theorem and Quantum Maxwellians

The Boltzmann's H-Theorem in the quantum context takes the following form:

$$\int_{\mathbb{R}^{d_v}} \ln \frac{f}{1 \pm \epsilon_0 f} \mathcal{Q}(f) dv \leq 0 \tag{2.15}$$

Let $\eta = -\frac{1}{\epsilon_0}\left[(\epsilon_0 f)\ln(\epsilon_0 f) \mp (1 \pm \epsilon_0 f)\ln(1 \pm \epsilon_0 f)\right]$, then

$$\frac{d}{dt}\int_{\mathbb{R}^{d_v}} \eta(f) dv = -\int_{\mathbb{R}^{d_v}} \ln \frac{\epsilon_0 f}{1 \pm \epsilon_0 f} \mathcal{Q}(f) dv \geq 0 \tag{2.16}$$

where $\int_{\mathbb{R}^{d_v}} \eta(f) dv$ is the entropy.

It is well-known that the entropy attains its maximum if and only if f reaches the local equilibrium. This holds when $\ln \frac{f}{1 \pm \epsilon_0 f}$ is a collision invariant. So one can assume

$$\frac{f}{1 \pm \epsilon_0 f} = A e^{-a(v-c)^2} \tag{2.17}$$

where A, a, c are the unknowns to be determined.

Clearly as $\epsilon_0 \to 0$, (2.17) becomes $f = Ae^{-a(v-c)^2}$, which implies that f is just the classical Maxwellian. For an ideal monatomic gas $c = u$, $a = \frac{m}{2k_B T}$ and $A = \rho\left(\frac{m}{2\pi k_B T}\right)^{\frac{d_v}{2}}$, where T is the temperature, k_B is the Boltzmann constant.

(2.17) can be rewritten as

$$f = \mathcal{M}_q = \frac{1}{A^{-1}e^{a(v-c)^2} \mp \epsilon_0} \tag{2.18}$$

Using the definitions of ρ and u, one can easily obtain $c = u$. Moreover, $a = \frac{m}{2k_BT}$ is also valid in the quantum case by statistical independence (see [3] pp. 333-335). To simplify the notation, we use a new variable $z = \epsilon_0 A$ rather than A from now on. Therefore, the quantum Maxwellian is given by

$$\mathcal{M}_q = \frac{1}{\epsilon_0} \frac{1}{z^{-1}e^{\frac{m(v-u)^2}{2k_BT}} \mp 1} = \frac{1}{A^{-1}e^{\frac{m}{2k_BT}(v-u)^2} \mp \epsilon_0}\,. \tag{2.19}$$

This is the well-known Bose-Einstein ('-') and Fermi-Dirac ('+') distributions.

2.2 The Quantum Euler Equations

Substituting $\mathcal{M}_q$ into (2.9)−(2.13), one can express all the moments in terms of T, u and z:

$$\rho = \frac{g}{\lambda^{d_v}} Q_{\frac{d_v}{2}}(z) \tag{2.20}$$

$$\rho u = \frac{g}{\lambda^{d_v}} Q_{\frac{d_v}{2}}(z) u \tag{2.21}$$

$$\rho e = \frac{d_v}{2m} k_B T \frac{g}{\lambda^{d_v}} Q_{\frac{d_v+2}{2}}(z) \tag{2.22}$$

$$\mathbb{P} = \frac{k_B T}{m} \frac{g}{\lambda^{d_v}} Q_{\frac{d_v+2}{2}}(z) I \tag{2.23}$$

$$q = 0 \tag{2.24}$$

where I is the identity matrix, $\lambda = \frac{h}{\sqrt{2\pi m k_B T}}$ is the thermal de Broglie wavelength, $Q_\nu(z)$ denotes the Bose-Einstein function $G_\nu(z)$ and the Fermi-Dirac function $F_\nu(z)$ respectively,

$$G_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}}{z^{-1}e^x - 1} dx \quad 0 < z < 1, \nu > 0; z = 1, \nu > 1 \tag{2.25}$$

$$F_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}}{z^{-1}e^x + 1} dx \quad 0 < z < \infty, \nu > 0 \tag{2.26}$$

where $\Gamma(\nu) = \int_0^\infty x^{\nu-1}e^{-x}dx$ is the Gamma function.

In physics z is called the fugacity. The physical range of interest for a Bose gas is $0 < z \leq 1$, where $z = 1$ corresponds to the degenerate case (the onset of Bose-Einstein condensation). For the Fermi gas we don't have such a restriction and the degenerate case is obtained when z is very large. For small z ($0 < z < 1$), the integrand in (2.25) and (2.26) can be expanded in powers of z,

$$G_\nu(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^\nu} = z + \frac{z^2}{2^\nu} + \frac{z^3}{3^\nu} + \ldots \tag{2.27}$$

$$F_\nu(z) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{z^n}{n^\nu} = z - \frac{z^2}{2^\nu} + \frac{z^3}{3^\nu} - \ldots \tag{2.28}$$

Thus, for $z \ll 1$, both functions behave like z itself and one recovers the classical limit. See [12] for more details about these functions.

