Numerical Approach of Interactions of Proton Beams and Dense Plasmas with Quantum-Hydrodynamic/Particle-in-Cell Model∗

ZHANG Ya (张雅)1, LI Lian (李莲)3, JIANG Wei (姜巍)1,2, YI Lin (易林) 1

1School of Physics, Huazhong University of Science and Technology, Wuhan 430074, China
2Centre for Mathematical Plasma-Astrophysics, Department of Mathematics, Katholieke Universiteit Leuven, B-3001 Leuven, Belgium

Abstract A one dimensional quantum-hydrodynamic/particle-in-cell (QHD/PIC) model is used to study the interaction process of an intense proton beam (injection density of \(10^{17} \text{ cm}^{-3}\)) with a dense plasma (initial density of \(\sim 10^{21} \text{ cm}^{-3}\)), with the PIC method for simulating the beam particle dynamics and the QHD model for considering the quantum effects including the quantum statistical and quantum diffraction effects. By means of the QHD theory, the wake electron density and wakefields are calculated, while the proton beam density is calculated by the PIC method and compared to hydrodynamic results to justify that the PIC method is a more suitable way to simulate the beam particle dynamics. The calculation results show that the incident continuous proton beam when propagating in the plasma generates electron perturbations as well as wakefields oscillations with negative valleys and positive peaks where the proton beams are repelled by the positive wakefields and accelerated by the negative wakefields. Moreover, the quantum correction obviously hinders the electron perturbations as well as the wakefields. Therefore, it is necessary to consider the quantum effects in the interaction of a proton beam with cold dense plasmas, such as in the metal films.

Keywords: proton beam, particle-in-cell, quantum hydrodynamics, wake field

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(Some figures may appear in colour only in the online journal)

1 Introduction

There has been great interest in the characteristics of beam-matter interactions due to their wide applications in basic and applied physics [1–4], such as laboratory accelerator [5], inertial confinement fusion (ICF) [6–10], astrophysics [11], heavy ion beam research [12,13], plasma physics [14], condensed matter physics [15] and high energy density physics (HEDP) [16–18]. For the laser-matter interactions, Bell et al. investigated the interaction of short-pulse, high-intensity lasers with solid targets [1]. Wang et al. [10] investigated laser beams interacting with compressed targets for the application of fast ignition (FI), by using an integrated particle-in-cell method. The case of a projectile charge interacting with a matter including electron gases and plasmas has been studied, not only within the framework of the linearized theories including the random phase-approximation (RPA) linear response theory [19], the dielectric [20] and binary collision [21] theories, but also with the inclusion of the nonlinear contributions by using kinetic theory [22] and numerical simulations based on particle-in-cell (PIC) simulation, molecular dynamics (MD) [14,23] and hydrodynamics [24]. However, much work was based on the linearized theories.

Moreover, a study of fundamental properties of the beam-matter interaction process is of considerable potential interest for the research of ICF [6–9]. It has been suggested that collimated laser-generated proton beam could offer an alternative path to fast ignition with simpler energy transport physics in ICF [25]. Again, recent progress in laser matter interaction makes it possible to produce intense, collimated, ultrashort picosecond proton beams with energy from few hundreds of electron volts up to several tens of MeV [2,26]. The mechanism used to generate the proton beam employs a high intensity ultra-short laser pulse incident on a thin metallic foil [27–29]. Therefore, it is suggested that proton beam interaction with matter offers new possibilities in HEDP through creating unique states of matter and that fast ignition with proton beams merits further study.

