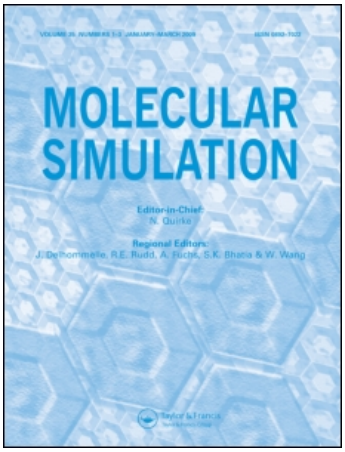

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Lattice Molecular Dynamics

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LATTICE MOLECULAR DYNAMICS

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We introduce a new method for simulating fluids in which the particles are constrained to lie on a lattice, but the momenta of the particles are permitted any continuous value. The model includes long-range interactions and is shown to obey the standard macroscopic fluid equations, microscopic time reversal symmetry, and detailed balance.

Keywords: Lattice molecular dynamics; Fluids; Fluid equations

INTRODUCTION

When modelling and simulating complex classical fluids, it is generally necessary to sacrifice some of the details of particle interactions in order to obtain useful information in a reasonable time. Molecular dynamics, which provides an accurate solution of the classical equations of motion, contains the most complete description of the system under study [1]. The calculation of the continuous forces in a molecular dynamics simulation, however, requires significant processing time at each time step, and the time steps used in the integration of the equations of motion are typically extremely short compared to most time scales of interest. For the simulation of macroscopic fluids, such complete simulations have proven impracticable.

Lattice gas automata (LGA) provide another method for the simulation of macroscopic fluid flow, which utilises a simplified phase space with

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discrete positions and velocities [2, 3]. The two-dimensional version consists of a set of particles on a hexagonal lattice with either unit velocities along the lattice directions or velocity set to zero. The particles interact according to simplified local collision rules that satisfy particle number and momentum conservation laws. In the small velocity limit, the macroscopic lattice gas has been shown to obey Navier-Stokes-type equations. Since the natural time step in a LGA simulation is the mean time between collisions, the LGA method provides an efficient scheme for simulating classical fluids. The single phase LGA has since been generalised to permit the simulation of immiscible fluids [4], and more recently the technique has been extended to model amphiphilic fluids comprised of oil, water, and surfactant [5].

While LGA methods have produced many impressive results, the approach suffers from some disadvantages. The underlying lattice causes a loss of Galilean invariance, and there is no sense of particle size or finite impact parameter. In addition, because of the limited velocity range (in the simplest models there are only two possible speeds), the study of energy relaxation processes is severely limited. There have been attempts to introduce LGA models with a particle size [6] and with a larger, though still finite, velocity range [7]. For multi-component fluids, however, LGA models do not observe detailed balance and so their equilibrium states are not known. The lattice-Boltzmann (LBE) approach, which operates with the real-valued single particle distribution function, provides another method to deal with these difficulties [8]. Unfortunately, LBE simulations of multi-component fluids also do not satisfy detailed balance and hence do not conform to an H theorem of the Boltzmann type. Thus, not only are the equilibrium states of LBE simulations not known, but they also suffer from poorly understood numerical instabilities. This poses a significant limitation to their application and their theoretical structure [2]. We note in passing that Boghosian, Yepez, Coveney and Wagner have addressed this problem by imposing an entropy-like function on lattice-Boltzmann schemes, and only performing lattice updates which ensure that this entropy monotonically increases with timestep [9].

Such considerations lead one to wonder if it is possible to develop a model with which one may study the approach to equilibrium but which still has some of the advantages of a lattice approach. In this paper we introduce a new method for modelling fluids which utilizes a lattice yet has a continuous velocity distribution, a notion of particle size and impact parameter, and potentials that govern particle interactions; which obeys detailed balance and microscopic time reversal invariance for both single and multi-component fluids; and which locally conserves momentum, mass, and

energy. We call this method lattice molecular dynamics (LMD) because in essence we are performing a simplified and probabilistic molecular dynamics simulation with particles constrained to lie on a lattice. For simplicity we consider a two dimensional fluid in which the particles all have the same mass, which we will set to unity. The extension to three dimensions is straightforward, and it is not difficult to show that if particles have varied masses, the equations below are only changed by constant factors involving the masses. We will consider the varied mass case in an Appendix.

