

Delays associated with elementary processes in nuclear reaction simulations

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Scatterings, particularly those involving resonances, and other elementary processes do not happen instantaneously. In the context of semiclassical nuclear reaction simulations, we consider delays associated with an interaction for incident quantum wave packets. As a consequence, we express delays associated with elementary processes in terms of elements of the scattering matrix and phase shifts for elastic scattering. We show that, within the second order in density, the simulation must account for delays in scattering consistently with the mean field in order to properly model thermodynamic properties such as pressure and free-energy density. Delays associated with nucleon-nucleon and pion-nucleon scattering in free space are analyzed with their nontrivial energy dependence. Finally, an example of *s*-channel scattering of massless partons is studied, and scattering schemes in nuclear reaction simulations are investigated in the context of scattering delays.

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I. INTRODUCTION

Semiclassical transport simulations have provided the theoretical backbone for interpreting heavy-ion reactions at energies in excess of few tens of MeV per nucleon. Simulations follow either a cascade approach [1,2] or a solution to the Boltzmann equation including the mean field effects and the Pauli principle [3–5]. Within these approaches particles move classically in-between collisions where momenta change abruptly and possibly new particles form. In practice, the Pauli principle appears primarily important for reactions below 150 MeV/nucleon. For beam energies of hundreds of MeV per nucleon, detailed comparisons of simulations with data have been carried out [6–9] in order to determine features of the momentum and density dependence of the nuclear mean field. Within many-body theory, efforts have been made to calculate nuclear optical potentials starting from elementary *NN* interactions [10–12]. In describing reactions with beam energies up to ~ 2 GeV/nucleon, pions and low-lying resonances have also been included in simulations.

It has been noted that results of heavy-ion reaction simulations can depend sensitively on prescriptions of space-time details of elementary scattering processes [13–16,9,17]. Such details of elementary processes may matter even more at higher beam energies than at those of the MSU or SIS accelerators, specifically, at those of AGS (14 GeV/nucleon), SPS (200 GeV/nucleon), and of the constructed and planned colliders, RHIC and LHC. This is because of high Lorentz dilation factors that can amplify space-time effects, and because of high particle densities early in the reactions.

In this paper we investigate the time duration of elementary processes in free space, in the context of semiclassical simulations. Both the forward-going and scattered waves get delayed in elementary processes. While delay of the forward wave is consistent with the effects of an optical potential for a particle in a medium, to the lowest order in particle density, both types of delay times, of the forward and scattered waves, affect the density of states in energy, to the lowest

nontrivial second order in particle density. As one important outcome of our work, we find that to describe the density of states and associated thermodynamic quantities such as pressure, heat capacity, etc., the delays for scattered particles must be properly accounted for in semiclassical simulations, in addition to the effects of the optical potential. If one relaxes the requirements on interactions in simulations, forsaking, e.g., the proper behavior of single-particle energies, but demanding that free energy as a fundamental thermodynamic function is properly reproduced to within the second order in density in equilibrium, then one can manipulate the mean field to entirely absorb effects of the delays for scattered particles. Alternatively, time delays for scattered particles may be manipulated to absorb the effects of the optical potential. Even in a degenerate Fermi gas, as we show, the delays in scattering can affect thermodynamic quantities. We investigate several examples of particle-particle scattering amplitudes describing, respectively, the scattering through a sharp Breit-Wigner resonance, the πN interaction in the Δ channel, and the *s*-channel scattering of massless partons. Using free-space amplitudes, we numerically calculate the time delays for the *NN* system. We show that the delay for scattering has some dependence on the scattering angle and that the delays become small at high energies. Finally, we investigate scattering schemes in simulations [2,4,5,13–17] in the context of time delays. The schemes include hard-sphere scattering and scattering at the distance of closest approach. We outline numerical strategies for determining the equation of state and transport coefficients to an arbitrary order in density given the scattering prescription.

The content of subsequent sections is as follows. In Sec. II we consider a wave packet traversing a region with a scatterer and derive expressions for the delays of scattered and forward-going waves in terms of scattering amplitudes (phase shifts) and their derivatives. In Sec. III we demonstrate that these delay times are consistent with an ergodic constraint stating that the extra time spent in the vicinity of a scatterer should be proportional to the change in the density of states brought about by that scatterer. We further show that

the delay time for a forward-going wave corresponds to the classical motion of a particle in a mean field given by the self-energy for a plane wave in a low-density medium. In that section, and further in the Appendix, we also discuss the modification of the scattering of two bodies brought about by the presence of a third body. Finally, we express the free-energy density and pressure in terms of different time delays. In Sec. IV we draw conclusions on the time delays in a Bose or Fermi degenerate medium by examining an expression for the change in the pressure due to two-particle interactions. Section V is devoted to the examples of resonance scattering. In Sec. VI we calculate spin-isospin averaged time delays for NN system and directly relate the delays to the second virial coefficient. Different scattering prescriptions and methods for the determination of equations of state and transport coefficients, to within arbitrary order in density for given prescriptions, are discussed in Sec. VII.

II. TIME DELAYS FROM WAVE-PACKET DYNAMICS

We consider a wave-packet incident on a large spherical volume of radius R , at the center of which interaction takes place. To make the derivation simpler we assume that this volume is much larger than the wave packet. The wave function is

$$\psi_\alpha(t) = \int dE g(E) \psi_\alpha^E(t), \quad (2.1)$$

where for large distances

$$\begin{aligned} \psi_\alpha^E &= \sum_\beta \phi_{\alpha\beta}(\mathbf{r}, t) \chi_\beta \\ &= \phi_\alpha^0(\mathbf{r}, t) \chi_\alpha + \sum_\beta f_{\alpha\beta}(\theta, E) \frac{e^{i(k_\beta r - Et)}}{r} \chi_\beta, \end{aligned} \quad (2.2)$$

and

$$\begin{aligned} \phi_\alpha^0 &= \frac{1}{2ik_\alpha r} \sum_{\ell=0}^{L_{\max}} (2\ell+1) P_\ell(\cos\theta) \\ &\quad \times [(-1)^{(\ell+1)} e^{-i(k_\alpha r + Et)} + e^{i(k_\alpha r - Et)}]. \end{aligned} \quad (2.3)$$

