(For presentation at T.D.H.F. Workshop, Paris, France, May 28 - June 1, 1979)

CONF-790545--3

CLASSICAL TRANSCRIPTION OF THE TDHF APPROXIMATION

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*Research sponsored by the Division of Physical Research, Department of Energy, under contract W-7405-eng-26 with the Union Carbide Corporation.

Abstract

We show that the time-dependent Hartree-Fock approximation is approximately equivalent to a purely classical pseudoparticle simulation. In this simulation, a collection of pseudoparticles are introduced to discretize the phase space of spatial and momentum coordinates. The dynamics is completely determined by following the pseudoparticle trajectories which are the same as the trajectories of real particles moving in the self-consistent field. An application of these concepts to nearly-head-on heavy-ion collisions leads to a better understanding of the origin of the low-ℓ fusion window obtained in the TDHF calculations.

I. Introduction

We seek a classical transcription of the TDHF approximation to help guide our intuition in order to understand the underlying physics. The procedure we take is a very well-known one. If we start from the Schrödinger equation, go to the Wigner space, interpret the Wigner function as a classical distribution function and take the limit of $\hbar \to 0$, then we obtain from quantum mechanical equations of motion purely classical equations of motion.[1-4] By following a similar procedure for the TDHF approximation, we are guaranteed to obtain classical equations of motion for the dynamics. What emerges out of such a transcription is the approximate equivalence of the TDHF approximation with a pseudoparticle simulation where the dynamics is completely determined by the motion of classical pseudoparticles following classical collisionless trajectories.

This paper contains a brief summary of the main results and their application to the discussion of the low-ℓ fusion window in heavy-ion collisions. The details of the discussion, as well as other extensions and

applications, are given elsewhere.[5]

II. Pseudoparticle Simulation as an Approximate Transcription of TDHF

The equation of motion for a single-particle state in the TDHF approximation is given by[6]

$$i\hbar \frac{\partial}{\partial t} \psi_\lambda(\vec{r},t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + \mathcal{V}(\rho(\vec{r},t)) \right] \psi_\lambda(\vec{r},t). \tag{1}$$

where ρ is the density and $\mathcal{V}(\rho)$ the mean-field potential.

In order to study the TDHF approximation from a classical viewpoint, we go to the Wigner space. The Wigner function is given by

$$f(\vec{r}\vec{p},t) = \int d^3s \, e^{i\vec{p}\cdot\vec{s}/\hbar} \sum_\lambda^{occ} \psi_\lambda(\vec{r} - \vec{s}/2,t)\psi_\lambda(\vec{r} + \vec{s}/2,t) \tag{2}$$

where the summation over λ extends over the occupied states. As is well known, the Wigner function is analogous with, but not identical to, the distribution function in classical statistical mechanics. Because of the usefulness of the distribution function in providing great insight and in guiding our intuition, we shall adopt the approximate interpretation of the Wigner function as the classical distribution function.

The equation of motion for the Wigner function in the TDHF approximation is[1-4]

$$\frac{\partial f}{\partial t}(\vec{r}\vec{p},t) + (\vec{p}/m)\cdot\nabla_r f(\vec{r}\vec{p},t) - \frac{2}{\hbar} \sin\left[\frac{\hbar}{2} \overleftarrow{\nabla}_r^v \cdot \overrightarrow{\nabla}_p^f\right] \mathcal{V}(\rho(\vec{r},t)) f(\vec{r}\vec{p},t) = 0 \tag{3}$$

where the superscripts v and f refer to the functions on which the gradient operators apply. One can expand the sine function in powers of $\hbar\nabla_r^v \cdot \nabla_p^f$. One expects that when the number of nucleons becomes large, the variation of the potential and the Wigner function in the interior region is relatively small so that the higher-order derivatives of v and f are unimportant. They are large only at the edge of the distribution where the density is however small. Thus, for large nuclei, we can retain only the term lowest order in $\hbar\nabla_r^v \cdot \nabla_p^f$ in the expansion. We obtain the Vlasov equation

$$\frac{\partial f}{\partial t}(\vec{r}\vec{p},t) + \frac{\vec{p}}{m}\cdot\nabla_r f(\vec{r}\vec{p},t) - \nabla_r \mathcal{V}(\rho(\vec{r}))\cdot\nabla_p f(\vec{r}\vec{p},t) = 0. \tag{4}$$

This equation, together with the equation of continuity for f, implies that

the phase space Wigner fluid in this approximation is incompressible. Because of the Pauli exclusion principle, the equilibrium distribution function has a uniform density in the phase space within a certain domain. The incompressibility of the phase space fluid guarantees that in the subsequent dynamics, the density of the fluid in phase space remains uniform, as would also be required by the Pauli exclusion principle.

