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NUMERICAL STUDIES ON THE PHASE-SPACE EVOLUTION OF
RELATIVE MOTION OF TWO HEAVY IONS

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NUMERICAL STUDIES ON THE PHASE-SPACE EVOLUTION OF RELATIVE MOTION
OF TWO HEAVY IONS

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Abstract:

The two-dimensional Fokker-Planck equation describing the phase-space evolution of the reduced density matrix $f(r,v;t)$ with respect to radial distance r and radial velocity v is numerically solved for various cases of inelastic heavy-ion collisions. A comparison of the exact solution with the global moment approach (GMA) used so far by several authors clearly shows that the GMA is not applicable for deeply inelastic collisions. A local moment approach (LMA) is proposed as an approximate solution to the Fokker-Planck equation.

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1. Introduction

Heavy-ion collisions in the energy range of a few MeV/n above the Coulomb barrier and induced nuclear fission have been interpreted as stochastic processes and described by classical transport equations of the Fokker-Planck type [1-3]. The standard procedure to solve the partial differential equations is to apply a moment expansion up to second order [2-4]. This global moment approach (GMA) yields exact solutions for harmonic driving potentials and approximate results in the case of a slightly perturbed potential, but as soon as the curvature of the potential changes sign within the domain where the density function is sizably different from zero, the GMA should loose its applicability [5,6]. Also for the nuclear mass transport in deeply inelastic collisions, described by a one-dimensional Fokker-Planck equation (FPE), anharmoniticities in the driving potential due to shell effects are found to be important [7,8] and require a more precise solution of the FPE. While approximate solutions for the one-dimensional problem are available for some time [5,8,9], a proper treatment of the two-dimensional problem, i.e. the time evolution of a phase-space density, has not yet been performed.

It is the aim of this publication to show that the GMA is not a useful tool for the description of radial motion in deeply inelastic reactions. As a replacement we propose the local moment approach (LMA) which can overcome the difficulties with the GMA.

2. Validity of the Global Moment Approach

One of the most interesting applications of classical transport equations is the description of the relative motion of two colliding heavy ions. Restricting ourselves to a single collective degree of freedom, i.e. the radial motion, the time evolution of the classical phase-space density $f(r,v;t)$ is given by

$$\frac{\partial}{\partial t} f(r,v;t) = \left\{ -v \frac{\partial}{\partial r} + \frac{1}{\mu} \frac{\partial U}{\partial r} \frac{\partial}{\partial v} + \frac{\partial}{\partial v} \gamma(r) v + D(r) \frac{\partial^2}{\partial v^2} \right\} f(r,v;t), \quad (1)$$

where the coordinates r, v correspond to the radial distance and radial velocity. The density function takes the initial values

$$f(r,v;0) = \delta(r-r_0) \delta(v-v_0) \quad (1a)$$

and has to fulfill the boundary conditions

$$f(r,v;t) \rightarrow 0 \text{ for } r \rightarrow 0, \quad r \rightarrow \infty, \quad |v| \rightarrow \infty. \quad (1b)$$

In eq. (1) the conservative potential is described by $U(r)$; $\gamma(r)$ and $D(r)$ denote the formfactors for friction and diffusion while the quantity μ corresponds to the reduced mass of the system. The conservative potential is a superposition of the attractive nuclear, the repulsive Coulomb, and the centrifugal potential, which yields a pocket for lower angular momenta ℓ to allow the description of fusion. Such a potential is depicted in fig. 1 for different angular momenta ℓ , generated by a Gaussian for the nuclear part, the Coulomb contribution corresponding to $Z_1 \cdot Z_2 = 3800$ and the reduced mass given by $\mu = 100 \text{ MeV } bs^2 \text{ fm}^{-2}$ ($bs = 10^{-23} \text{ s}$). The formfactor for friction is supposed to be a Gaussian

$$\gamma(r) = \gamma_0 \cdot \exp \left\{ -r^2 / 2a^2 \right\}, \quad (2)$$

with $\gamma_0 = 7 \text{ bs}^{-1}$ and $a = 6 \text{ fm}$. This choice leads to the mean trajectories shown in fig. 1 (dashed lines) for an incident collective energy of $E_{CM} = 400 \text{ MeV}$. In this model the critical angular momentum is given by $\ell_{crit} = 23 \hbar$; trajectories with lower angular momentum are trapped and lead to fusion in the classical sense. The formfactor for diffusion is chosen according to an Einstein relation with constant temperature