As is well known, when ion beams interact with a matter, wakefields will be present due to the collective excitations of the target electrons, and the inci-
dent protons will lose energy. Thus the wakefield and energy loss measurements of charged particles penetrating plasmas are of fundamental importance to understand beam-plasma interactions. The energy loss of intense ion beams in plasmas that is available at high energy heavy ion accelerators at GSI (1Gesellschaft für Schwerionenforschung), has been investigated by Hoffmann et al. [18]. The wakefield has been studied widely, for example, by the AWAKE experiment at CERN (European Council for Nuclear Research) and by the cooperation group of the Institute of Modern Physics and Dalian University of Technology in China [30]. Strongly-coupled cold and dense plasmas at 0.01 to 0.1 times solid density are of considerable scientific importance as well as of great technological interest for studies of the beam-plasma interaction process in the field of HEDP. For the interaction of proton beams with dense plasmas, the plasma electron density can be larger than $10^{21} \text{ cm}^{-3}$, forming a high density degenerate quantum plasma. Thus, the quantum effects are necessary to be considered. Quantum plasmas are regarded as extremely dense plasmas (comparable or larger than 0.01 times solid density) behave like a quantum ideal gas, due to the exclusion principle [31].

In addition, dilute plasmas can also exhibit quantum features, when the dimensions of the system can be comparable to the de Broglie wavelength. Again, the quantum plasma approaches the classical limit when the temperature is much higher than the Fermi temperature, as is well known [31–33]. Recently, most researchers adopted one-dimensional (1D) hydrodynamic models [26,34] to simulate the interaction of laser produced proton beams with an aluminum target, however, they still employed classic treatment and quantum effects were not considered. Again, quantum molecular dynamics simulations [35] are too computationally costly to study the properties of charged particles moving through a quantum plasma, such as the wakefield and energy loss, especially for the microscope level.

The quantum hydrodynamical model (QHD) [32,33,36], with considering the quantum effects, has been developed by solving the nonlinear Schrödinger-Poisson or the Wigner-Poisson kinetic models. In our previous works, we simulated the wake potential and energy loss of a proton propagating in a 1D solid target by using the 1D QHD theory [24]. Again, the two-dimensional (2D) QHD model was also employed to study a proton cluster [37] and a continuous proton beam [38] interacting with a solid aluminum target. The continuous proton beam was treated as a continuous fluid in the above work [38] due to the pure hydrodynamic model. However, the dynamics of beam particles cannot be considered by the QHD model. At present, the PIC simulations have been adopted to study the interaction process of a test point charge [14] and a test ion-cluster beam including the dynamics of beam particles [39] with classic plasmas. To the best of our knowledge, a self-consistent QHD/PIC hybrid model has not been performed to study the interaction process of an intense proton beam ($\sim 10^{17} \text{ cm}^{-3}$) with a quantum plasma carefully. In this work, the PIC method is employed to consider the beam particle dynamics, while the QHD model is used to describe the collective excitation of the plasma electrons with considering the quantum effects, for an intense proton beam interacting with a 1D quantum plasma. When a continuous proton beam is propagating in quantum plasmas, oscillating wakefields are generated and the quantum effects obviously hinder the wakefields. The paper is organized as follows. In section 2.1 the physical model is described, and in section 2.2 the QHD/PIC simulation model coupled with the Poisson equation is presented. In section 3, simulation results are shown to analyze the beam properties propagating in the plasma target and the wakefields driven by this beam. Comparisons between with and without considering the quantum effects are also made in this section, to show their visible contributions not only to the plasma electron dynamics but also to the beam proton dynamics. A short summary is given in section 4. Gauss units will be used throughout the paper except in specific definitions.

2 Physical and numerical model

2.1 Physical model

The physical parameters of the proton beams are selected according to the experiment carried out by Patel et al. [8]. A continuous proton beam with injection velocities $v_0 = 1v_B$, $3v_B$ and $5v_B$, and injection density $n_{id} = 10^{17} \text{ cm}^{-3}$, is considered, with the duration about several ps. Here $v_B = e^2/\hbar$ is the Bohr velocity. Electron gases, with an initial density $n_0 = 1.8 \times 10^{21} \text{ cm}^{-3}$, or 0.01 times solid aluminum density, is assumed to be equilibrium at the initial time. The ions are treated as a motionless background, due to the fact that the interaction time is so small. The proton beam is injected into a planar film with the thickness of $z = 2.3 \times 10^{-4} \text{ cm}$. In experiments, this µm film can be prepared from solid aluminum foams [40]. In our future work, we will try to simulate the interaction processes of the proton beams with aluminum foams that are exactly linked with experiments.