METHOD

We consider a fluid of N particles in a volume V, a two dimensional space with periodic boundary conditions. The particles are constrained to lie at the vertices of a square lattice, and each particle has a real-valued vector momentum pointing in an arbitrary direction which is decomposed into its components along the lattice directions. Time advances in discrete steps of length τ. At the beginning of the time step, we choose a particle i and lattice direction k randomly. In practice, each particle and direction will be chosen once in each time step and operated upon in a random order. We then set x'_{ik}, the lattice site to which particle i may move, to the neighbouring site in the direction of the k-component of momentum for particle i, p_{ik}. We now look for other particles which may interact with particle i, *i.e.*, particles that are within the effective radius of the interaction potential. Though it is possible for the effective radius to be infinite, typically we will use potentials with a small cut-off radius for computational efficiency. We label the interacting particles with an index j and the particle nearest to particle i as particle n. All distances are calculated from the average of the current and possible future position of particle i.

Once the list of interacting particles is compiled, we calculate the following quantity:

$$\Psi = \left(\frac{p_{ik} - p_{nk}}{2}\right)^2 - \Delta U \tag{1}$$

This quantity tells us if there is sufficient kinetic energy to overcome an increase in the potential energy due to the movement of particle i. The first term on the right hand side of (1) is the total kinetic energy of particles i and n available to offset an increase in the potential energy, *i.e.*, it is the total kinetic energy of the particles in the centre of mass rest frame. The potential

energy term, represented by ΔU, is the change in the total potential energy due to the interactions of particle i and all of the particles j that would result from particle i moving from its current position to x'_{ik}. If $\Psi < 0$ there is insufficient kinetic energy available, and the transition is not allowed. In this case, particle i and particle n exchange their momenta in the k-direction. This corresponds to the two particles recoiling from each other elastically in the centre of mass frame. If $\Psi > 0$ there is sufficient kinetic energy to overcome the potential energy increase (or the potential energy is decreasing, yielding extra kinetic energy for the two particles), so we may allow particle i to move to its new position. However, we will need to adjust the k-component of the momenta of particle i and particle n so that total energy and total momentum are conserved.

Let us set

$$\begin{aligned} p'_{ik} &= p_{ik} + \Delta p \\ p'_{nk} &= p_{nk} - \Delta p \end{aligned} \tag{2}$$

These values clearly conserve momentum. Substituting the primed momenta into the energy conservation equation and solving for Δp yields

$$\Delta p = \frac{p_{nk} - p_{ik}}{2} \pm \sqrt{\left(\frac{p_{nk} - p_{ik}}{2}\right)^2 - \Delta U} \tag{3}$$

The ambiguity of the $\pm$ sign in the equation for Δp is resolved by requiring that the relative momentum of the two particles maintains its sign, which is what one would expect in a collision. Finally, because we wish to have real-valued momenta for particles constrained to a lattice, we will connect the velocity of a particle to its actual motion by a Monte Carlo procedure. Once we have determined that a transition for particle i is allowed and have calculated its new momentum, we only complete the move with probability

$$\pi_{ik} = \left|\frac{p'_{ik} + p_{ik}}{2}\right| \frac{\tau}{ml} \tag{4}$$

where l is the lattice spacing and m is the mass of a particle. The right hand side is clearly interpreted as the average k-component of the velocity of particle i as it moves from its current position to x'_{ik}. Hence, a particle moves from one lattice site to the next with a probability proportional to its velocity. The expectation value of the displacement of a particle after many time steps is simply the velocity of the particle multiplied by the duration of the interval observed. Thus we have a very natural link between

the real-valued velocity of a particle and its actual motion on the lattice. Once particle i has had its chance to move in direction k, we continue by choosing another particle and direction. The process repeats until every particle and direction has been treated. Once this is completed, we start a new time step.