$$D(r) = \gamma(r) \cdot D_0 \quad (3)$$

with $D_0 = 5 \cdot 10^{-2} \text{ fm}^2 \text{ bs}^{-2}$. In this way all coefficients in eq. (1) are specified and supposed to approximately simulate the dynamics of a heavy-ion collision. The standard procedure for the solution of eq. (1) is to expand the function $f(r,v;t)$ in moments up to 2nd order in r and v [2-4] which yields

$$\frac{d}{dt} \langle r \rangle = \langle v \rangle, \quad (4a)$$

$$\frac{d}{dt} \langle v \rangle = - \frac{1}{\mu} \frac{dU}{dr}(\langle r \rangle) - \gamma(\langle r \rangle) \langle v \rangle, \quad (4b)$$

$$\frac{d}{dt} \bar{\sigma}_r^2 = 2\bar{\sigma}_{rv} \quad (4c)$$

$$\frac{d}{dt} \bar{\sigma}_v^2 = -2\gamma(\langle r \rangle) \bar{\sigma}_v^2 + 2D(\langle r \rangle) - \frac{2}{\mu} \frac{d^2 U}{dr^2}(\langle r \rangle) \cdot \bar{\sigma}_{rv} \quad (4d)$$

$$\frac{d}{dt} \bar{\sigma}_{rv} = \bar{\sigma}_v^2 - \gamma(\langle r \rangle) \cdot \bar{\sigma}_{rv} - \frac{1}{\mu} \frac{d^2 U}{dr^2}(\langle r \rangle) \cdot \bar{\sigma}_r^2 \quad (4e)$$

with

$$\bar{\sigma}_r^2 = \langle (r - \langle r \rangle)^2 \rangle,$$

$$\bar{\sigma}_v^2 = \langle (v - \langle v \rangle)^2 \rangle \quad \text{and}$$

$$\bar{\sigma}_{rv} = \langle (rv - \langle r \rangle \langle v \rangle) \rangle.$$

The approach is expected to break down if the second derivative

of $U(r)$ changes sign. In this case the variance $\bar{\sigma}_r^2$ increases according to eqs. (4) much too strong because the mean value $\langle r \rangle$ remains in the domain of

instability (negative d^2U/dr^2) for quite a long time, whereas in the FPE (1) large fractions of the density function $f(r,v;t)$ extend to regions of positive $d^2U(r)/dr^2$, where a spreading of $f(r,v;t)$ in r is suppressed. To be more specific, we compare the results of eqs. (4) with the solution of eq. (1) according to the computer code ADIP which is described in the appendix. For reasons of computational time we let the system evolve in time up to 10bs according to the GMA (4), and then solve the FPE (1) on a grid of 81×61 meshpoints in the $r \times v$ plane. The distribution in r space was restricted to the interval [5fm, 25 fm] for $\lambda = 0 \hbar$, $\lambda = 23 \hbar$ and to [10fm, 30fm] for $\lambda = 30 \hbar$ because friction and diffusion become negligible for $r > 23$ fm.

The results of these calculations are shown in fig. 2 (r -h.s.) in comparison with the GMA (1.h.s.); for orientation the motion of the center of the distribution function in the $r \times v$ plane is depicted in the upper part of the figures. A comparison of these results clearly shows that $f(r,v;t)$ due to the GMA (1.h.s.) significantly differs from the exact solution (r -h.s.) in the outgoing channel, i.e. for $\langle v \rangle > 0$. This is basically due to the large spreading of $f(r,v;t)$ in r space which no longer allows to approximate the potential by a local oscillator. Projections on coordinate or velocity space,

$$\rho(r;t) = \int dv f(r,v;t), \quad (5a)$$

$$g(v;t) = \int dr f(r,v;t), \quad (5b)$$

show almost no similarity for $t > 25$ bs except for the case of zero angular momentum (2c) where the system is almost entirely trapped (99.8%) in the pocket of the potential (cp. fig. 1). The only interesting quantity which is reproduced by the GMA is the spreading in velocity for $t \rightarrow \infty$ if the distribution function does not split into two parts. This of course is trivial because the potential either is zero for $t \rightarrow \infty$ ($\lambda = 30 \hbar$) or well reproduced by an oscillator ($\lambda = 0 \hbar$; within the pocket region) and the limiting value of $\bar{\sigma}_v^2$ is given by D_0 according to the Einstein relation (3).