Here α and β denote the initial and final channels, respectively, and χ is the internal wave function. Most often we shall consider elastic scattering of particles with no internal degrees of freedom, hence

$$f(\theta, E) = -\frac{1}{2k} \sum_{\ell} (2\ell+1) P_\ell(\cos\theta) \mathcal{T}_\ell(E), \quad (2.4)$$

where the amplitude \mathcal{T}_ℓ is related to scattering matrix and phase shift by

$$\mathcal{T}_\ell = i(S_\ell - 1) = -2 \sin\delta_\ell \exp i\delta_\ell, \quad (2.5)$$

$S_\ell = \exp 2i\delta_\ell$. For the asymptotic form to be valid r must be much larger than L_{\max}/k and T_ℓ must vanish for $\ell > L_{\max}$.

The average time τ_{vol} that a particle spends in the volume can be written as

$$\tau_{\text{vol}} = R^2 \frac{\sum_\gamma \int dt d\Omega \mathbf{j}_\gamma(R, \Omega, t) \cdot \hat{\mathbf{r}} t}{N}, \quad (2.6)$$

where current density in channel γ is

$$\mathbf{j}_\gamma = \frac{1}{2\mu_\gamma i} \phi_\gamma^*(\mathbf{r}, t) \vec{\partial} \phi_\gamma(\mathbf{r}, t), \quad (2.7)$$

and N is integrated incident flux through the surface. The time in (2.6) is represented as the average time for the particle to leave the volume minus the average time for the particle to enter the volume, as $\mathbf{j} \cdot \hat{\mathbf{r}}$ is positive when a particle exits and negative when a particle enters. We decompose \mathbf{j} into incoming and outgoing pieces and, as there is no interference between incoming and outgoing waves for a large volume, we write explicitly

$$\tau_{\text{vol}} = \tau_{\text{out}} - \tau_{\text{in}}. \quad (2.8)$$

With the incoming wave having only a contribution from the unscattered wave packet, one finds, from (2.3) and (2.6), that $\tau_{\text{in}} = -R/v_\alpha$.

The outgoing wave has contributions from both the scattered and unscattered portions of the wave packet. Correspondingly, the outgoing current has three contributions: from the scattered wave, from the unscattered wave, and from the interference between the two. We first calculate the exit time associated with the scattered wave in the single-channel case, for particles leaving at the center of mass angle θ , using the partial-wave expansion

$$\begin{aligned} \tau_s(\theta) &= R^2 \frac{\int dt \mathbf{j}_s(R, \theta, t) \cdot \hat{\mathbf{r}} t}{dN_s/d\Omega} \\ &= \frac{1}{Z} \sum_{\ell, \ell'}^{L_{\max}} \int dt dE dE' g(E) g(E') e^{i(k-k')R} (2\ell+1) \\ &\quad \times P_\ell(\cos\theta) (2\ell'+1) P_{\ell'}(\cos\theta) \mathcal{T}_{\ell'}^*(E') \\ &\quad \times \mathcal{T}_\ell(E) t e^{-i(E-E')t} \left(\frac{1}{k} + \frac{1}{k'} \right), \end{aligned} \quad (2.9)$$

where Z is the same expression as the sum on the rhs of the last equation, only without the time t in the integrand,

$$\begin{aligned} Z &= \sum_{\ell, \ell'}^{L_{\max}} \int dt dE dE' g(E) g(E') e^{i(k-k')R} (2\ell+1) \\ &\quad \times P_\ell(\cos\theta) (2\ell'+1) P_{\ell'}(\cos\theta) \mathcal{T}_{\ell'}^*(E') \mathcal{T}_\ell(E) \\ &\quad \times e^{-i(E-E')t} \left(\frac{1}{k} + \frac{1}{k'} \right). \end{aligned} \quad (2.10)$$

By making the substitution

$$t = \frac{i}{2} \left\{ \frac{\partial}{\partial E} - \frac{\partial}{\partial E'} \right\}, \quad (2.11)$$

then carrying out integration by parts to make the derivatives with respect to E and E' act on g , $\exp i(k-k')R$, and \mathcal{T} , and further integrating over the time coordinate and one of the

energy variables, one obtains a simple expression for τ_s . For a well-defined energy this expression is

$$\begin{aligned}\tau_s(\theta) &= \frac{R}{v} + \Delta\tau_s(\theta) \\ &= \frac{R}{v} + \frac{1}{Z'} \sum_{\ell, \ell'}^{L_{\max}} (2\ell+1) P_{\ell}(\cos\theta)(2\ell'+1) \\ &\quad \times P_{\ell'}(\cos\theta) \frac{1}{2i} \left[\mathcal{F}_{\ell'}^*(E) \left(\frac{d}{dE} \mathcal{F}_{\ell}(E) \right) \right. \\ &\quad \left. - \left(\frac{d}{dE} \mathcal{F}_{\ell'}^*(E) \right) \mathcal{F}_{\ell}(E) \right],\end{aligned}\quad (2.12)$$

where

$$\begin{aligned}Z' &= \sum_{\ell, \ell'}^{L_{\max}} (2\ell+1) P_{\ell}(\cos\theta)(2\ell'+1) \\ &\quad \times P_{\ell'}(\cos\theta) \mathcal{F}_{\ell'}^*(E) \mathcal{F}_{\ell}(E).\end{aligned}\quad (2.13)$$

The more general result when many channels are open, in terms of the scattering amplitude f , is

$$\tau_s^{\alpha\beta}(\Omega) = \frac{R}{v_{\beta}} + \frac{1}{2i|f_{\alpha\beta}|^2} \left\{ f_{\alpha\beta}^* \frac{df_{\alpha\beta}}{dE} - f_{\alpha\beta} \frac{df_{\alpha\beta}^*}{dE} \right\}.\quad (2.14)$$

This is of use when determining time delays for a NN system in Sec. VI. In that case the indices refer to spin components.