We now move on to note some of the interesting properties of the LMD fluid, beginning with its microscopic time reversal symmetry. Let us begin by defining the vectors $\mathbf{x}$ and $\mathbf{p}$ as follows: $\mathbf{x}$ is a $2N$ dimensional vector whose components are the x and y components of the position of each of the N particles. The vector $\mathbf{p}$ is similarly a $2N$ dimensional vector whose components are the x and y components of the momentum of each of the N particles. Thus, the vector pair $(\mathbf{x}, \mathbf{p})$ describes the exact point in phase space occupied by the system at a given time. The time reversal symmetry obeyed by an LMD fluid states that the probability of a particle going from a state $(\mathbf{x}, \mathbf{p})$ to a state $(\mathbf{x}', \mathbf{p}')$ forward in time is equal to the probability of a particle going from a state $(\mathbf{x}', -\mathbf{p}')$ to a state $(\mathbf{x}, -\mathbf{p}')$ backward in time.

That this symmetry holds can be seen by considering the various factors that combine to form the transition probability. The first aspect to consider is whether a transition from the state $(\mathbf{x}, \mathbf{p})$ to the state $(\mathbf{x}', \mathbf{p}')$ is allowed. Such a transition is only allowed in a single time step if the vectors $\mathbf{x}$ and $\mathbf{x}'$ are identical except for one component x_{ik} which differs only by unity. Similarly, the vectors $\mathbf{p}$ and $\mathbf{p}'$ must be identical except in the components p_{ik} and p_{nk}. We also require that the total energy and momentum of the system are the same for both the primed and unprimed states. Finally, the transition is only allowed if $\Psi > 0$. It is straightforward to demonstrate that if these conditions are met for a given direction of time, they will also be met for reverse time.

Further, because the particles are treated in a random order, the probability of a given particle being treated at a certain point in the time step is unaffected by a time reversal transformation. The particles that interact with the chosen particle are determined by calculations based on the average position of the particle during the time step, and the probability that the chosen particle moves is calculated based on the average momentum of the particle during the time step (see Eq. (4)). These last two considerations, and thus the entire transition probability, are unaffected by a time reversal transformation.

We note that the system is not deterministic, and simply reversing the sign of time does not guarantee a return to the initial state. However, this symmetry is significant in that an observer looking only at the motions of individual particles would have no means of determining the direction of

time. We will also see shortly that on macroscopic length and time scales the expected irreversible behaviour will emerge. Thus, the LMD fluid provides an interesting opportunity to study in detail the development of irreversible macroscopic phenomena from reversible microscopic rules.

From this time reversal symmetry and two other symmetries of the system, one can also show that for systems in which it is meaningful to discuss collisions, detailed balance holds in equilibrium. To illustrate the proof, we will consider binary collisions. The extension to higher order collisions is straightforward. The transition rate, w, between one state and another due to a collision is a function only of the velocities of the particles and the impact parameter, b. Due to the time reversal symmetry of the system, the transition rate $w(\mathbf{v}, \mathbf{v}_1|\mathbf{v}', \mathbf{v}_1'; b)$ must be equal to the time-reversed transition rate $w(-\mathbf{v}', -\mathbf{v}_1'| -\mathbf{v}, -\mathbf{v}_1; b)$. This rate is equal, in turn, to $w(-\mathbf{v}_1' - \mathbf{v}'| -\mathbf{v}_1, -\mathbf{v}; b)$ because of symmetry under a relabelling of the particles, and finally due to the symmetry of the system under rotations by 180°, this rate must be equal to $w(\mathbf{v}', -\mathbf{v}_1'|\mathbf{v}, -\mathbf{v}_1; b)$. Thus, we have found that

$$w(\mathbf{v}, \mathbf{v}_1|\mathbf{v}', \mathbf{v}_1'; b) = w(\mathbf{v}', \mathbf{v}_1'|\mathbf{v}, \mathbf{v}_1; b) \tag{5}$$

which is the detailed balance condition.

We now turn to a study of the macroscopic properties of a dilute LMD fluid. Let us consider the evolution of $f(\mathbf{x}, \mathbf{v}, t)$, the single particle distribution function which is defined as the number of particles in a cell of phase space surrounding the point $(\mathbf{x}, \mathbf{v})$ at time t. We assume that a cell contains a large number of lattice sites, but is small compared to the size of the system. It is also assumed that f is sufficiently smooth that it may be expanded to first order in a Taylor series in both space and time. We will consider changes in this function over a time, dt, which is long compared to a single time step but is short compared to the time scales of interest. Such changes may be written as