The other quantity of physical interest is the probability of fusion as a function of orbital angular momentum λ . Looking at fig. 2b for $t \geq 20$ bs, there is a splitting of $f(r,v;t)$ into two parts; one of these gets trapped in the pocket region of the potential, the other escapes from the interaction region and runs into our imaginary detector at $r \rightarrow \infty$. The probability for fusion P is simply given by the integral over r and v of the part which stays in the pocket for $t \rightarrow \infty$. This quantity is plotted in fig. 3 as a function of λ (full line) in comparison with the predictions of the trajectory model (dashed line) which corresponds to the sharp cut-off limit. The results show that the transition from zero capture at high angular momentum to total capture for central collisions is very smooth in accordance with experimental findings [11]. In this transition region ($10 \hbar \leq \lambda \leq 26 \hbar$) the GMA does not yield any reasonable result because the moment expansion diverges (cp. fig. 2b). In addition fig. 3 explains why trajectory models may succeed in reproducing fusion cross sections [12], but fail to reproduce the deflection characteristics of deeply inelastic collisions [13]. While the fusion cross-section σ_f is related to the area under the P_λ curve weighted by λ , the smooth cut-off in angular momentum is not essential for an estimate of σ_f . The low energy part of every Wilczynski plot ($d^2\sigma/d\theta dE$) instead is mainly produced by small angular momentum partial waves which are attributed to fusion in the trajectory models.

We thus find that the description of deeply inelastic heavy-ion collisions by a transport equation of the Fokker-Planck type requires a full numerical solution of the problem in order to learn anything reliable about the reaction process and to allow for a proper comparison with experimental data. Only in case of peripheral collisions where $\bar{\sigma}_r^2$ remains less than 0.5 fm^2 in the interaction region the GMA remains applicable.

3. The Local Moment Approach

The main impediment for the solution of partial differential equations is the dimensionality of the problem. Equations with more than four independent variables (time included) seem to be inaccessible by computations on a grid. Physics, however, forces us to take more degrees of freedom into account than just v and r . Therefore we propose a method to reduce the dimensionality of the original FPE, the local moment approach (LMA), and examine its usefulness for the problem of section 2, where we can compare it with the guaranteed approximations from ADIP.

The idea of introducing a local moment approach to eq. (1) is guided by the results for $f(r,v;t)$ for fixed r depicted in fig. 4 ($\lambda = 23H$, $t = 23bs$). The distribution very much resembles Gaussians with different centers and widths, and a harmonic expansion of eq. (1) with respect to v appears promising. This is, of course, connected with the fact that all coefficients in eq. (1) are linear with respect to v . Defining the density ρ , the local velocity V , and the local spreading σ_v^2 by

$$\rho(r,t) = \int dv f(r,v;t) , \quad (6a)$$

$$V(r,t) = \int dv \frac{v \cdot f(r,v;t)}{\rho(r,t)} \quad (6b)$$

and

$$\sigma_v^2(r,t) = \int dv \frac{(v-V(r,t))^2}{\rho(r,t)} f(r,v;t) , \quad (6c)$$

we obtain

$$\frac{\partial}{\partial t} \rho(r,t) = -V(r,t) \frac{\partial}{\partial r} \rho(r,t) - \rho(r,t) \frac{\partial}{\partial r} V(r,t) , \quad (7)$$

$$\begin{aligned} \frac{\partial}{\partial t} V(r,t) = & -V(r,t) \frac{\partial}{\partial r} V(r,t) - \frac{\partial}{\partial r} \sigma_v^2(r,t) \\ & - \frac{1}{\mu} \frac{\partial U}{\partial r} - \gamma(r) \cdot V(r,t) - \sigma_v^2(r,t) \frac{\partial \ln \rho(r,t)}{\partial r} , \end{aligned} \quad (8)$$

and

$$\begin{aligned} \frac{\partial}{\partial t} \sigma_v^2(r,t) = & -2 \sigma_v^2(r,t) \frac{\partial V(r,t)}{\partial r} - V(r,t) \frac{\partial \sigma_v^2(r,t)}{\partial r} \\ & - 2\gamma(r) \sigma_v^2(r,t) + 2 D(r) \end{aligned} \quad (9)$$

by neglecting 3rd and higher moments of $f(r,v;t)$ with respect to v .