For the case of elastic scattering in only one partial wave, the exit time from (2.12) may be written as

$$\tau_s = \frac{R}{v} + \frac{d\delta_{\ell}}{dE}.\quad (2.15)$$

Thus, the extra time delay due to the scattering is $d\delta/dE$ which is not the naive guess that one would make from considering an incoming partial wave reflecting off a potential. In that case the answer should be $2d\delta/dE$ since the potential modifies the scattered wave by a factor $e^{2i\delta}$. This discrepancy is associated with the interference between the forward-going wave and the scattered wave.

Next, we consider the current and the average exit time associated with the interference of the forward wave ϕ^0 with itself and with the scattered wave. The angular integration must extend up to $\theta \approx L_{\max}/kR$ which limits the forward wave, and it may, in particular, extend over the whole angular range. Analogous procedure to that before yields

$$\tau_f = \frac{R}{v} - \frac{1}{2Z''} \sum_{\ell=0}^{L_{\max}} (2\ell+1) \frac{d}{dE} [\mathcal{F}_{\ell}(E) + \mathcal{F}_{\ell}^*(E)],\quad (2.16)$$

where

$$Z'' = \sum_{\ell=0}^{L_{\max}} (2\ell+1) \{1 - i[\mathcal{F}_{\ell}(E) - \mathcal{F}_{\ell}^*(E)]\}.\quad (2.17)$$

In terms of phase shifts this gives

$$\tau_f = \frac{R}{v} + \frac{\sum_{\ell}^{L_{\max}} (2\ell+1) 2 \cos 2\delta_{\ell} \frac{d\delta_{\ell}}{dE}}{\sum_{\ell}^{L_{\max}} (2\ell+1) (1 - 4 \sin^2 \delta_{\ell})}.\quad (2.18)$$

The more general result in terms of the scattering amplitude f is

$$\begin{aligned}\tau_f^{\alpha} &= \frac{R}{v_{\alpha}} + \frac{2}{\sum_{\ell}^{L_{\max}} (2\ell+1) - 4k_{\alpha} \text{Im}f_{\alpha\alpha}(0)} \frac{d}{dE} \\ &\quad \times \{k_{\alpha} \text{Re}f_{\alpha\alpha}(0)\}.\end{aligned}\quad (2.19)$$

By combining the results for scattered and forward waves, we obtain the average exit time in the single-channel case

$$\begin{aligned}\tau_{\text{out}} &= \tau_f \left(1 - \frac{N_s}{N} \right) + \int d\Omega \tau_s(\Omega) \frac{dN_s/d\Omega}{N} \\ &= \frac{R}{v} + \frac{\sum_{\ell}^{L_{\max}} (2\ell+1) 2 \frac{d\delta_{\ell}}{dE}}{\sum_{\ell}^{L_{\max}} (2\ell+1)}.\end{aligned}\quad (2.20)$$

The total number of scattered particles is N_s . The delay time (2.20) is the same that one would have guessed assuming that different partial waves acted independently and each was delayed by $2d\delta_{\ell}/dE$. The complexity of Eqs. (2.18) and (2.12) stems from the interference of partial waves. In the next section we discuss the consistency of these results with equilibrium expectations. We show that the forward delay time agrees with a delay in the motion through a mean field.

III. THE ERGODIC CONSTRAINT AND THE MEAN FIELD

A. Ergodicity

All thermodynamic variables such as the pressure can be found if one knows the density of states within a system. Assuming that particles do not interact, and that statistical effects can be ignored, one can obtain thermodynamic quantities to lowest order in particle density. Assuming that particles interact only two at a time allows one to calculate these quantities to the next order in the density. To account for the interaction of two particles at a time, one needs to find the correction to the density of states of relative motion. This correction to the density of states $\rho(E) \equiv dn/dE$ is given by phase shifts for two-particle scattering [18,19],

$$\rho(E) = \rho_0(E) + \Delta\rho(E) = \frac{4\pi V}{(2\pi)^3} \frac{k^2}{v} + \frac{1}{\pi} \sum_{\ell} (2\ell+1) \frac{d\delta_{\ell}}{dE},\quad (3.1)$$

where k is the reduced relative momentum, V is the volume, and v is the velocity of relative motion. This is the complete quantum-mechanical answer for the single-channel case. If processes such as $a+b \rightarrow c+d$ can occur, a similar answer can be obtained by diagonalizing the S matrix and finding the eigenphases [20].

In a simulation, the equations of motion should modify the probability for two particles of a specific energy to be in

the vicinity of each other, such that it should be proportional to the change in the density of states for these particles. If the equations of motion accomplish this, the classical simulation will yield correct thermodynamic quantities. We consider a subvolume V in relative-coordinate space and a narrow relative-energy range $|E - E_0| < \delta E$. Given that particles spend a portion of time τ_0 within V in the absence of interactions, when sampling is carried out over a long time T , in the presence of interactions, the time within V should change by $\Delta\tau$ such that

$$\frac{\Delta\tau}{\tau_0} = \frac{\Delta\rho}{\rho_0} = \frac{1}{\pi} \sum_{\ell} (2\ell + 1) \frac{d\delta_{\ell}}{dE}. \quad (3.2)$$

This can be thought of as an ergodic constraint, since a system continuously sampled over a long time should be populated according to its contribution to the density of states. In this section we explore the case of elastic scattering and wish to see if the results of the preceding section are consistent with the ergodic constraint and with the picture of particles moving through a mean field.