The transcription of the Vlasov equation to a pseudoparticle simulation can be readily made. One follows the coordinates of the fluid element initially located at a representative point $\vec{r}_o$, $\vec{p}_o$ at time t_o. The location of the fluid element at time t is denoted by $\vec{R}(\vec{r}_o\vec{p}_o,t)$ and $\vec{P}(\vec{r}_o\vec{p}_o,t)$. In terms of the fluid elements ("pseudoparticles") initially located at $\vec{r}_o$ and $\vec{p}_o$, the distribution function can be decomposed to be

$$f(\vec{r}\vec{p},t) = \int d\vec{r}_o d\vec{p}_o f(\vec{r}_o\vec{p}_o,t_o)\delta[\vec{r}-\vec{R}(\vec{r}_o\vec{p}_o,t)]\delta[\vec{p}-\vec{P}(\vec{r}_o\vec{p}_o,t)] \tag{5}$$

where $f(\vec{r}_o\vec{p}_o,t_o)$ is the initial distribution function at time t_o. By substituting Eq. (5) into Eq. (4), one finds that the coordinates $\vec{R}$ and $\vec{P}$ satisfy the following Newtonian equations of motion

$$\frac{\partial\vec{R}}{\partial t} = \frac{\vec{P}}{m} \tag{6}$$

and

$$\frac{\partial\vec{P}}{\partial t} = -\vec{\nabla}_R V(\rho(\vec{R})). \tag{7}$$

These equations are the classical equations of motion for a single particle of mass m moving in a self-consistent potential well V. Thus, when the distribution function is given at time $t = t_o$, the dynamics is completely solved by following the classical collisionless trajectories of all the points (pseudoparticles) in the Wigner space using Eqs. (5-7).

III. Pseudonucleon Dynamics in a Single Nucleus

A good approximation to the Wigner function of a nucleus in its ground state, with the neglect of the diffuseness of the edges and oscillations, is

$$f(\vec{r}\vec{p}) \sim \theta(\hbar k_f - |\vec{p}|)\theta(R_o - |\vec{r}|) \tag{8}$$

where $\hbar k_f$ is the Fermi momentum, R_o the radius of the nucleus, and θ the step function. Such a uniformity of distribution in phase space is a

consequence of the Pauli exclusion principle.

When one looks at the distribution function as a whole, it is time independent, but if one follows an elementary volume (pseudonucleon or simply "nucleon") in the $(\vec{r},\vec{p})$ space as a function of time, it exhibits classical-type motions and traverses in the phase space following a unique trajectory. Each of these pseudonucleons traverses in nearly straight line trajectory in the interior of the nucleus and suffers an elastic reflection at the surface. When static equilibrium is achieved, the motion is such that for every group of nucleons leaving a phase space cell, it is replenished by another group of nucleons from some other location.

IV. Pseudonucleon Dynamics in Heavy-Ion Collisions

We consider first a head-on collision of two equal nuclei. When the common boundary between the two nuclei disappears, there are two effects on the dynamics of the nucleons. Those nucleons originating from a point near the boundary and coming to the boundary will follow straight line trajectories and proceed to the other nucleus. Secondly, in the absence of the boundary and the subsequent change of the trajectories of these nucleons, part of the original Fermi sphere near the boundary points are not replenished by nucleons from the same nucleus. In place of these vacated phase space points now arrive the nucleons from the other nucleus, the most energetic ones being the first to arrive.

At a time approximately $2R_o/(\text{Fermi velocity})$ after the removal of the common boundary, the most energetic pseudonucleons from one nucleus arrive at the far surface point of the other nucleus. They are not expected to suffer much loss of energy. They are now ready to give an assault to the "walls" at the surface points. Whether or not the wall can contain these most energetic nucleons depends on the "height" of the wall and the energy of these nucleons. Furthermore, besides these nucleons that have just arrived, a large array of energetic nucleons originally from the other nucleus have positioned themselves at more distant points to prepare for an assault of the wall at a later time. Such a "collective" behavior of the nucleons is a consequence of the initial condition of colliding nuclei. How the dynamics will proceed further depends on the containment of these most energetic nucleons by the wall.

V. The Low-ℓ Fusion Window in TDHF Calculations

From the TDHF results,[7,8] we know that the ℓ-window occurs at a threshold energy of $E_{lab} = 54$ MeV for the $^{16}O + ^{16}O$ system and that the ℓ-window can be specified by[7,8] an absence of fusion when

$$\ell \leq \left[\frac{2\mu R_B^2}{\hbar^2}\left(\frac{E_{lab}-E_o}{2}\right)\right]^{1/2} \tag{9}$$

where μ is the reduced mass, R_B is the interaction barrier radius, and E_o is the threshold energy. Threshold energies for other colliding systems have also been obtained.[9,10]