On the other hand, equation (2.20) can also be written as

$$Q_{\frac{d_v}{2}}(z) = \rho\frac{\lambda^{d_v}}{g} = \rho\left(\frac{m}{2\pi k_B T}\right)^{\frac{d_v}{2}}\epsilon_0 \tag{2.29}$$

where $\rho\left(\frac{m}{2\pi k_B T}\right)^{\frac{d_v}{2}}$ is the coefficient of the classical Maxwellian, which should be an $O(1)$ quantity. Now if $\epsilon_0 \to 0$, then $Q_{\frac{d_v}{2}}(z) \to 0$, which means $z \ll 1$ by the monotonicity of the function Q_ν. This is consistent with the fact that one gets the classical Boltzmann equation in QBE (2.1) by letting $\epsilon_0 \to 0$.

Now with the above computed moments (2.20)−(2.24), system (2.14) can be closed and gives the quantum compressible Euler equations. Note here the macroscopic quantities ρ, e and T, z are related by a nonlinear 2 by 2 system:

$$\rho = \frac{g}{\lambda^{d_v}}Q_{\frac{d_v}{2}}(z) \tag{2.30}$$

$$e = \frac{d_v}{2m}k_B T\frac{Q_{\frac{d_v+2}{2}}(z)}{Q_{\frac{d_v}{2}}(z)} \tag{2.31}$$

3 KFVS Schemes

In this section, we give a KFVS scheme for the quantum Euler equations. We will first review some previous kinetic schemes for both classical and quantum fluid equations.

3.1 Classical KFVS Schemes

To illustrate the basic idea, consider the 1-D classical compressible Euler equations,

$$\begin{pmatrix} \rho \\ \rho u \\ \frac{1}{2}\rho\frac{k_B T}{m} + \frac{1}{2}\rho u^2 \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + \rho\frac{k_B T}{m} \\ \left(\frac{3}{2}\rho\frac{k_B T}{m} + \frac{1}{2}\rho u^2\right)u \end{pmatrix}_x = 0 \tag{3.1}$$

This system can be obtained by taking the moments of

$$\partial_t \mathcal{M}_c + v\partial_x \mathcal{M}_c = 0 \tag{3.2}$$

where $\mathcal{M}_c$ is the classical Maxwellian (assume $d_v = 1$),

$$\mathcal{M}_c = \rho\sqrt{\frac{m}{2\pi k_B T}}e^{-\frac{m(v-u)^2}{2k_B T}} \tag{3.3}$$

To derive a kinetic scheme, we divide the spatial domain into a number of cells $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$, $i \in \mathbb{Z}$. Each cell is centered at x_i with a uniform length Δx. Then a first order upwind scheme for equation (3.2) can be written as

$$\partial_t M_i + \frac{\frac{v+|v|}{2}M_i + \frac{v-|v|}{2}M_{i+1} - \frac{v+|v|}{2}M_{i-1} - \frac{v-|v|}{2}M_i}{\Delta x} = 0 \tag{3.4}$$

Multiply (3.4) by $\left(1, v, \frac{1}{2}v^2\right)^T$ and integrate with respect to v, one can get

$$\partial_t U_i + \frac{F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}}{\Delta x} = 0 \tag{3.5}$$

with

$$U_i = \left(\rho_i,\ \rho_i u_i,\ \frac{1}{2}\rho_i \frac{k_B T_i}{m} + \frac{1}{2}\rho_i u_i^2\right)^T \tag{3.6}$$

$$F_{i+\frac{1}{2}} = \int_{-\infty}^{\infty} \left(1, v, \frac{1}{2}v^2\right)^T \frac{v+|v|}{2} M_i dv + \int_{-\infty}^{\infty} \left(1, v, \frac{1}{2}v^2\right)^T \frac{v-|v|}{2} M_{i+1} dv \tag{3.7}$$

Define

$$F_i^{\pm} = \int_{-\infty}^{\infty} \left(1, v, \frac{1}{2}v^2\right)^T \frac{v \pm |v|}{2} M_i dv \tag{3.8}$$

then $F_{i+\frac{1}{2}} = F_i^+ + F_{i+1}^-$. Plugging (3.3) into (3.8), $F_i^{\pm}$ can be evaluated in closed form in terms of error functions as [4]

$$F_i^{\pm} = \begin{pmatrix} \rho_i u_i A_i^{\pm} \pm \rho_i B_i \\ \left(\rho_i \frac{k_B T_i}{m} + \rho_i u_i^2\right) A_i^{\pm} \pm \rho_i u_i B_i \\ \left(\frac{3}{2}\rho_i \frac{k_B T_i}{m} u_i + \frac{1}{2}\rho_i u_i^3\right) A_i^{\pm} \pm \left(\frac{1}{2}\rho_i u_i^2 + \rho_i \frac{k_B T_i}{m}\right) B_i \end{pmatrix} \tag{3.9}$$

where

$$A_i^{\pm} = \frac{1}{2}\left(1 \pm \mathrm{erf}(s_i)\right),\ B_i = e^{-s_i^2}\sqrt{\frac{k_B T}{2\pi m}} \text{ and } s_i = u_i \sqrt{\frac{m}{2k_B T_i}} \tag{3.10}$$