In the context of a classical simulation, the additional time $\Delta\tau$ will come from three causes. First, the particle kinetic energy within the volume V will be different as compared to free space, reduced by the mean potential within the volume, $-u(k)$. The change in the energy gives a change in the momentum and in the velocity and, in consequence, in the time spent within subvolume by an amount denoted $\Delta\tau_1^{\text{clas}}$. In addition, the energy dependence of the mean potential generally changes the velocity by $\Delta v = du/dk$. The corresponding change in the time spent within the volume is denoted as $\Delta\tau_2^{\text{clas}}$. Both these contributions to the time follow from classical equations of motion within a potential. A third contribution $\Delta\tau^{\text{coll}}$ stems from collisions. Because of collisions the particles will emerge on the average earlier or later (particularly in the case of resonance scattering) from the volume than in absence of collisions. Summing the three contributions should yield

$$\frac{\Delta\tau_1^{\text{clas}} + \Delta\tau_2^{\text{clas}} + \Delta\tau^{\text{coll}}}{\tau_0} = \frac{1}{\pi} \sum_{\ell} (2\ell + 1) \frac{d\delta_{\ell}}{dE}. \quad (3.3)$$

The time $\Delta\tau_1^{\text{clas}}$ can be easily obtained from the ergodic theorem for a *classical* potential. Otherwise, one can resort to geometric considerations, caring for the fact that to the lowest order in u , the velocity changes its direction as well as the magnitude. As the relative change in time spent within the subvolume should be proportional to the relative change in the density of states brought about by the change in kinetic energy, we obtain

$$\frac{\Delta\tau_1^{\text{clas}}}{\tau_0} = \frac{\Delta\rho_0}{\rho_0} = - \frac{u(E)}{\rho_0} \frac{d\rho_0}{dE}. \quad (3.4)$$

The contribution $\Delta\tau_2^{\text{clas}}$ is obtained by noting that the time it takes to traverse a given path through the subvolume is proportional to the inverse of velocity,

$$\frac{\Delta\tau_2^{\text{clas}}}{\tau_0} = - \frac{\Delta v}{v} = - \frac{1}{v} \frac{du}{dk} = - \frac{du}{dE}. \quad (3.5)$$

The contribution due to collisions, $\Delta\tau^{\text{coll}}$, will be determined by the collision rate and the change $\Delta\tau_s$ in the average time spent within the collision range compared to free flight time,

$$\Delta\tau^{\text{coll}} = \tau_0 \frac{\sigma v}{V} \Delta\tau_s. \quad (3.6)$$

Combining the expressions for different contributions to the change in time on account of interactions, we find that, according to the ergodic constraint, we should have

$$\frac{1}{\pi} \sum_{\ell} (2\ell + 1) \frac{d\delta_{\ell}}{dE} = - \frac{d\rho_0}{dE} u - \rho_0 \frac{du}{dE} + \rho_0 \frac{\sigma v}{V} \Delta\tau_s. \quad (3.7)$$

In the following we shall express u in terms of phase shifts and then determine $\Delta\tau_s$ from (3.7) and examine whether the result is consistent with what was obtained in preceding section. The potential u in (3.7) is identified with the correction to the kinetic energy at which the single-particle Green's function has a pole,

$$\begin{aligned} g(k_1, E_1) &= \frac{1}{E_1 - e(k_1) - u + i\gamma/2} \\ &= \frac{1}{E_1 - e(k_1) - \langle \mathbf{k} | \mathcal{T} | \mathbf{k} \rangle / V}, \end{aligned} \quad (3.8)$$

where we use the fact that the self-energy can be expressed in terms of the forward element of the \mathcal{T} matrix. Here, k continues to be the relative particle momentum. Assuming that angular momentum is conserved, we obtain

$$\begin{aligned} \frac{1}{V} \langle \mathbf{k} | \mathcal{T} | \mathbf{k} \rangle &= \frac{1}{V} \sum_{\ell, m} \langle \mathbf{k} | \ell, m \rangle \langle \ell, m | \mathcal{T} | \ell, m \rangle \langle \ell, m | \mathbf{k} \rangle \\ &= \sum_{\ell} (2\ell + 1) \frac{\mathcal{T}_{\ell}}{2\pi\rho_0}. \end{aligned} \quad (3.9)$$

The imaginary part of the matrix times -2 can be shown to be equal to σv by using the standard expression for the cross section involving $\sin^2\delta$. Then γ is indeed the geometric scattering rate one expects. Turning now to the real part of \mathcal{T} matrix, the potential associated with the presence of other particle within subvolume becomes

$$u(E) = - \frac{\sum_{\ell} (2\ell + 1) \sin 2\delta_{\ell}}{2\pi\rho_0}. \quad (3.10)$$

The sum of the times $\Delta\tau_1^{\text{clas}}$ and $\Delta\tau_2^{\text{clas}}$ in (3.7) involve the derivative $d[u(E)\rho_0(E)]/dE$. With (3.10), we obtain

$$\begin{aligned} \frac{\Delta\tau_1^{\text{clas}} + \Delta\tau_2^{\text{clas}}}{\tau_0} &= - \frac{1}{\rho_0} \frac{d}{dE} [\rho_0 u(E)] \\ &= \frac{1}{\pi\rho_0} \sum_{\ell} (2\ell + 1) \cos 2\delta_{\ell} \frac{d\delta_{\ell}}{dE}. \end{aligned} \quad (3.11)$$

Upon inserting the above result into Eq. (3.7) we find

$$\Delta\tau_s = \frac{\sum_{\ell}(2\ell+1)\sin^2\delta_{\ell}\frac{d\delta_{\ell}}{dE}}{\sum_{\ell}(2\ell+1)\sin^2\delta_{\ell}}. \quad (3.12)$$

If only one partial wave is scattered, then the change in time reduces to

$$\Delta\tau_s = \frac{d\delta_{\ell}}{dE}. \quad (3.13)$$

This result is consistent with Eq. (2.15) of the last section. If many waves are scattered, then there is generally interference between various scattered partial waves giving rise to a variation of the change in time with scattering angle, cf. Eq. (2.12). Equation (3.12) represents, in such a case, an average of the change of time over scattering angles, weighted with the flux or cross section.