Furthermore we have to determine the initial values and the boundary conditions for the functions $\rho(r,t)$, $V(r,t)$ and $\sigma_v^2(r,t)$. The initial conditions are simply derived from (1a) and the definitions (6)

$$\rho(r,0) = \delta(r-r_0) \quad (11a)$$

$$V(r,0) = v_0 \quad (11b)$$

$$\sigma_v^2(r,0) = 0 . \quad (11c)$$

The boundary conditions can be obtained by the requirement of compatibility at $t = 0$ and by the physical conditions at $r = 0$, where the density distribution must vanish due to the repulsive core of the potential, and at $r \rightarrow \infty$, which the system cannot reach within a finite time;

$$\rho(0,t) = \rho(\infty,t) = 0 \quad (12a)$$

$$V(0,t) = V(\infty,t) = v_0 \quad (12b)$$

$$\sigma_v^2(0,t) = \sigma_v^2(\infty,t) = 0 . \quad (12c)$$

However, (11a,b) and (12b) are not suitable for practical purposes where we wish to limit all calculations to a grid as small as possible. We apply physical arguments to ameliorate the situation.

For short times, GMA is a good approximation, since the density function $f(r,v;t)$ covers only a small domain within which all coefficients in (1) are nearly linear functions. Choosing some small time t_1 , we therefore replace the δ function in (11a) by a Gaussian determined by the GMA equations (4).

Furthermore, since $f(r,v;t)$ is so sharply localized, $V(r,t_1)$ and $\sigma_v^2(r,t_1)$ have to be accurately known only in a vicinity of $\langle r \rangle(t_1)$ where they can be well approximated by the solution given by eqs. (4),

$$V_{GMA}(r,t_1) = \langle v \rangle(t_1) + \bar{\sigma}_{rv}(t_1) (r - \langle r \rangle(t_1)) / \bar{\sigma}_r^2(t_1) \quad (13a)$$

$$\sigma_{GMA}^2(r,t_1) = \bar{\sigma}_v^2(t_1) + \bar{\sigma}_{rv}^2 / \sigma_r^4 \cdot ((r - \langle r \rangle(t_1))^2 - \bar{\sigma}_r^2(t_1)) \quad (13b)$$

for $\langle r \rangle(t_1) - \bar{\sigma}_r(t_1) < r < \langle r \rangle(t_1) + \bar{\sigma}_r(t_1)$.

The range of integration is given by $U(r_{min}) = E_{CM}$, and r_{max} sufficiently far away from the barrier in fig. 1 ($r_{max} = 30$ fm).

The boundary conditions for $t \geq t_1$ then read

$$\rho(r_{min},t) = \rho(r_{max},t) = 0, \quad (14a)$$

$$\sigma_v^2(r_{min},t) = \sigma_v^2(r_{max},t) = 0, \quad (14b)$$

and

$$V(r_{min},t) = 0, \quad V(r_{max},t) = \left\{ \frac{2}{\pi} (E_{CM} - E^* - U(r_{max})) \right\}^{1/2}. \quad (14c)$$

The boundary values (14c) are determined by the condition that the mean velocity of the outgoing wavepacket at r_{max} should coincide with the mean velocity of the trajectory calculations (4a,b) at this point. Accordingly the energy loss E^* in (14c) is calculated via (4a,b) requiring total energy conservation.