3.2 Quantum KFVS Schemes

3.2.1 An Old Quantum KFVS Scheme

A direct generalization of the above scheme to the quantum system was done by Yang *et al* in [22]. They obtained the numerical fluxes by integrating the quantum Maxwellian $\mathcal{M}_q$. For instance, when $d_v = 1$ the first component of $F^{\pm}$ at cell i is

$$F_i^{\pm(1)} = \sqrt{\frac{\pi k_B T_i}{2m}} u_i A_i^{\pm} + \frac{k_B T_i}{m} B_i^{\pm} \tag{3.11}$$

$$A_i^{\pm} = \frac{1}{\epsilon_0}(Q_{\frac{1}{2}}(z_i) \pm \mathrm{sgn}(u_i) Q_{\frac{1}{2}}(h_i, z_i)),\quad B_i^{\pm} = \pm\frac{1}{\epsilon_0}\tilde{Q}_1(h_i, z_i) \tag{3.12}$$

where $h_i = \frac{m u_i^2}{2k_B T_i}$, $Q_\nu(h,z)$ and $\tilde{Q}_\nu(h,z)$ are the incomplete Bose-Einstein or Fermi-Dirac functions,

$$Q_\nu(h,z) = \frac{1}{\Gamma(\nu)} \int_0^h \frac{x^{\nu-1}}{z^{-1}e^x \mp 1} dx,\quad \tilde{Q}_\nu(h,z) = Q_\nu(z) - Q_\nu(h,z) \tag{3.13}$$

These functions are not as easy to evaluate as the error function. Furthermore, one needs the values of u_i, T_i and z_i to evaluate $F_i^{\pm}$. While u_i can be computed directly from the conserved quantities (density, momentum and energy), to get z_i and T_i one has to solve the nonlinear 2 by 2 system (2.30) (2.31) at every spatial point and every time step. This is very expensive and selecting a good initial guess for the iterative method is sometimes tricky due to the complexity of the function Q_ν.

3.2.2 A New Quantum KFVS Scheme

By the definition of the moments in (2.20)−(2.24), one finds that the stress tensor $\mathbb{P} = \frac{2}{d_v}\rho e I$, so the quantum Euler equations can be written in terms of ρ, u and e as

$$\begin{aligned}
&\partial_t \rho + \nabla_x \cdot (\rho u) = 0 \\
&\partial_t (\rho u) + \nabla_x \cdot \left(\rho u \otimes u + \frac{2}{d_v}\rho e I \right) = 0 \\
&\partial_t \left(\rho e + \frac{1}{2}\rho u^2 \right) + \nabla_x \cdot \left(\left(\frac{d_v+2}{d_v}\rho e + \frac{1}{2}\rho u^2 \right) u \right) = 0 \\
&\text{sound speed } c = \sqrt{\gamma \frac{p}{\rho}}, \quad \gamma = \frac{d_v+2}{d_v}, \quad p = \frac{2}{d_v}\rho e
\end{aligned} \tag{3.14}$$

which are the same as the classical Euler equations! This suggests our new idea: we can just use the classical Maxwellian instead of the quantum Maxwellian. To be specific, replace the temperature T with the internal energy e in the classical Maxwellian using relation $e = \frac{d_v}{2m} k_B T$ (true for classical monatomic gases) and get

$$\mathcal{M}_c = \rho \left(\frac{d_v}{4\pi e} \right)^{\frac{d_v}{2}} e^{-\frac{d_v}{4e}(v-u)^2} \tag{3.15}$$

then this $\mathcal{M}_c$ has the same (first five) moments as $\mathcal{M}_q$ and can be used to construct the quantum KFVS scheme. Correspondingly, we only need to replace T with e in the fluxes of the classical KFVS (3.9). Here we give a general formula for velocity space of dimension d_v,

$$F_i^{\pm} = \begin{pmatrix} \rho_i u_i A_i^{\pm} \pm \rho_i B_i \\ \left(\frac{2}{d_v}\rho_i e_i + \rho_i u_i^2 \right) A_i^{\pm} \pm \rho_i u_i B_i \\ \left(\frac{d_v+2}{d_v}\rho_i u_i e_i + \frac{1}{2}\rho_i u_i^3 \right) A_i^{\pm} \pm \left(\frac{1}{2}\rho_i u_i^2 + \frac{d_v+1}{d_v}\rho_i e_i \right) B_i \end{pmatrix} \tag{3.16}$$

where

$$A_i^{\pm} = \frac{1}{2}\left(1 \pm \operatorname{erf}\left(u_i \sqrt{\frac{d_v}{4e_i}} \right) \right), \; B = e^{-\frac{d_v}{4e_i}u_i^2} \sqrt{\frac{e_i}{d_v \pi}} \tag{3.17}$$

It is important to notice that z and T are not present at all in this new scheme, thus one does not need to invert the 2 by 2 system (2.20) (2.31) during the time evolution. If they are desired variables for output, one only needs to convert between ρ, e and z, T at the final output time.

Remark 3.1: *If one uses a BGK approximation to the quantum Boltzmann equation (2.1), then the observation in this subsection suggests that the quantum BGK equation*

$$f_t + v \cdot \nabla_x f = \frac{1}{\tau}(\mathcal{M}_q - f) \tag{3.18}$$

and the classical BGK equation

$$f_t + v \cdot \nabla_x f = \frac{1}{\tau}(\mathcal{M}_c - f) \tag{3.19}$$

where $\mathcal{M}_c$ is defined by (3.15), have the same fluid limit as the relaxation parameter $\tau \to 0$, as long as one relates the internal energy e and temperature T by (2.31). Thus our approach somewhat resembles the Jin-Xin relaxation scheme for hyperbolic systems of conservation laws [8].