One can further see that the time delay of the forward wave, as derived in the last section, may be identified with $\Delta\tau_1^{\text{clas}} + \Delta\tau_2^{\text{clas}}$. The wave packet in the last section was of a transverse size $B = L_{\text{max}}/k$. We further assume that the length of the packet is W . The time for such a packet to move by the potential in the absence of interactions is $\tau_0 = W/v$. Using Eq. (2.16) in the limit of large L_{max} we obtain

$$\frac{\Delta\tau_f}{\tau_0} = \frac{\sum_{\ell}(2\ell+1)2\cos 2\delta_{\ell}\frac{d\delta_{\ell}}{dE}}{\frac{W}{v}\sum_{\ell}(2\ell+1)}. \quad (3.14)$$

For wide packets we can approximate $\sum_{\ell}(2\ell+1) \approx 2f\ell d\ell = k^2 B^2$ and, with the volume of a packet being equal to $V = \pi B^2 W$, we can rewrite (3.14) as

$$\frac{\Delta\tau_f}{\tau_0} = \frac{\sum_{\ell}(2\ell+1)\cos 2\delta_{\ell}\frac{d\delta_{\ell}}{dE}}{\frac{WB^2k^2}{v}} = \frac{\sum_{\ell}(2\ell+1)\cos 2\delta_{\ell}\frac{d\delta_{\ell}}{dE}}{\pi\rho_0}, \quad (3.15)$$

where ρ_0 is the density of states inside V . One can see that this agrees with (3.11).

Given a uniform many-body system, with density n and temperature T treated as independent variables, all intensive thermodynamic quantities can be obtained from the free energy per unit volume f . In terms of the correction to the density of states of relative motion in energy in (3.1), the free energy f , to the second order in the density, can be written as

$$f(n, T) = f_0(n, T) + \Delta P(n, T), \quad (3.16)$$

where f_0 is free energy for a noninteracting system and ΔP is the correction to the pressure [21,18]

$$P = P_0 + \Delta P = nT - Tn^2 \left(\frac{4\pi}{mT} \right)^{3/2} \frac{1}{2} \int dE e^{-E/T} \frac{1}{\pi} \times \sum_{\ell} (2\ell+1) \frac{d\delta_{\ell}}{dE}, \quad (3.17)$$

and where the effects of statistics are ignored. It can be verified by a direct calculation that the correction to pressure may be further expressed as

$$\begin{aligned} \Delta P &= \frac{1}{2} \int \frac{d\mathbf{p}_1}{(2\pi)^3} \frac{d\mathbf{p}_2}{(2\pi)^3} f(p_1)f(p_2) \\ &\quad \times \text{Re}\langle (\mathbf{p}_1 - \mathbf{p}_2)/2 | \mathcal{S} | (\mathbf{p}_1 - \mathbf{p}_2)/2 \rangle \\ &\quad - T \frac{1}{2} \int \frac{d\mathbf{p}_1}{(2\pi)^3} \frac{d\mathbf{p}_2}{(2\pi)^3} f(p_1)f(p_2) \int d\Omega \frac{d\sigma}{d\Omega} v \Delta\tau_s(\Omega). \end{aligned} \quad (3.18)$$

Here $f = e^{(\mu-E)/T}$ is phase-space occupancy. The first term on the rhs of (3.18) accounts for the forward time delay or mean field. The second term accounts for delay in scattering and, depending on the sign of $\Delta\tau_s$, allows further for an interpretation in terms of the reduction in the number of degrees of freedom or in terms of excluded volume.

B. Limitation of the considerations

Two important conclusions can be reached regarding the method of the previous section. First, the sum of time delays for scattered and forward-going waves is consistent with ergodic constraints. Second, the time delay of the forward-going wave is consistent with motion of a particle through a mean field. However, this consistency was derived assuming that the size of the region used to determine the densities was large. The limitations of this approximation are discussed below.

A problem with incorporating a mean field which depends on the number of particles within a given volume element, is that such field can result in classically bound states for attractive potentials, or impenetrable potential barriers for repulsive potentials. Considerations in this section required that the potential $u(E)$ was much smaller than any characteristic energy. This requires that $\Delta\rho \ll \rho_0$. For a sufficiently large volume V this is not a problem. However, for a finite V there exists phase space that is either bound (attractive potentials) or unavailable (repulsive potentials), of a magnitude

$$\Delta = \frac{V}{(2\pi)^3} \frac{4\pi}{3} [2mu(k=0)]^{3/2}. \quad (3.19)$$

On using $\sin\delta_0 \approx -ka$, where a is scattering length, for low k in the expression for optical potential (3.10), one finds that

$$\Delta = \frac{4}{3\pi^{1/2}} \frac{a^{3/2}}{V^{1/2}}. \quad (3.20)$$

Thus one finds that for a *strict* validity of our considerations the volume V containing a single scatterer must be chosen large compared to the scattering length. On examining Eq. (2.16) from the previous section, one finds that such a condition must be satisfied to allow for a proper definition of

τ_f . Scattering lengths are of the order of the interaction range, unless a resonance or bound state exist close to the threshold. Unfortunately, this is precisely the case for nucleon-nucleon scattering near threshold where scattering lengths approach 20 fm.

C. Scattering in the presence of third bodies

When considering the interaction of two particles in Secs. II and III A, we neglected the probability that a third body could interact with any of the two particles within the subvolume used to define the mean field. In Eq. (3.3) the contributions to the extra time spent within the subvolume, $\Delta\tau_1^{\text{clas}}$ and $\Delta\tau_2^{\text{clas}}$, arose because the particle trajectories were modified by the mean field. The first contribution arose because the kinetic energy and direction were altered on entering the mean field. The second contribution arose due to dependence of the mean field on momentum that led to the change of velocity by $du(E)/dE$. When many scatterings occur, the time spent in a given relative state does not just depend on trajectories and velocity, but further on the manner in which such state is populated and depopulated. If the population of different states is to be consistent with the first two of the time delays in Eq. (3.3) due to interactions, the scattering prescriptions need to be modified in the presence of third bodies.