2.2 Numerical model

Consider the propagation of a continuous proton beam through a 1D quantum plasma with constant injection density $n_{id}$ and velocity $v_0$ in the z-direction. A 1d1v explicit electrostatic PIC code is used for the proton beam simulation. All the charged particles are considered to move along the z axis [41]. The PIC model calculates the charge density $n_B$ of the proton beam based on the position of the protons. The simulation length is composed of $N = 440$ grids in the z direction. The space and time steps are fixed to $10^6 n_B$ with the Bohr radius $a_B = \hbar^2/m_e e^2 = 0.529 \times 10^{-8} \text{ cm}$ and $2.4 \times 10^{-17} \text{ s}$, respectively. Here $m_e$ is the electron
mass and $e$ is the elementary charge. We adopt averaged 2000 super particles per cell, which is varied to check the stability and accuracy of the results. The open boundary condition is used at the left boundary $z = 0$ and the absorption boundary condition is applied at the right boundary $z = 2.3 \times 10^{-4}$ cm in the $z$ direction. In other words, as the time progresses, the beam protons are continually injected into the plasma with the injection velocity prescription on the left boundary $z = 0$ and absorbed as they reach the right boundary $z = 2.3 \times 10^{-4}$ cm.

Here we adopt the explicit and electrostatic PIC model, with a standard leap-frog particle push \[^{[41]}\], which is robust and easy to deploy. It is well known that in particle-in-cell/Monte Carlo (PIC/MC) simulating the spatiotemporal steps must satisfy the constraints as

$$
\Delta t < \frac{2}{\omega_b},
\Delta t < \frac{\Delta z}{u_{\text{bmax}}},
\Delta x < \xi \lambda_D,
$$

(1)

where $\omega_b = \sqrt{4\pi \varepsilon_n n_b/\mu_p}$ is the beam oscillating frequency, $u_{\text{bmax}}$ is the maximum injection velocity of the proton beam, $\lambda_D$ is the Debye length, and $\xi$ is a factor about 3 depending on the specific problem. Here $m_p$ is the proton mass and $t$ represents time. For our simulations, all three conditions are satisfied. Furthermore, the PIC model is noisy, since it is a statistical method. By adopting 2000 particles per cell, this harmful effect is successfully suppressed.

The electric field $E_z$ satisfies the Poisson equation

$$
\frac{\partial E_z}{\partial z} = -4\pi e(n_e - n_0 - n_b).
$$

(2)

To solve the Poisson equation, it needs to know the total charge density consisting of the plasma electron charge density $n_e$ that can be obtained from the QHD model and the proton charge density $n_b$ is obtained from the PIC model.

We consider a 1D quantum plasma composed of non-relativistic degenerate electron fluids and motionless ions with equilibrium density $n_0 = n_{\text{e0}} = n_0$, where the quantum effects are taken into account. In this quantum plasma with degenerate electrons ($T \ll E_F$), the quantum coupling parameter—the ratio of the characteristic potential energy of plasma particle interactions to their characteristic kinetic energy \[^{[33]}\], is given by $\Gamma_q = E_{\text{pot}}/E_F \sim (\hbar \omega_p/E_F)^2$, with the plasma electron frequency $\omega_p = \sqrt{4\pi \varepsilon n_e/m_e}$, the Fermi energy $E_F = (\hbar^2/2m_e)(3\pi^2 n_e)^{2/3}$ and the electron temperature $T$ in unit of eV. The characteristic potential \[^{[33]}\] is estimated as $E_{\text{pot}} = 4\pi e^2 n_e^{1/3}$. The quantum plasma is collisionless, provided $\Gamma_q \ll 1$. Thus, the quantum N-body problem can be reduced to a one-particle Wigner equation. The Wigner-Poisson system is therefore capable of describing a quantum electrostatic plasma in the collisionless approximation. Finally, the QHD model is derived from the Wigner-Poisson system. Compared to the Wigner-Poisson system, the QHD model is more simple for numerical studies and has a straightforward interpretation in terms of fluid quantities that are employed in classical physics.