Remark 3.2: *One does not have to use a kinetic scheme for the quantum Euler equations (3.14). Clearly any shock capturing method can be used.*

3.2.3 High Resolution Schemes

The above first order method can be easily extended to higher orders. To do so, we rewrite the fluxes in (3.5) as $F_{i+\frac{1}{2}} = F^+_{i+\frac{1}{2}} + F^-_{i+\frac{1}{2}}$. In the first order scheme, the positive flux $F^+_{i+\frac{1}{2}} = F^+_i$ and the negative flux $F^-_{i+\frac{1}{2}} = F^-_{i+1}$; $F^\pm_i$ is given by (3.16). One can use the slope limiter method [10] to get a formally second order TVD scheme:

$$F^{+(j)}_{i+\frac{1}{2}} = F^{+(j)}_i + \frac{\Delta x}{2}\sigma^{+(j)}_i \tag{3.20}$$

$$F^{-(j)}_{i+\frac{1}{2}} = F^{-(j)}_{i+1} - \frac{\Delta x}{2}\sigma^{-(j)}_{i+1} \tag{3.21}$$

$j = 1, 2, 3$. The slope limiter $\sigma^\pm_i$ is defined as

$$\sigma^{+(j)}_i = \frac{F^{+(j)}_{i+1} - F^{+(j)}_i}{\Delta x}\phi\left(\frac{F^{+(j)}_i - F^{+(j)}_{i-1}}{F^{+(j)}_{i+1} - F^{+(j)}_i}\right) \tag{3.22}$$

$$\sigma^{-(j)}_i = \frac{F^{-(j)}_i - F^{-(j)}_{i-1}}{\Delta x}\phi\left(\frac{F^{-(j)}_{i+1} - F^{-(j)}_i}{F^{-(j)}_i - F^{-(j)}_{i-1}}\right) \tag{3.23}$$

where $\phi(\theta)$ is the flux limiter function, e.g. the van Leer limiter [9] is given by

$$\phi(\theta) = \frac{|\theta| + \theta}{1 + |\theta|} \tag{3.24}$$

4 Numerical Examples

In this section we present some numerical results using the new quantum KFVS schemes. The test example is the 1-D shock tube problem with the initial condition

$$\begin{cases} (\rho_l, u_l, T_l) = (1, 0, 1) & \text{if } 0 \le x \le 0.5 \\ (\rho_r, u_r, T_r) = (0.4, 0, 0.6) & \text{if } 0.5 < x \le 1 \end{cases} \tag{4.1}$$

In all of the simulations, we assume the dimension of the velocity space $d_v = 3$; the particle mass m, spin degeneracy g and Boltzmann constant k_B are all taken to be 1. We adjust the Planck constant h to get z that corresponds to different physical regimes.

Besides the directly computed macroscopic quantities, we will show the fugacity z and temperature T as well. The next subsection is devoted to a discussion of inverting the system (2.30) (2.31).

4.1 Computing z and T

First, (2.30) (2.31) lead to

$$\frac{Q^{\frac{d_v+2}{d_v}}_{\frac{d_v}{2}}(z)}{Q_{\frac{d_v+2}{2}}(z)} = \frac{\rho^{\frac{2}{d_v}}}{e}\frac{d_v h^2}{g^{\frac{2}{d_v}} 4\pi m^2} \tag{4.2}$$

In our computation, we treat the left hand side of (4.2) as one function of z, and invert it by the secant method. Once z is obtained, T can be computed easily using for example (2.30).

The next question is how to evaluate the quantum function $Q_\nu(z)$? Expansions (2.27) and (2.28) are valid for the Bose and Fermi gases in the classical regime ($z \ll 1$) and the Bose gas

in the nearly degenerate regime (z close to but less than 1). Since (2.27) (2.28) are convergent series, one can just terminate the approximation whenever the difference of two successive terms is less than a tolerance. For the Fermi gas in the degenerate regime, the well-known Sommerfeld expansion [19] is widely used by physicists to approximate the Fermi-Dirac integral. However, this expansion works well when z is extremely large ($\ln z \gg 1$). In the nearly degenerate regime z is not very large, we compute the functions by numerical integration. The approach adopted here is taken from [15] (chapter 6.10).

4.2 Bose Gas in Classical Regime

Let $h = 1$, then the initial condition (4.1) corresponds to $z_l = 0.0621$, $z_r = 0.0536$. Here $z \ll 1$ characterizes the classical regime. Figure 1 shows the computed density ρ, velocity u, internal energy e, pressure P, fugacity z and temperature T at time $t = 0.18$. The behaviors are similar to a classical gas.

4.3 Bose Gas in Nearly Degenerate Regime

Increase h to 3.3, then the initial condition (4.1) corresponds to $z_l = 0.9906$, $z_r = 0.9611$. z close to 1 implies that the gas is in the nearly degenerate regime. Figure 2 shows the computed density ρ, velocity u, internal energy e, pressure P, fugacity z and temperature T at time $t = 0.18$. The solutions are quantitatively quite different from those in the classical regime.

4.4 Fermi Gas in Classical Regime

Let $h = 1$, the initial condition (4.1) corresponds to $z_l = 0.0649$, $z_r = 0.0557$, which is in the classical regime. Figure 3 shows the computed density ρ, velocity u, internal energy e, pressure P, fugacity z and temperature T at time $t = 0.18$. We can see that the behaviors of the Fermi gas and the Bose gas are more or less the same in this regime.

4.5 Fermi Gas in Nearly Degenerate Regime

Increase h to 6, the initial condition (4.1) corresponds to $z_l = 901.2840$, $z_r = 459.5218$. z is large, thus the Fermi gas is in the nearly degenerate regime. Figure 4 shows the computed density ρ, velocity u, internal energy e, pressure P, fugacity z and temperature T at time $t = 0.18$. Again the solutions are very different from those in the classical regime.