$$\frac{\partial f(\mathbf{x}, \mathbf{v}, t)}{\partial t} = \Delta_A + \Delta_C \tag{6}$$

where Δ_A is the change in f due to advection, or free motion, of the particles and Δ_C is the change due to collisions. From the fact that particles move from one lattice site to the next with a probability proportional to their velocity, it can be shown assuming that particles are evenly distributed within a cell that the number of particles moving from one cell to a neighbour is proportional to the velocity of the particles in that cell. Thus,

following the classical derivation (see for example [10]), we find that Δ_A is simply $\mathbf{v} \cdot \nabla f(\mathbf{x}, \mathbf{v}, t)$. The collision term may be found by first considering the collision term for a Newtonian fluid [10]

$$\Delta_C^{\text{Newton}} = \int dbd\mathbf{v}_1 g[f(\mathbf{x}, \mathbf{v}', t) f(\mathbf{x}, \mathbf{v}_1', t) - f(\mathbf{x}, \mathbf{v}, t) f(\mathbf{x}, \mathbf{v}_1, t)] \tag{7}$$

In the Newtonian collision term, the outgoing (primed) velocities are a function of the incoming velocities. In the LMD fluid, for a given pair of incoming velocities, the resulting outgoing velocities are drawn from all possible velocities with probability $w(\mathbf{v}, -\mathbf{v}_1 | \mathbf{v}', \mathbf{v}_1'; b)$. Thus, we must integrate the Newtonian collision term multiplied by this probability function over all possible outgoing velocities. This leads to the LMD Boltzmann equation

$$\frac{\partial f(\mathbf{x}, \mathbf{v}, t)}{\partial t} + \mathbf{v} \cdot \nabla f(\mathbf{x}, \mathbf{v}, t) = \int dbd\mathbf{v}_1 d\mathbf{v}' d\mathbf{v}_1' g[f(\mathbf{x}, \mathbf{v}', t) f(\mathbf{x}, \mathbf{v}_1', t) - f(\mathbf{x}, \mathbf{v}, t) f(\mathbf{x}, \mathbf{v}_1, t)] w(\mathbf{v}, \mathbf{v}_1 | \mathbf{v}', \mathbf{v}_1', b) \tag{8}$$

We note that the Boltzmann equation for the LMD fluid differs from the two dimensional Boltzmann equation for a Newtonian fluid only in the collision term. The connection between this equation and the corresponding equation for a Newtonian fluid is clear in that the transition probabilities go to delta functions in the continuum limit. Integrating over these delta functions yields the classical Boltzmann equation.

The collision integral for the LMD fluid, though, has the same symmetries as the collision integral for the Newtonian fluid. By using these symmetries, one can demonstrate an H-theorem for the LMD fluid by methods similar to those used for the Newtonian fluid. Such an analysis also leads to an equilibrium distribution that is Maxwellian and the classical conservation equations of fluid dynamics. Applying the approximations used to derive the Navier-Stokes equations for a Newtonian fluid yields identical results for the LMD fluid. In a similar way, transport coefficients may also be calculated for the LMD fluid. We also note that if the single particle distribution function is isotropic in velocity, the pressure tensor will be as well. Since the direction of a particle's velocity is independent of the lattice directions, there are no preferred directions in the velocity distribution function. This makes it possible to use a square lattice in LMD simulations without the symmetry problems faced in conventional LGA models [3]. Thus, we have developed a simulation method that in the large scale limit behaves like a Newtonian fluid.

RESULTS

We report here a simple numerical study to confirm the validity of our model. The simulation was performed with 10,000 particles spread out over a $6{,}000 \times 6{,}000$ lattice with periodic boundary conditions, yielding an average distance between the particles of 60 lattice sites. We used a $1-(r/s)^2$ potential, where s is the cut-off radius which was set to 20 lattice sites. The particles were assigned positions with uniform probability throughout the volume, and momenta were assigned with uniform probability in all directions and magnitudes in the range 0 to 0.5 such that the total momentum of the system was zero. We found a rapid convergence to a two-dimensional Maxwell distribution. The points in Figure 1 represent values averaged over 20 snapshots taken of the system each separated by 5,000 time steps. The error bars signify one standard deviation from the mean, and the solid curve is a two dimensional Maxwell-Boltzmann distribution with $k_BT=0.181$.