In a dense quantum plasma, $\Gamma_q \simeq 1$; however, at strictly zero temperature ($T \ll E_F$), all electrons have energies below $E_F$, and no collision is possible, simply due to the exclusion principle. Thus the collisionless QHD model is valid \[^{[33,42,43]}\].

When the proton beam moves through the plasma along the $z$ axis, the homogeneous electron plasma is perturbed by the projectiles and can be regarded as a charged fluid with the velocity field $u_e(z, t)$ and the density $n_e(z, t)$. By employing the collisionless QHD model as discussed above, the excitations of the degenerate electrons can be described by the continuity equation

$$
\frac{\partial n_e}{\partial t} + \frac{\partial (u_n u_e)}{\partial z} = 0,
$$

(3)

and the momentum-balance equation

$$
\frac{\partial u_e}{\partial t} + u_n \frac{\partial u_e}{\partial z} = -\frac{e}{m_e} E_z - \frac{1}{m_e} \frac{\partial w_e}{\partial z} + \frac{\hbar^2}{2m_e^2} \sqrt{\pi e} \frac{1}{\sqrt{n_e}} \frac{\partial^2}{\partial z^2} \sqrt{n_e}.
$$

(4)

Note that the energy-balance equation is neglected as the degenerate electron fluids ($T = 0$) are considered. Here, to close the equations above, an equation of state (EOS) with the form of

$$
P = \frac{\hbar^2}{5m_e^2}(3\pi^2 n_e)^{2/3},
$$

(5)

is used, where the quantum statistical pressure $P$ is obtained at zero temperature \[^{[42]}\]. Thus, the second term on the right-hand side of Eq. (4) is the quantum statistical effect with $w_e = \hbar^2(3\pi^2 n_e)^{2/3}/(2m_e)$. The third term is the quantum diffraction effect with the quantum Bohm potential $\frac{\hbar^2}{2m_e^2} \sqrt{\pi e} \frac{1}{\sqrt{n_e}} \frac{\partial^2}{\partial z^2} \sqrt{n_e}$.

The flux corrected transport (FCT) method \[^{[44]}\] is adopted to numerically solve Eqs. (3) and (4) by split-time integration from the initial time $t = 0$ when the values of all quantities are known. At initial time $t = 0$, the plasma electrons are unperturbed with equilibrium density $n_e(z, t = 0) = n_0$ and the velocity $u_e(z, t = 0) = 0$. The 1D coupled conservative equations can be solved by the 1D FCT algorithm in the context of a two stage Runge-Kutta time integration. However, to ensure the stability and positivity satisfied by the continuity and momentum balance equations, that is the physical requirement in the fluid equations, Eulerian convection involves a certain amount of numerical diffusion. This numerical diffusion may invalidate numerical calculations. Thus, higher-order approximations to the convective derivatives are required to reduce this diffusion. The general idea of the FCT
algorithms is that: (a) for solving the conservative fluid equations, a minimum amount of numerical diffusion must be added to assure numerical stability and positivity, since these equations are subject to a numerical instability due to steep gradients; (b) an antidiiffusion term that should not generate new maxima or minima in the solution, nor accentuate already existing extrema, is considered to remove this additional diffusion and correct the flux.

In general, the above Eqs. (2)–(4) involve a self-consistent determination of the plasma electron density \( n_e \), beam proton density \( n_0 \), and the total electric field \( E_z \). \( E_z \) can be obtained by solving the Poisson equation with the successive over relaxation (SOR) method when the values of \( n_e \) and \( n_0 \) are known, therefore, the wakefield \( E_{\text{ind}} \) is obtained numerically. Again, the PIC simulation cycle consists of the following steps: (a) weighting: proton density \( n_0 \) is calculated from its position, (b) move: proton position and velocity are updated from \( E_z \). Whereas, the one timestep cycle of the QHD simulation with a previously determined timestep \( \Delta t \) is concluded as: (a) integrate the Eqs. (3)–(4) from the initial time \( t^0 \) (\( t = 0 \)) to a half timestep \( t^0 + \Delta t/2 \) to obtain first-order accurate approximations of the density \( n_e \) and momentum \( n_{eb} \) at the middle of the timestep, (b) integrate the equations from \( t^0 \) to a full timestep \( t^0 + \Delta t \) to obtain second-order accurate approximations of the density and momentum at the end of the timestep, and (c) repeat these two procedures to calculate the density and momentum at any timestep.