4.6 Another Example for Fermi Gas in Nearly Degenerate Regime

For comparison, we solve the Example 4 in [22] with our new scheme. The initial condition is given by

$$\begin{cases} (\rho_l, u_l, T_l) = (3.086455, 0, 8.053324) & \text{if } 0 \le x \le 0.5 \\ (\rho_r, u_r, T_r) = (3.084272, 0, 8.067390) & \text{if } 0.5 < x \le 1 \end{cases} \tag{4.3}$$

This corresponds to $z_l = 2000$, $z_r = 1500$. Figure 5 shows the computed density ρ, velocity u, fugacity z and temperature T at time $t = 0.1$. The results are comparable to those of [22] computed with a fifth-order WENO scheme.

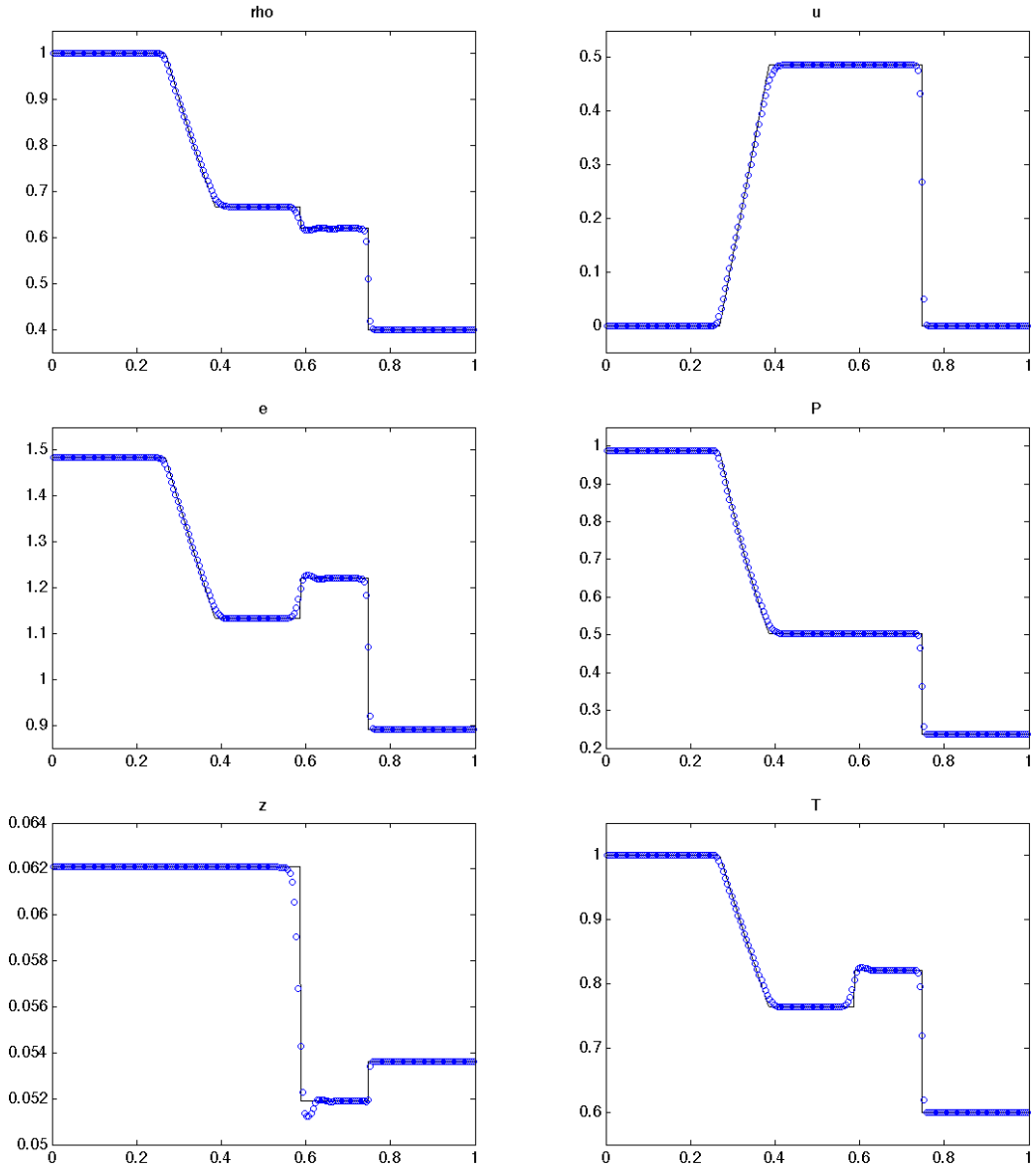

Figure 1: Bose gas in the classical regime: $z_l = 0.0621$, $z_r = 0.0536$. Density ρ, velocity u, internal energy e, pressure P, fugacity z and temperature T. $t = 0.18$, $\Delta t = 0.0002$, $\Delta x = 0.005$. Solid line: exact solution; $\circ$: the high resolution scheme with the van Leer limiter.