Transition rates per unit time from an initial state are given by a transition matrix element to a final state squared multiplied by the final-state density in energy. For example, in the case of particles 1 and 3 scattering in the presence of particle 2, the final-state density would be obtained from a product of single-particle densities for 1 and 3. Latter densities, up to a factor, are identical with imaginary parts of single-particle Green's functions (3.8). When shifting the single-particle energies by mean fields generally dependent on relative momenta of 1 and 2, and 3 and 2, one precisely accounts for the change in the density of relative states, in feeding of the states. Besides the change of relative momenta due to the mean field that corresponds to $\Delta\tau_1^{\text{class}}$, the levels of 1 and 2 or 3 and 2 are pulled apart or pushed together when the mean field is energy dependent, changing the density that corresponds to $\Delta\tau_2^{\text{class}}$. Then the rates calculated with single-particle energies in the final density of states would yield a population of states consistent with these first two times in Eq. (3.3), if the particles could leave these states during the whole time such as obtained with an inclusion of the forward time delay or adoption of the mean field.

Ergodicity when many scatterings occur is discussed in more detail in the Appendix, together with the single-particle spectral densities. There, we show that the population of different states could be made consistent with an ergodic constraint involving all three delay times in (3.3), i.e., also the scattering delay, if one included in the Green's function (3.8) the imaginary part of the \mathcal{T} matrix and allowed for a separate dependence of the matrix on energy and relative momentum. Modification of the scattering or transition rates in terms of such complete spectral functions, nonetheless, might not be practical except for fully equilibrated situations. Also, it needs to be stated that a modification of the final-state density for two particles such as 1 and 3 on account of scattering with a third particle, *independent* of a modification

of matrix element for 1 and 3, might not be proper. With regard to scattering, correlations could be important, persisting throughout the interaction process.

It will be seen in the examples of Secs. V and VI that the contribution to the density of states from the mean field alone can be very significant. If scattering is then done in the presence of strong mean fields, it is important that matrix elements get modified too. In the case of momentum-independent mean fields, this amounts to the calculation of scattering rates in terms of kinetic particle energies only. Situations can be more cumbersome in the case of momentum-dependent fields as one generally loses the convenience of working in the rest frame of the scattering particles. A particularly strong momentum dependence of the mean field is expected for pions in nuclear matter due the derivative coupling to nucleons and deltas [22,23].

Rates and scattering prescriptions may be complicated when the time delay is negative. In such a case the prescription may effectively exclude a relative volume, e.g., an energy-dependent hard core. One may not want to fill the excluded phase-space volume in the scattering with a third body to be consistent with the ergodic theorem. Scattering prescriptions are investigated in Sec. VII, including one with a hard-core prescription and one where effective time delays are generated by correlating the outgoing scattering angle with the impact parameter.

D. Manipulating time delays

If one solely aims at satisfying the ergodic constraint, and thus properly reproducing thermodynamic properties of a system, while ignoring the physical differences behind the mean field or forward time delay and the delays for scattered waves, then one can absorb all interaction effects, in the lowest nontrivial order in density, exclusively into the mean field or, alternatively, into the delays for scattered particles. We shall illustrate our points by considering the correction to the pressure in (3.17) and (3.18).

Thus, from (3.2), (3.10), and (3.11), it follows that the density of two-particle states in energy would be properly reproduced when ignoring the delays for scattered waves and, in place of the mean field u in the center expression in (3.10), using a field u' given by (3.10) with $\sin 2\delta_\ell$ replaced by $2[\delta_\ell(E) - \delta_\ell(0)]$. As far as the correction to the pressure is concerned, this corresponds to rewriting the expression (3.18) as

$$\Delta P = \frac{1}{2} \int d\mathbf{p}_1 d\mathbf{p}_2 f(p_1)f(p_2) \times \langle (\mathbf{p}_1 - \mathbf{p}_2)/2 | \text{Re} \mathcal{T}' | (\mathbf{p}_1 - \mathbf{p}_2)/2 \rangle, \quad (3.21)$$

where

$$\langle p | \text{Re} \mathcal{T}' | p \rangle = \frac{2\pi v}{k^2} \sum_{\ell} (2\ell + 1) [\delta_\ell(0) - \delta_\ell(E)]. \quad (3.22)$$

The replacement of the sine by its argument in the field is actually a good approximation when the phase shifts are low compared to $\pi/4$. The general conclusion then is that the delays for scattered waves are relatively unimportant for the

thermodynamic properties when the phase shifts are low, no matter what are the values of these delays.

If the mean field were to be ignored, then, in order to properly reproduce the density of two-particle states, from (3.2) and (3.6), the mean delay time for scattering should be taken equal to

$$\Delta\tau'_s = \frac{\sum_{\ell}(2\ell+1)\frac{d\delta_{\ell}}{dE}}{2\sum_{\ell}(2\ell+1)\sin^2\delta_{\ell}}, \quad (3.23)$$

and for scattering in only one partial wave

$$\Delta\tau'_s = \frac{1}{2} \frac{d\delta_{\ell}}{\sin^2\delta_{\ell} dE}, \quad (3.24)$$

in place of (3.12). The correction to the pressure (3.18) is then rewritten as

$$\Delta P = -T \frac{1}{2} \int d\mathbf{p}_1 d\mathbf{p}_2 f(p_1)f(p_2)\sigma v \Delta\tau'_s. \quad (3.25)$$

Some advantage of an approach with delays put into scattering is that particles move with uniform velocities. One problem, though, is that the delay times $\Delta\tau'_s$ diverge at thresholds, where phase shifts go to zero linearly in the momentum with the coefficient of proportionality being equal to the negative of scattering length. In Sec. V when we evaluate resonant scattering and pion-nucleon scattering, we further discuss the implication of these various schemes. Now we turn to the role of statistics.