For this simulation, we also calculated the normalised pressure tensor, *i.e.*, the pressure tensor with each component divided by the number of

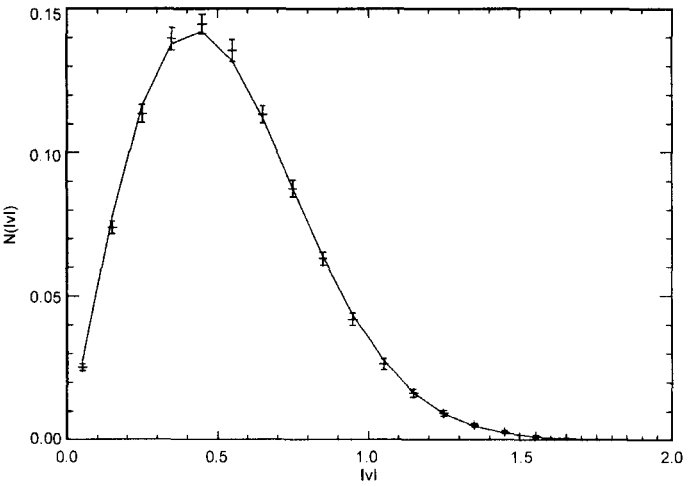

FIGURE 1 The average velocity distribution for an LMD simulation of a 10,000 particle dilute fluid with zero fluid velocity compared to a Maxwell distribution with $k_BT=0.181$. The error bars signify one standard deviation from the mean. The average was taken over 20 snapshots of the system each taken 5000 time steps apart. The velocity bins are of width 0.1 lattice sites per time step.

TABLE I The normalised components of the pressure tensor evaluated at several different angles for an LMD fluid with zero fluid velocity. The first line contains the theoretical values. The averages were performed over 20 snapshots taken of the system each separated by 5000 time steps. The errors represent one standard deviation from the mean

ϕ	P_{xx}	P_{xy}	P_{yx}	P_{yy}
–	0.181	0.000	0.000	0.181
0	0.1812 ± 0.0028	-0.0001 ± 0.0017	-0.0001 ± 0.0017	0.1810 ± 0.0026
9	0.1813 ± 0.0029	-0.0000 ± 0.0017	-0.0000 ± 0.0017	0.1810 ± 0.0026
18	0.1813 ± 0.0030	0.0000 ± 0.0017	0.0000 ± 0.0017	0.1810 ± 0.0025
27	0.1812 ± 0.0031	0.0001 ± 0.0015	0.0001 ± 0.0015	0.1810 ± 0.0025
36	0.1812 ± 0.0032	0.0001 ± 0.0014	0.0001 ± 0.0014	0.1810 ± 0.0026
45	0.1812 ± 0.0032	0.0001 ± 0.0013	0.0001 ± 0.0013	0.1811 ± 0.0027

particles. The result is the second line in Table I. On the first line are the theoretical values calculated from the measured temperature of the fluid, the assumed isotropy of the pressure tensor, and the ideal gas relation

$$\frac{1}{2}\mathrm{Tr}(\mathbf{P})/n = k_B T \tag{9}$$

where n is the number density of the fluid and k_B is Boltzmann's constant. We see good agreement between the measured and calculated values of the pressure tensor. For the other lines of the table, we rotated the velocities of the particles and recalculated the pressure tensor. This is equivalent to measuring the pressure tensor along axes at some angle to the lattice, and we can see from the table that the pressure tensor is independent of the lattice directions. The angles measured here are sufficient due to the symmetry of the square lattice.

CONCLUSION

We have presented a new method for modelling fluids that utilizes a lattice yet avoids several of the significant problems faced by traditional lattice methods. Our model locally and globally conserves energy, mass, and momentum. It obeys detailed balance and microscopic time reversal symmetry for single and multi-component fluids as well as obeying the macroscopic fluid equations. There is a continuous velocity distribution along with potentials that govern the particle interactions and give meaning to particle size and impact parameter. Overall, the model is a lattice gas that closely resembles a fluid of Newtonian particles.