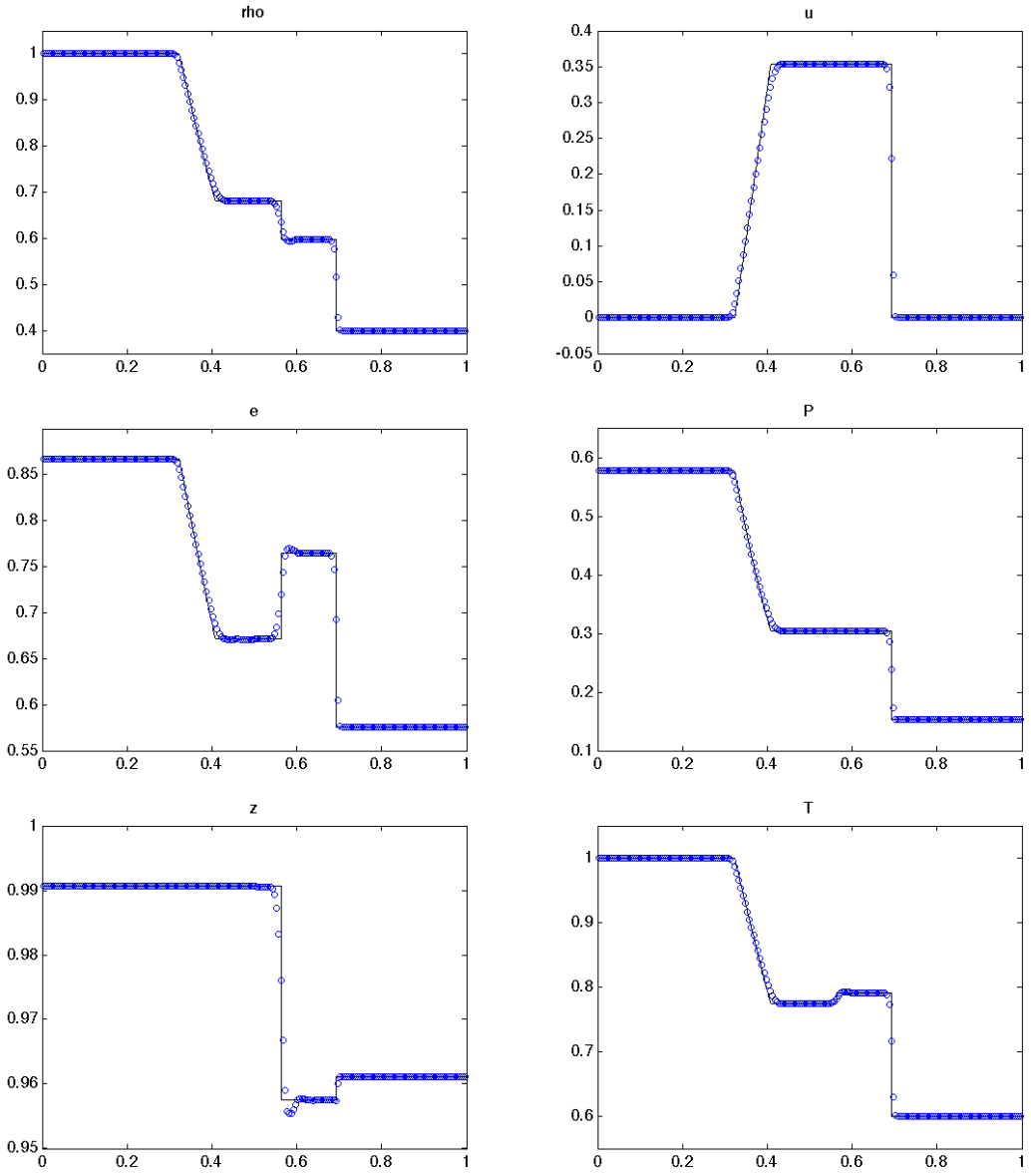

Figure 2: Bose gas in the nearly degenerate regime: $z_l = 0.9906$, $z_r = 0.9611$. Density ρ, velocity u, internal energy e, pressure P, fugacity z and temperature T. $t = 0.18$, $\Delta t = 0.0002$, $\Delta x = 0.005$. Solid line: exact solution; $\circ$: the high resolution scheme with the van Leer limiter.