The initial values (13a,b) are only appropriate for r close to $\langle r \rangle(t_1)$ and the extension to all values of r is done in such a way that they fulfill the boundary conditions (14a-c). We thus assume

$$\rho(r,t_1) = \{2\pi\bar{\sigma}_r^2(t_1)\}^{-1/2} \exp \{-(r - \langle r \rangle(t_1))^2 / (2\bar{\sigma}_r^2(t_1))\}, \quad (15a)$$

$$V(r,t_1) = \begin{cases} V_{GMA}(r,t_1) \cdot \exp \{-(r - \langle r \rangle(t_1))^2 / (2\bar{\sigma}_r^2(t_1))\} & \text{for } r \leq \langle r \rangle(t_1) \\ V_{GMA}(r,t_1) & \text{for } \langle r \rangle(t_1) \leq r \leq r_c \\ V(r_{max},t) & \text{else} \end{cases} \quad (15b)$$

$$\sigma_v^2(r,t_1) = \sigma_{GMA}^2(r,t_1) \cdot \exp \{-(r - \langle r \rangle(t_1))^2 / (2\bar{\sigma}_r^2(t_1))\} \quad (15c)$$

In eq. (15b) r_c is given by

$$r_c = \langle r \rangle(t_1) + (V(r_{max},t_1) - \langle v \rangle(t_1)) \cdot \bar{\sigma}_r^2(t_1) / \bar{\sigma}_{rv}^2(t_1). \quad (16)$$

Extensions of the initial values (13) different from (15) are numerically checked to be insignificant as long as the boundary conditions (14) are fulfilled.

In order to compactly display our results within the LMA, we choose the form

$$f(r,v;t) = \{2\pi\sigma_v^2(r,t)\}^{-1/2} \cdot \exp \{-(v - V(r,t))^2 / (2\sigma_v^2(r,t))\} \cdot \rho(r,t), \quad (17)$$

though a direct insertion of (17) into eq. (1) yields more complicated nonlinear equations for $V(r,t)$ and $\sigma_v^2(r,t)$.

The numerical solution of eqs. (7-9) with the boundary conditions (14) and initial values (15) for $t_1 = 10$ fs are displayed in fig. 5 (r.h.s) for $\lambda = 23$ Å together with the ADIP solution of the FPE (1) (l.h.s). The contour lines correspond to the same values of $f(r,v;t)$ as in figs. 2a - 2c. The graphs show that the LMA reproduces the splitting of the distribution function and approximately yields similar shapes for constant $f(r,v;t)$. It may be taken as a minor point that the fall off of the distribution function for small r is too steep. The velocity fields $V(r,t)$, however, agree within an accuracy of 5%. The velocity distribution $g(v,t)$ (5b) consequently is much better reproduced than the coordinate distribution $\rho(r,t)$ (5a) which 'fortunately' can not be observed experimentally.

4. Summary

We would like to point out that the conventional global moment approach (GMA) (4) appears to be no approximation to the correct solution of the Fokker-Planck equation (1) in case of deeply inelastic heavy-ion collisions because the moment expansion tends to diverge if the physical solution splits into parts describing partial fusion and inelastic scattering. Unfortunately (w.r.t. the GMA) the transition from inelastic scattering to complete fusion is very soft in angular momentum in accordance with experimental findings. Thus the Fokker-Planck equation seems to be a reliable description of deeply inelastic heavy-ion collisions and to be applicable to the dynamics of fusion, but does not permit the conventional approximation schemes. Therefore we proposed a local moment approach (LMA) formally close to hydrodynamics which yielded approximative solutions for the Fokker-Planck equation in this case.

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Appendix

Peaceman and Rachford [14] developed the alternating directions implicit procedure (ADIP) for the numerical solution of the two-dimensional heat equation. We applied their method to the two-dimensional Fokker-Planck equation

$$\partial_t P(x_1, x_2, t) = \sum_{i=1}^2 -\partial_{x_i} [V^i P(x_1, x_2, t)] + \partial_{x_i}^2 [d^i P(x_1, x_2, t)], \quad (A.1)$$

where the drift coefficients $V^i(x_1, x_2, t)$ and the diffusion coefficients $d^i(x_1, x_2)$ are given functions of the coordinates x_1 and x_2 .