IV. TIME DELAYS AND STATISTICS

For any finite energy the density of states in energy increases by symmetrization and decreased by antisymmetrization. Corrections to thermodynamic quantities, such as the free-energy density or pressure, arise within the second order in density even in the absence of interactions. Symmetrization also affects scattering processes both in that the outgoing states may be Pauli blocked or Bose enhanced and in that the scattering amplitude may be internally modified [24]. In the following, we consider pressure in an equilibrated many-body system in terms of the \mathcal{T} matrix. In a nonequilibrium system, for low scattering rates, the \mathcal{T} -matrix approximation [25] in the single-particle equations of motion leads to the Boltzmann equation with rates corresponding to two-particle collisions, enhanced or reduced on account of statistics of final states and with medium-modified amplitudes. We assess implications for time delays and scattering processes in simulations, following from ergodicity.

The pressure in a many-body system at a given temperature T and chemical potential μ may be generally represented as [26]

$$P(\mu, T) = P_0(\mu, T) + \Delta P(\mu, T), \quad (4.1)$$

where

$$\begin{aligned} \Delta P(\mu, T) = & \frac{1}{2} \int \frac{d\mathbf{P}}{(2\pi)^3} \frac{d\mathbf{p}}{(2\pi)^3} dE_t \frac{1}{e^{(E_t - 2\mu)/T} - 1} \\ & \times \int_0^1 d\lambda \left(-\frac{1}{\pi} \right) \text{Im} \langle \mathbf{p} | \mathcal{T} G_{\lambda}(\mathbf{P}, E_t) (|\mathbf{p}\rangle \pm |-\mathbf{p}\rangle) \rangle. \end{aligned} \quad (4.2)$$

Here \mathcal{T} is the interaction, \mathbf{p} and \mathbf{P} are relative and total momenta, respectively, E_t is the total energy, and G_{λ} is the two-particle Green's function within a system with the interaction scaled down by a factor of λ . The negative of the imaginary part of this function, divided by π , plays the role of the two-particle spectral function. The statistical factor in (4.2) is bosonic, as is appropriate for a state of two particles with the same statistics. The apparent change in sign of the correction to the pressure above compared to (3.17), is associated with the fact that there the pressure is expressed as a function of density while in (4.2) it is expressed as a function of μ .

In the \mathcal{T} -matrix approximation [25] the two-particle Green's function satisfies

$$G = G_0 + G_0 \mathcal{T} G, \quad (4.3)$$

and explicitly

$$\begin{aligned} \langle \mathbf{k} | G(\mathbf{P}, E_t) | \mathbf{k}_1 \rangle = & \langle \mathbf{k} | G_0(\mathbf{P}, E_t) | \mathbf{k}_1 \rangle \\ & + \int \frac{d\mathbf{k}_2}{(2\pi)^3} \frac{d\mathbf{k}_3}{(2\pi)^3} \langle \mathbf{k} | G_0(\mathbf{P}, E_t) | \mathbf{k}_2 \rangle \\ & \times \langle \mathbf{k}_2 | \mathcal{T} | \mathbf{k}_3 \rangle \langle \mathbf{k}_3 | G(\mathbf{P}, E_t) | \mathbf{k}_1 \rangle. \end{aligned} \quad (4.4)$$

The noninteracting Green's function in the above is equal to

$$\langle \mathbf{p} | G_0(\mathbf{P}, E_t) | \mathbf{p}' \rangle = (2\pi)^3 \delta(\mathbf{p} - \mathbf{p}') \frac{N(\mathbf{p}, \mathbf{P})}{E_t - P^2/4m - p^2/m + i\epsilon}. \quad (4.5)$$

The factor of N stems from an equal-time commutator of the operators for two particles,

$$\begin{aligned} N(\mathbf{k}, \mathbf{P}) = & [1 \pm f(\mathbf{P}/2 + \mathbf{k})][1 \pm f(\mathbf{P}/2 - \mathbf{k})] \\ & - f(\mathbf{P}/2 + \mathbf{k})f(\mathbf{P}/2 - \mathbf{k}) \\ = & 1 \pm f(\mathbf{P}/2 + \mathbf{k}) \pm f(\mathbf{P}/2 - \mathbf{k}), \end{aligned} \quad (4.6)$$

and the upper signs refer to bosons and lower to fermions. The \mathcal{T} matrix and Green's function are related with

$$\mathcal{T} = \mathcal{T}' + \mathcal{T}' G \mathcal{T}', \quad (4.7)$$

and thus the \mathcal{T} matrix satisfies

$$\mathcal{T} = \mathcal{T}' + \mathcal{T}' G_0 \mathcal{T}. \quad (4.8)$$

The factor of N in G_0 in the above equation, on considering the case of a resonance, can be related to the fact that, for a bosonic two-particle state, the width is equal to the difference between the decay and the formation rates [25].

On integrating in (4.2), we obtain, from (4.3),

$$\begin{aligned}
& \int_0^1 d\lambda \operatorname{Im} \langle \mathbf{p} | \mathcal{V} G_\lambda(|\mathbf{p}\rangle \pm |-\mathbf{p}\rangle) \\
&= \operatorname{Im} \langle \mathbf{p} | \sum_{n=1}^{\infty} \frac{1}{n} (\mathcal{V} G_0)^n (|\mathbf{p}\rangle \pm |-\mathbf{p}\rangle) \\
&= -\operatorname{Im} \langle \mathbf{p} | \ln(1 - \mathcal{V} G_0) (|\mathbf{p}\rangle \pm |-\mathbf{p}\rangle) \\
&= \langle \mathbf{p} | \arctan(\mathcal{V}(1 - \mathcal{V} \operatorname{Re} G_0)^{-1} \operatorname{Im} G_0) (|\mathbf{p}\rangle \pm |-\mathbf{p}\rangle) \\
&= \langle \mathbf{p} | \arctan(\mathcal{R} \operatorname{Im} G_0) (|\mathbf{p}\rangle \pm |-\mathbf{p}\rangle), \tag{4.9}
\end{aligned}$$

where \mathcal{R} satisfies

$$\mathcal{R} = \mathcal{V} + \mathcal{V} \operatorname{Re} G_0 \mathcal{R}. \tag{4.10}$$