3 Results and discussion

We first show in Fig. 1 the comparison of the proton beam density and corresponding wake electron density between the PIC method and a pure hydrodynamic simulation. Note that the incident beam motion is simulated by the PIC model and the hydrodynamic method, respectively, while the QHD model is used to calculate the background plasma electron motion throughout this paper. The proton beam density (a) and the wake electron density \( n_{e1} = n_e - n_0 \) (normalized by \( n_0 = 1.8 \times 10^{21} \text{~cm}^{-3} \)) (b) as a function of \( z \) at time \( t = 0.72 \) fs without quantum effects, for proton beams with injection velocity \( u_b = 3c_B \) and density \( n_{b0} = 10^{17} \text{~cm}^{-3} \). The PIC method (solid line) is compared to the pure hydrodynamic method (dashed line) for simulating the proton beam dynamics, while electron dynamics are simulated by the QHD model throughout the paper.

In order to display more clearly the incident beam dynamics, Fig. 2 shows the beam propagating properties in the electron plasma with initial density \( n_0 = 1.8 \times 10^{21} \text{~cm}^{-3} \), by the space evolution of the proton density distribution at four different times 0.72 fs (solid line), 0.97 fs (dashed line), 1.2 fs (dotted line) and 1.4 fs (dash-dotted line), without considering the quantum effects. Here a continuous proton beam with injection velocity \( u_b = 3c_B \) and density \( n_{b0} = 10^{17} \text{~cm}^{-3} \) is considered. It is seen from Fig. 2 that two density peaks appear at these four different times. The proton density \( n_b \) increases and the distance of these two peaks becomes larger as time increases. Because the beam
protons are continually injected into the plasma and the forgoing peak is not absorbed yet, which can give an increasing density as time increases. In other words, the proton beam is compressed to two density peaks with larger values compared to the injection density $n_{b0} = 10^{17} \text{ cm}^{-3}$, in which the maximum density compression ratio reaches $n_{bmax}/n_{b0} = 12$, also shown in the following Fig. 3. Again, at a later time after 1.4 fs, the forgoing peak may propagate to the right boundary and be absorbed, then a new forgoing peak may be generated from the left boundary, which will be shown and justified clearly in Fig. 3 in picosecond time and micrometer space scales that can link with the space-time scales of laboratory laser-accelerated proton beams.

The maximum compression ratio of the proton density is $n_{bmax}/n_{b0} = 2.6$ at $u_b = 1v_B$ with considering quantum effects, while $n_{bmax}/n_{b0} = 9.4$ at $u_b = 3v_B$ and $n_{bmax}/n_{b0} = 7.7$ at $u_b = 5v_B$ without quantum effects.