We want to compute the time evolution of the probability density $P(x_1, x_2, t)$ provided the initial distribution $P(x_1, x_2, 0)$ is known. In our problem (1) it is given by

$$P(x_1, x_2, 0) = \delta(x_1 - x_{10}) \cdot \delta(x_2 - x_{20}) \quad (A.2)$$

and the boundary values are specified by

$$P(x_1, x_2, t) \rightarrow 0 \quad \text{for } x_1^2 + x_2^2 \rightarrow \infty, \quad (A.3)$$

In a sufficiently small neighborhood of (x_{10}, x_{20}) , the drift and diffusion coefficients can be approximated by linear expressions

$$V^i \approx a_i + \sum_{j=1}^2 b_{ij}(x_j - x_{j0}), \quad d^i \approx c_i \quad \text{if } x_i \approx x_{i0}, \quad (A.4)$$

a_i , b_{ij} , and c_i being constants. In this case the Fokker-Planck equation (A.1) is solved in closed form

$$P(x_1, x_2, t) = \exp(-\arg/\det) / (2\pi/\det) \quad (A.5)$$

where

$$\begin{aligned} \arg &= \sigma_{22}^2 (x_1 - \langle x_1 \rangle)^2 + \sigma_{11}^2 (x_2 - \langle x_2 \rangle)^2 - 2\sigma_{12}^2 (x_1 - \langle x_1 \rangle)(x_2 - \langle x_2 \rangle), \\ \det &= \sigma_{11}^2 \sigma_{22}^2 - \sigma_{12}^4. \end{aligned} \quad (A.6)$$

The mean values $\langle x_i \rangle$ and the variances σ_{ij}^2 depend on time and are easily determined from the ordinary differential equations

$$\begin{aligned} \frac{d}{dt} \langle x_i \rangle &= \sum_{j=1}^2 b_{ij} \langle x_j \rangle + a_i \\ \frac{d}{dt} \sigma_{ii}^2 &= 2 \sum_{j=1}^2 b_{ij} \sigma_{ij}^2 + 2c_i, \quad \sigma_{12}^2 = \sigma_{21}^2 \\ \frac{d}{dt} \sigma_{12}^2 &= \sum_{j=1}^2 b_{jj} \sigma_{12}^2 + b_{21} \sigma_{11}^2 + b_{12} \sigma_{22}^2 \end{aligned} \quad (A.7)$$

with the initial conditions

$$\langle x_i \rangle(0) = x_{i0}, \quad \sigma_{ij}^2(0) = 0. \quad (A.8)$$

Thus (A.5) describes the initial broadening of the delta peak (A.2), and we use it as the initial distribution for the numerical solution. The condition for its usefulness is that the distribution (A.5) is still narrow enough to keep (A.4) valid. On the other hand the Gaussian (A.4) must already be wide enough to allow for a reasonably small number of grid points.

For the numerical solution of (A.1), we span a two-dimensional grid over the $x_1 \times x_2$ plane,

$$\begin{aligned} x_{1m} &= x_{1min} + m \Delta x_1 & m &= 0, 1, \dots, m_{max} \\ x_{2n} &= x_{2min} + n \Delta x_2 & n &= 0, 1, \dots, n_{max} \end{aligned} \quad (A.9)$$

and have to discuss the choice of x_{1min} , x_{2min} , and $x_{1max} = x_{1min} + m_{max} \Delta x_1$, $x_{2max} = x_{2min} + n_{max} \Delta x_2$. As the analogue of (A.2) we impose the requirement

$$P(x_1, x_2, t) = 0, \quad x_1 = x_{1min}, x_{1max} \quad \text{or} \quad x_2 = x_{2min}, x_{2max} \quad (A.10)$$

on the boundaries of the grid. Therefore the grid's extension has to be so large that $P(x_1, x_2, t)$ never reaches its boundaries during the time of interest. Otherwise a steadily increasing part of the probability is absorbed.

To explain ADIP, we conveniently introduce the operators F_1 and F_2 .

$$\begin{aligned} F_1 P(t) &:= - (V_{m+1n}^1 P_{m+1n}(t) - V_{m-1n}^1 P_{m-1n}(t)) / (2\Delta x) \\ &\quad + (d_{m+1n}^1 P_{m+1n}(t) - 2d_{mn}^1 P_{mn}(t) + d_{m-1n}^1 P_{m-1n}(t)) / \Delta x^2, \end{aligned} \quad (A.11)$$

and a similar expression for $F_2 P(t)$ where the upper index 1 has to be replaced by 2 and m stays fixed while n varies between $n-1$ and $n+1$.

$P_{mn}(t)$ is just shorthand for $P(x_{1m}, x_{2n}, t)$ (cp. (A.9)). The difference operators F_1 and F_2 obviously correspond to the differential operators under the sum in (A.1).