In order to understand the phenomena of the ℓ-window in the TDHF calculation, we examine the dynamics of the nucleons at the time when the most energetic nucleons from one nucleus reaches the far surface of the other nucleus. If these nucleons are bound inside the potential, they are then reflected backward after proceeding to the classical turning point and are therefore contained. The containment of these nucleons will eventually lead to a fused compound system. On the other hand, if the energy is such that they are unbound in the mean-field potential, these nucleons will proceed forward and emerge outside of the surface point. When this happens, they will lower the potential at the new points because of the self-consistency effect. The turning points of many of the other nucleons are shifted so that more nucleons emerge out of the far side of the surface. This will lower the potential even more to allow more and more nucleons to emerge outward. It is reasonable to expect that such a coherent flow-through motion will continue on and may perhaps be the origin of the non-fusion (break-up) events in the low-ℓ fusion window of the TDHF calculations.

A flow-through motion occurs when the most energetic nucleons become unbound. That is, when

$$\frac{\hbar^2}{2m}\left[k_f + m\, v_o/\hbar\right]^2 \geq \frac{\hbar^2}{2m} k_f^2 + B \tag{10}$$

where v_o is the velocity of one of the nuclei in the center-of-mass system, B is the separation energy of the ground-state nucleons. Here, the velocity of the wall at the surface points is neglected. In terms of the Fermi energy ϵ_F and B, the threshold energy is

$$\tfrac{1}{2} m v_o^2 \geq [(1 + B/\epsilon_F)^{1/2} - 1]^2 \epsilon_F. \qquad (11)$$

Upon using a separation energy of B = 8 MeV and ϵ_F = 35 MeV, one finds the threshold energy per nucleon in the center-of-mass system given by

$$\tfrac{1}{2} m v_o^2 \geq 0.411 \text{ MeV}. \qquad (12)$$

The foregoing consideration can be generalized to non-head-on collisions of unequal nuclei in the presence of Coulomb repulsion. One finds the threshold energy as given by

$$E_{CM}(\text{threshold}) = \frac{Z_1 Z_2 e^2}{R_B} + \frac{A_2(A_1+A_2)}{A_1} [(1 + B/\epsilon_F)^{1/2} - 1]^2 \epsilon_F \qquad (13)$$

and the ℓ-window below which no fusion occurs as

$$\ell^2 \leq \frac{2\mu R_B}{\hbar^2} \left\{ E_{CM} - \frac{Z_1 Z_2 e^2}{R_B} - \frac{A_2(A_1+A_2)}{A_1} [(1 + B/\epsilon_F)^{1/2} - 1]^2 \epsilon_F \right\}. \qquad (14)$$

where $A_2 \geq A_1$.

TABLE I. *Threshold energies for the onset of no fusion in head-on collisions.*

System	Threshold Energy E_{cm} in MeV from Eq. (13)	Threshold Energy E_{cm} in MeV from TDHF
$^{16}O + ^{16}O$	28.40	27[a]
$^{28}Si + ^{28}Si$	61.76	55[b]
$^{16}O + ^{40}Ca$	89.86	100[b]
$^{40}Ca + ^{40}Ca$	103.08	97.5[c]
$^{12}C + ^{12}C$	36.5[d]	35.0[e]

a) Ref. 8.
b) Ref. 12.
c) Ref. 9.
d) We use a different set of B and ϵ_f as different interactions are used in Ref. 10.
e) Ref. 10.

For $^{16}O + ^{16}O$, $^{28}Si + ^{28}Si$, $^{16}O + ^{40}Ca$, and also $^{40}Ca + ^{40}Ca$, we use the above equation (13) and obtain the threshold energies as given in Table I. They compare favorably with those obtained from the TDHF calculations. For the $^{12}C + ^{12}C$ system, a different interaction was used[10] and the important parameters of B and ϵ_f which are interaction-dependent and enter into the estimates of the threshold energies should rather be B ~ 12 MeV and ϵ_f ~ 23 MeV.[11] When this set of parameters is used in Eq. (13), one obtains the threshold energy which agrees well with the results from TDHF calculations.[10] Besides the threshold energies, the functional dependence of the

ℓ window given by (14) agrees with that of (9) obtained from TDHF calculations. These agreements indicate the approximate validity of the simple picture presented here.

It is of interest to note that the low-ℓ fusion window can be well utilized to provide an experimental test on the validity of the TDHF approximation. If the collisions of nucleons are allowed, there is a finite probability for the most energetic nucleons to suffer a loss of radial kinetic energy before reaching the far surface. What in the collisionless TDHF case will lead to the flow-through motion and the subsequent break-up may become a case of fusion in the presence of particle collisions. One expects therefore that with the inclusion of the particle collisions, the onset of the occurrence of no fusion in a head-on collision will move to a higher energy. A careful search for the ℓ-window for various systems and a subsequent comparison with the results from TDHF calculations will indicate either the validity of the TDHF approximation or the need to introduce particle collisions.

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