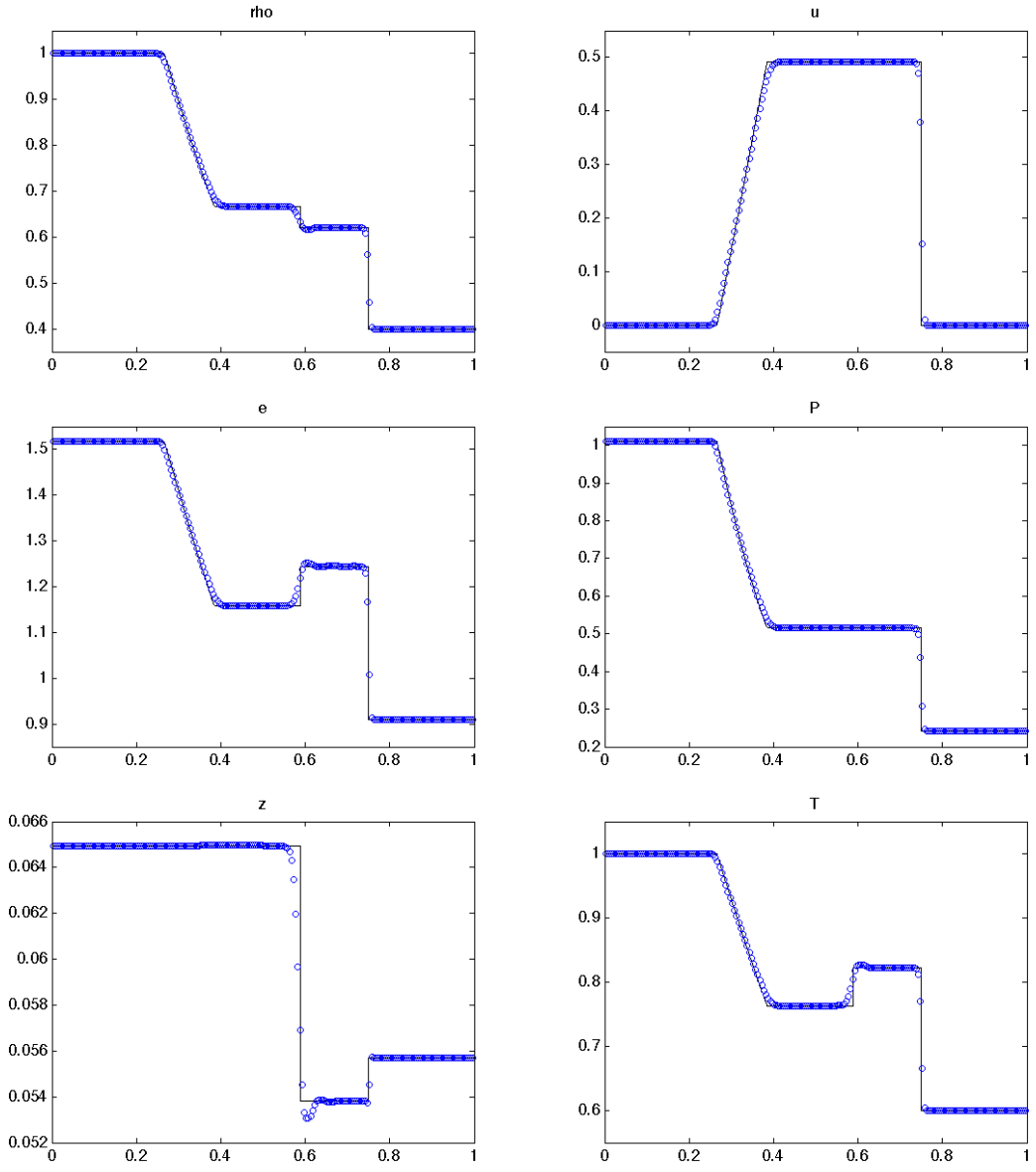

Figure 3: Fermi gas in the classical regime: $z_l = 0.0649$, $z_r = 0.0557$. Density ρ, velocity u, internal energy e, pressure P, fugacity z and temperature T. $t = 0.18$, $\Delta t = 0.0002$, $\Delta x = 0.005$. Solid line: exact solution; $\circ$: the high resolution scheme with the van Leer limiter.