Henceforth we shall suppress the coordinates in the notation of the probability density $P(x_1, x_2, t)$ and shall retain only the time since it is this dependence which ADIP tackles in a peculiar way.

Let us now assume that all values of $P(t)$ are known and we wish to calculate $P(t+\Delta t)$. To this end we first content ourselves with the halved time step $\Delta t/2$ and write instead of (A.1)

$$(P(t+\Delta t/2) - P(t)) / (\Delta t/2) = F_1 P(t+\Delta t/2) + F_2 P(t).$$

The remarkable point in the equation is that the space differences in x_2 direction are taken at the old time t whereas those in x_1 direction already necessitate the knowledge of $P(t+\Delta t/2)$. This leads to difference equations which are explicit with respect to x_2 , but implicit in x_1 :

$$[1 - (\Delta t/2) F_1] \cdot P(t+\Delta t/2) = \Delta t/2 \cdot F_2 P(t). \quad (A.12)$$

They can be quickly solved since, as insertion of (A.11) into (A.12) shows, they constitute a tridiagonal system [15]. To proceed further from $t + \Delta t/2$ to $t + \Delta t$, we repeat the step, but alternate the implicit direction. This time the x_1 direction is treated explicitly:

$$[1 - (\Delta t/2) F_2] \cdot P(t+\Delta t) = (\Delta t/2) \cdot F_1 P(t+\Delta t/2). \quad (A.13)$$

The equations (A.12) and (A.13) represent ADIP. The method is stable and accurate. The error of the solution of the difference equations (A.12,13) relative to that of the differential equation (A.1) is $O(\Delta x_1^2 + \Delta x_2^2 + \Delta t^2)$. However, this is only true for the solution at the full time steps $t, t + \Delta t, t + 2\Delta t, \dots$. The values at the intermediate steps $t + \Delta t/2, t + 3\Delta t/2, \dots$ are auxiliaries and should not be used for the calculation of moments and similar purposes.

We are aware that ADIP loses its unconditional stability if the drift coefficients become too large:

$$|V^i| > 2d^i/\Delta x_i. \quad (A.14)$$

For this case, the linear systems in (A.12) or (A.13) forfeit diagonal dominance, and the standard methods to solve them, being basically all Gaussian eliminations without pivoting, cease to be stable. But ADIP is still conditionally stable if the inequalities

$$\frac{2\Delta x_i}{\Delta t} > |v_i| \quad (A.15)$$

are fulfilled. This is nothing else than the Courant-Friedrichs-Lewy criterion [16] for time step size $\Delta t/2$. We are aware of means which re-introduce unconditional stability [17], but in the present application we could do without them.

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Figure captions

- 1 Model potential U for some orbital angular momenta ℓ . The dashed lines indicate the mean trajectories obtained with the friction formfactor (2)
- 2a-c Contour plot of $f(r, v; t)$ for various times and different angular momenta [a) $\ell=30\hbar$, b) $\ell=23\hbar$, c) $\ell=0\hbar$] for the global moment approach (l.h.s.) in comparison with the exact solution (r.h.s.). The dashed line in the upper part indicates the mean trajectory of the GMA. The contour lines correspond to constant $f(r, v; t)$ in the sequence $(10^{-2}, 5 \cdot 10^{-2}, 10^{-1}, 2 \cdot 10^{-1}, 5 \cdot 10^{-1}, 1.0)$
- 3 Probability for fusion P_ℓ as a function of angular momentum in comparison with the sharp cut off limit (dashed line)
- 4 Distribution function $f(r, v; t)$ for $\ell=23\hbar$, $t=32\text{fs}$ at various fixed distances r [fm]
- 5 Contour plot of $f(r, v; t)$ for $\ell=23\hbar$ and several times for the local moment approach (LMA) (r.h.s.) in comparison with the exact result (l.h.s.). The contour lines correspond to constant $f(r, v; t)$ in the sequence $(10^{-2}, 5 \cdot 10^{-2}, 10^{-1}, 2 \cdot 10^{-1}, 5 \cdot 10^{-1}, 1.0)$

fig. 2a

Fig. 26

Fig. 24

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Fig. 5