Figs. 3(a)–(c) show the space evolution of the proton beam density at 5 ps for a continuous proton beam propagating in the electron plasma of initial density $n_0 = 1.8 \times 10^{21} \text{ cm}^{-3}$, with injection velocity $u_b = 1v_B$ (a), $u_b = 3v_B$ (b) and $u_b = 5v_B$ (c), and injection density $n_{b0} = 10^{17} \text{ cm}^{-3}$, with (solid line) and without (dashed line) quantum effects (quantum statistical and quantum diffraction effects). One can clearly observe from Figs. 3(a)–(c) that the incident continuous proton beam is modulated into many pulsed beams of high densities with oscillating density peaks. Again the peak value of the proton density that varies with different injection velocity is the largest at $u_b = 3v_B$, larger at $u_b = 5v_B$ while is the smallest at $u_b = 1v_B$. Moreover, the incident proton distribution is strongly influenced by the quantum effects through the wakefields. From Fig. 3(a) at $u_b = 1v_B$, we can see that, the amplitude of the proton density oscillation with quantum effects is much larger than that with quantum effects near the beam injection boundary ($z < 0.33 \mu \text{m}$), while in the region of $z \geq 0.33 \mu \text{m}$ the situation is reversed. Similarly, at $u_b = 3v_B$ in Fig. 3(b), the quantum effects weaken and strengthen the pulsed beams in the region of $z < 0.5 \mu \text{m}$ and $z \geq 0.5 \mu \text{m}$, respectively. Whereas, at $u_b = 5v_B$ in Fig. 3(c), the quantum effects significantly weaken the generated pulsed beam when the continuous beam is propagating through the plasma.
positive and negative wakefields, respectively. In particular, we can see that both the wake density and wakefield with large perturbations are depressed while with very small oscillations are enhanced with considering the quantum effects, because the quantum effects tend to hinder the collective electron motion and make them be in an equilibrium state, which is an essence of the quantum correction. Thus in our calculation, when a proton beam is propagating through a 1D cold dense electron plasma ($\sim 10^{21}$ cm$^{-3}$), the quantum effects are evident both on the wake density and wakefield, and it is necessary to take into account the quantum effects including the quantum statistical and quantum diffraction effects. However, quantum effects become smaller when the electron density decreases, which is clearly shown in Fig. 6. Here the initial electron density is $8.5 \times 10^{20}$ cm$^{-3}$ smaller than 0.01 times of the metallic electron density. For dilute plasmas thus the quantum effects can be neglected, unless the dimensions of the system are small enough that they are comparable to the de Broglie wavelength.

Fig. 4 The wake electron density $n_{e1} = n_e - n_0$ (normalized by $n_0 = 1.8 \times 10^{21}$ cm$^{-3}$) as a function of $z$ at 5 ps, for proton beams with three different injection velocities $u_b = 1v_B$ (a), $3v_B$ (b) and $5v_B$ (c), and injection density $n_{b0} = 10^{17}$ cm$^{-3}$, with (solid line) and without (dashed line) quantum effects.

Fig. 5 The wakefield $E_{\text{ind}}$ (normalized by $e/a_B^2$) as a function of $z$ at 5 ps, for proton beams with three different injection velocities $u_b = 1v_B$ (a), $3v_B$ (b) and $5v_B$ (c), and injection density $n_{b0} = 10^{17}$ cm$^{-3}$, with (solid line) and without (dashed line) quantum effects.

Fig. 6 (a) The wake electron density $n_{e1} = n_e - n_0$ (normalized by $n_0 = 8.5 \times 10^{20}$ cm$^{-3}$), (b) proton beam density $n_b$ and (c) wakefield $E_{\text{ind}}$ (normalized by $e/a_B^2$) as a function of $z$ at 5 ps, for proton beams with an injection velocity of $u_b = 3v_B$ and an injection density $n_{b0} = 10^{17}$ cm$^{-3}$, with (solid line) and without (dashed line) quantum effects.

4 Summary

In conclusion, QHD/PIC simulation is performed to investigate a continuous proton beam interacting with 1D cold dense quantum plasmas with considering quantum statistical and quantum diffraction effects, where the PIC method is employed to consider the beam particle dynamics and the QHD model is applied to describe
the wake density and wakefield induced by the collective electron motion. Comparisons are made between the PIC and a hydrodynamic method for simulating the proton beams to show that the PIC method gives more accurate results than the hydrodynamic model, because the hydrodynamic model treats the proton beam as a continuous fluid while the PIC method can track an individual particle. In our calculation, the incident continuous fluid is compressed to two pulsed beams with two density peaks in a femtosecond time scale, in which the maximum density compression ratio reaches $n_{b\text{max}}/n_{b0} = 12$. When time continues to increase to picoseconds, the proton beam is modulated into many pulsed beams of high densities. In particular, the quantum effects strongly hinder the collective electron motion as well as the wakefields, thus cannot be neglected in the interaction of a proton beam with quantum plasmas. The results indicate that the hybrid model with the PIC method for simulating the beam particles and the QHD model for considering the quantum effects, is a powerful tool to study the interaction of an intense ion beam with a quantum plasma. As for our plan for the future, this 1D QHD/PIC model will be upgraded to a cylindrical 2D simulation and used to simulate the experimental parameters.

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E-mail address of corresponding author YI Lin: yilin@hust.edu.cn


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