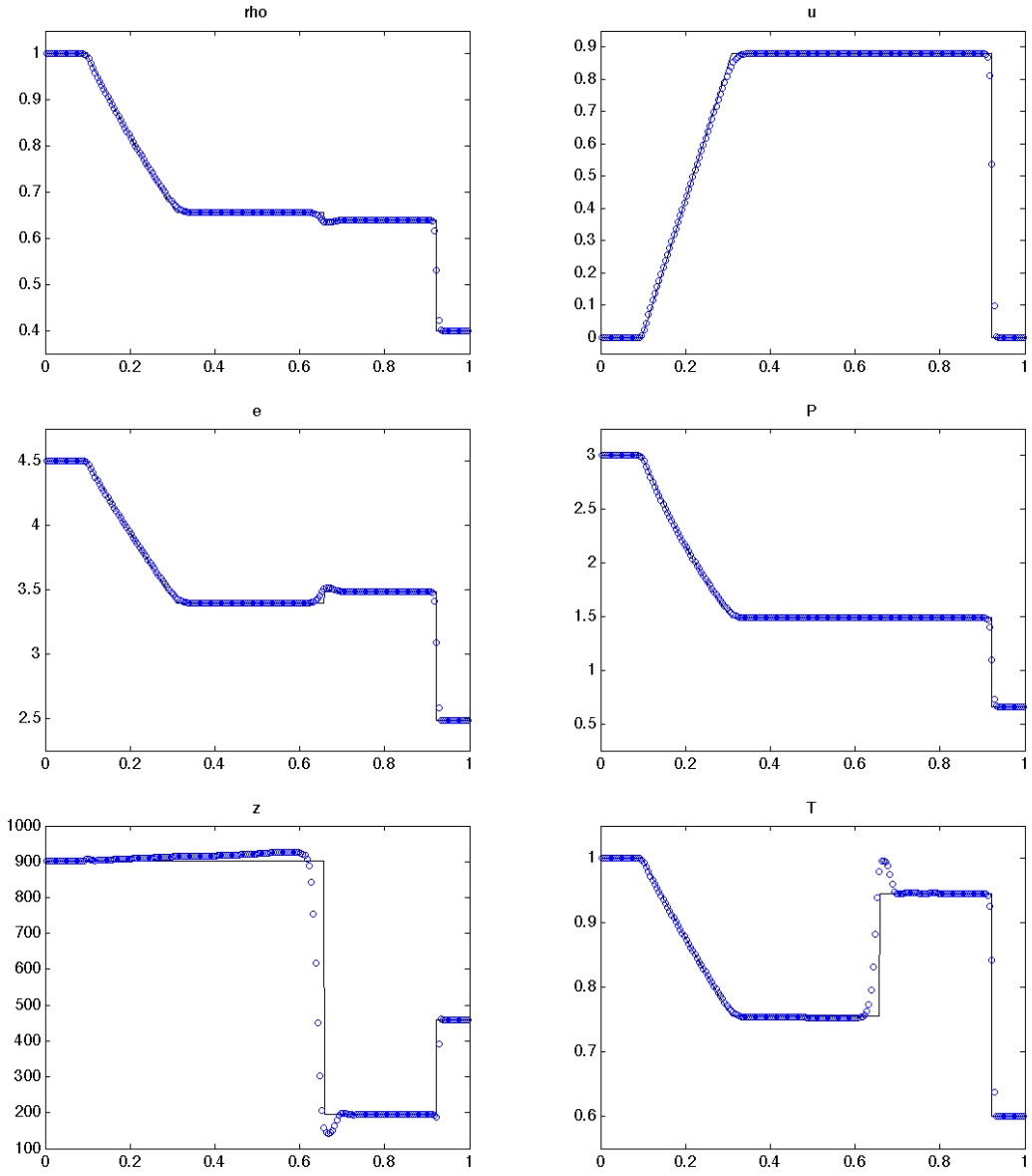

Figure 4: Fermi gas in the nearly degenerate regime: $z_l = 901.2840$, $z_r = 459.5218$. Density ρ, velocity u, internal energy e, pressure P, fugacity z and temperature T. $t = 0.18$, $\Delta t = 0.0002$, $\Delta x = 0.005$. Solid line: exact solution; $\circ$: the high resolution scheme with the van Leer limiter.

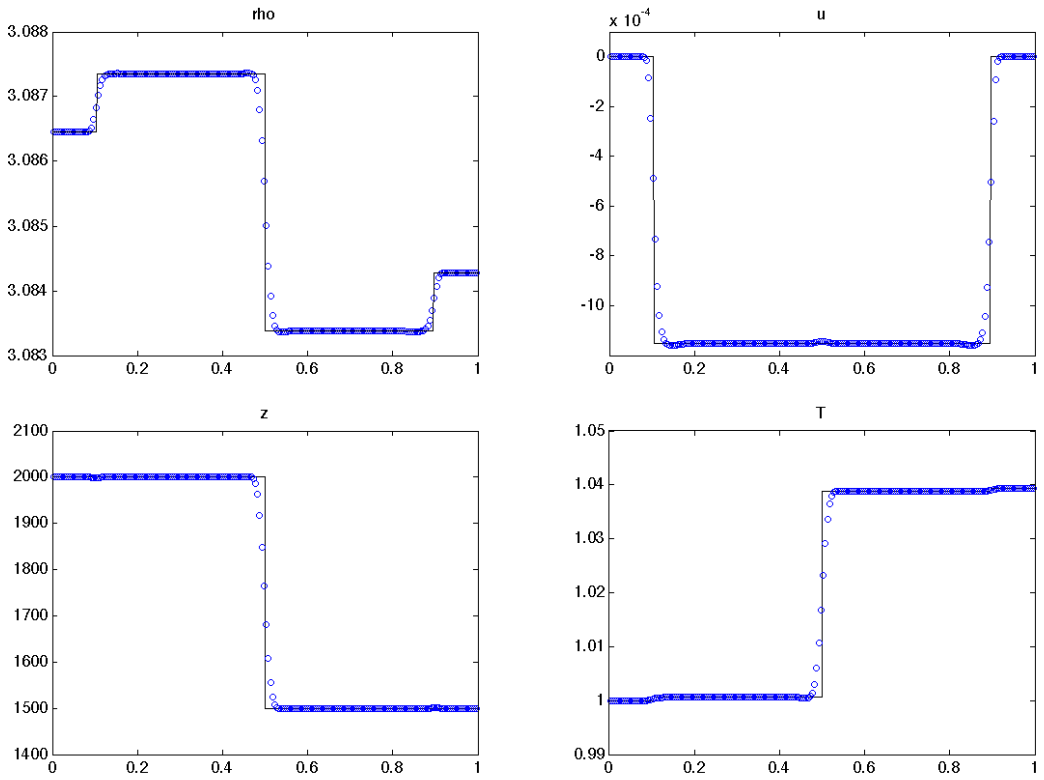

Figure 5: Example 4 in [22]. The Fermi gas in the nearly degenerate regime: $z_l = 2000$, $z_r = 1500$. Density ρ, velocity u, fugacity z and temperature T. $t = 0.1$, $\Delta t = 0.0002$, $\Delta x = 0.005$. Solid line: exact solution; $\circ$: the high resolution scheme with the van Leer limiter.

5 Conclusion

In this paper, a Kinetic Flux Vector Splitting scheme was proposed for the quantum Euler equations. The key observation here is that the quantum and classical Euler equations can be written in the same form as long as one uses density, velocity and internal energy as the variables. This motivates us to use the *classical* Maxwellian – based on the internal energy rather than temperature – to construct the numerical flux. This avoids the complexity of evaluating the quantum functions and the overall scheme is basically classical except at the final output time one needs to invert the nonlinear system $\rho = \rho(z,T)$, $e = e(z,T)$ to get the fugacity and temperature if they are desired. Numerical examples for the 1-D shock tube problem are presented to demonstrate that the behaviors of both the Bose and Fermi gases in different physical regimes can be captured well with our scheme.

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