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APPENDIX: THE CASE OF PARTICLES WITH DIFFERING MASSES

In the main part of this paper, the discussion was restricted to a fluid containing particles each with an identical mass. This was done in order to simplify the notation and thus illustrate more clearly several aspects of the model. In this Appendix a brief account of the more general case in which each particle may have a unique mass is presented. The Appendix begins with a derivation of the formula for the momentum of each particle following an interaction subject to the conservation constraints. This is followed by an examination of an interaction in the centre of mass frame that shows that the interpretations of the terms offered in the main text is consistent with the general case.

The rules of the algorithm in the general case are identical to those outlined in the main text. The particles i and n and the direction k have been chosen in the same manner as before. Now let us consider how to adjust their momenta and begin by writing (suppressing the index k):

$$\begin{aligned} p_i' &= p_i + \Delta p \\ p_n' &= p_n - \Delta p \end{aligned} \tag{10}$$

This choice clearly conserves momentum. Next, let us consider the conservation of energy:

$$K' + U' = K + U \tag{11}$$

where the primes indicate the values following the collision. The kinetic energy takes on the usual value, so one may write the following two equations for the kinetic energy following the interaction:

$$\begin{aligned} K' &= \frac{p_i^2}{2m_i} + \frac{p_n^2}{2m_n} - \Delta U \\ K' &= \frac{p_i'^2}{2m_i} + \frac{p_n'^2}{2m_n} = \frac{p_i^2 + 2p_i\Delta p + \Delta p^2}{2m_i} + \frac{p_n^2 - 2p_n\Delta p + \Delta p^2}{2m_n} \end{aligned} \tag{12}$$

Combining these equations and simplifying yields:

$$\left(\frac{m_i + m_n}{m_i m_n}\right)\Delta p^2 + 2\left(\frac{p_i}{m_i} - \frac{p_n}{m_n}\right)\Delta p + 2\Delta U = 0 \tag{13}$$

Solving this equation yields the following form for Δp:

$$\Delta p = \frac{m_i p_n - m_n p_i}{m_i + m_n} \pm \sqrt{\left(\frac{m_i p_n - m_n p_i}{m_i + m_n}\right)^2 - \frac{2m_i m_n}{m_i + m_n}\Delta U} \tag{14}$$

Substituting (14) back into (10), one gets for the new momenta:

$$\begin{aligned} p_i' &= \frac{m_i p_n + m_i p_i}{m_i + m_n} \pm \sqrt{\left(\frac{m_i p_n - m_n p_i}{m_i + m_n}\right)^2 - \frac{2m_i m_n}{m_i + m_n}\Delta U} \\ p_n' &= \frac{m_n p_n + m_n p_i}{m_i + m_n} \mp \sqrt{\left(\frac{m_i p_n - m_n p_i}{m_i + m_n}\right)^2 - \frac{2m_i m_n}{m_i + m_n}\Delta U} \end{aligned} \tag{15}$$

All of the other formulae discussed in the main text related to the rules of the algorithm remain the same.

Now consider the meaning of the terms in (14). Let us begin by making a Galilean transformation of the interaction to the centre of mass rest frame by adding to the velocity of each particle

$$v_T = -\frac{p_i + p_n}{m_i + m_n} \tag{16}$$

Thus one finds for the centre-of-mass momentum for particle i and particle n:

$$p_{i,CM} = -p_{n,CM} = p = \frac{m_n p_i - m_i p_n}{m_i + m_j} \tag{17}$$

and thus (14) can be written as

$$\Delta p = -p \pm \sqrt{p^2 - 2M\Delta U} \tag{18}$$

where we have defined the reduced mass

$$M = \frac{m_i m_n}{m_i + m_n}. \tag{19}$$

Noting that:

$$K_{CM} = \frac{p^2}{2m_i} + \frac{p^2}{2m_n} = \frac{p^2}{2M} \tag{20}$$

one sees that the condition requiring that the transition only be allowed when the square root in (14) is real is simply:

$$K_{CM} - \Delta U > 0 \tag{21}$$

which is the same conclusion arrived at when the masses of all the particles had been set to unity. Also, the ambiguity of the $\pm$ sign in (14) is resolved as before, *i.e.*, we choose the sign in front of the square root so that the relative momentum maintains its sign if the transition is allowed. It can also be seen from the above that the prescription for prohibited transitions, an exchange of the momenta of the two particles, corresponds to the two particles bouncing back elastically in the centre-of-mass rest frame.

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