On introducing then the matrix $\tilde{\mathcal{R}}$ that is Hermitian in the spherical angle and may be diagonalized,

$$\begin{aligned}
\tilde{\mathcal{R}}(p, \Omega, \Omega', \mathbf{P}) &= \operatorname{sgn}(E_t - 2\mu) |N(p, P, \Omega) N(p, P, \Omega')|^{1/2} \\
&\quad \times \langle p, \Omega | \mathcal{R}(\mathbf{P}, E_t) | p, \Omega' \rangle \\
&= \sum_n r_n(p, P) \mathcal{Y}_n(p, P, \Omega) \mathcal{Y}_n^*(p, P, \Omega'), \tag{4.11}
\end{aligned}$$

where $E_t = P^2/4m + p^2/m$, and $\{\mathcal{Y}_n\}$ form an orthonormal set in spherical angle (with a definite symmetry under inversion), we can rewrite (4.2) as

$$\begin{aligned}
\Delta P(\mu, T) &= \frac{1}{2} \int \frac{d\mathbf{P}}{(2\pi)^3} \frac{dE}{\pi} \frac{1}{e^{(E + P^2/4m - 2\mu)/T} - 1} \\
&\quad \times \sum_n \delta_n(p, P), \tag{4.12}
\end{aligned}$$

where $\delta_n = \operatorname{atan}(-p^2 r_n / 8\pi^2 v)$.

In terms of the phase shifts δ_n introduced above, the on-shell \mathcal{S} matrix can be expressed as

$$\begin{aligned}
\langle p, \Omega | \mathcal{S}(\mathbf{P}, E_t) | p, \Omega' \rangle &= -\frac{8\pi^2 v}{p^2} \operatorname{sgn}(E_t - 2\mu) \\
&\quad \times |N(p, P, \Omega) N(p, P, \Omega')|^{-1/2} \\
&\quad \times \sum_n \sin \delta_n e^{i\delta_n} \mathcal{Y}_n(p, P, \Omega) \\
&\quad \times \mathcal{Y}_n^*(p, P, \Omega'). \tag{4.13}
\end{aligned}$$

On carrying partial integrations in (4.12), the correction to the pressure may be decomposed into the mean-field and scattering contributions that take the form, in terms of the \mathcal{S} matrix,

$$\begin{aligned}
\Delta P(\mu, T) &= -\frac{1}{2} \int \frac{d\mathbf{p}_1}{(2\pi)^3} \int \frac{d\mathbf{p}_2}{(2\pi)^3} f(p_1) f(p_2) \\
&\quad \times \operatorname{Re} \langle \mathbf{p} | \mathcal{S}(\mathbf{P}, e(p_1) + e(p_2)) (|\mathbf{p}\rangle \pm |-\mathbf{p}\rangle) \\
&\quad + \frac{1}{2} \int \frac{d\mathbf{P}}{(2\pi)^3} \frac{P^2}{6m} \int \frac{d\mathbf{p}}{(2\pi)^3} \int d\Omega \\
&\quad \times \left(f(p_1) f(p_2) \frac{d\sigma}{d\Omega} v \Delta \tau_s [1 \pm f(p'_1)] [1 \pm f(p'_2)] \right. \\
&\quad \left. - f(p_1) f(p_2) \frac{d\sigma}{d\Omega} v \Delta \tau_s f(p'_1) f(p'_2) \right), \tag{4.14}
\end{aligned}$$

where $f = (e^{[e(p) - \mu]/T} \mp 1)^{-1}$, $d\sigma/d\Omega = (m/4\pi)^2 |\langle \mathbf{p} | \mathcal{S}(\mathbf{P}, E_t) (|\mathbf{p}'\rangle \pm |-\mathbf{p}'\rangle)|^2$, integration is over the spherical angle of 2π , and the time delay for scattering is

$$\begin{aligned}
\Delta \tau_s &= \left(\frac{\partial}{\partial(p^2/m)} - \frac{\partial}{\partial(P^2/4m)} \right) \\
&\quad \times \operatorname{Im} [\ln \langle \mathbf{p} | \mathcal{S}(\mathbf{P}, E_t) (|\mathbf{p}'\rangle \pm |-\mathbf{p}'\rangle)]. \tag{4.15}
\end{aligned}$$

Following (4.1) and (4.14), in order to produce proper changes in the pressure in simulations, associated with two-particle interactions, it is necessary to include the effects of the mean field on particle motion, and to delay the collision processes, according to the expressions in terms of the \mathcal{S} matrix, with an internal symmetrization and symmetrization with other particles in the medium accounted for in the final and intermediate states [Eqs. (4.8), (4.5), (4.14), and (4.15)]. Besides delaying direct collisions, where two particles alter their momenta and spins, by $\Delta \tau_s$, it is necessary to delay exchange collision processes, where pairs of particles meet and interchange pairwise quantum numbers, by $-\Delta \tau_s$. (The latter holds for particles of one statistics. In the case of particles of opposite statistics, the exchange collisions should be delayed by $\Delta \tau_s$.) The exchange collisions may be thought of as processes [26] where two particles collide and, while in an intermediate 2p-2h state, encounter two more particles, ending up in the interchange of the quantum numbers. The cross section, from (4.14), is the same as for the direct collisions. Notably, there is no room for the exchange collisions in the Boltzmann equation that ignores the duration of interactions, since these processes leave the occupations of single-particle states unaltered. These processes should, nonetheless, appear in a possible quantum Enskog equation, since their duration affects thermodynamic quantities.

V. RESONANCE SCATTERING

A. Sharp Breit-Wigner resonance

An obvious example, that can serve to illustrate the time delays and different prescriptions, is that involving a sharp resonance. If the width of the resonance Γ is small compared to its energy E_R , then the phase shift in the vicinity of E_R is given by

$$\tan \delta = -\frac{\Gamma/2}{E - E_R}. \tag{5.1}$$

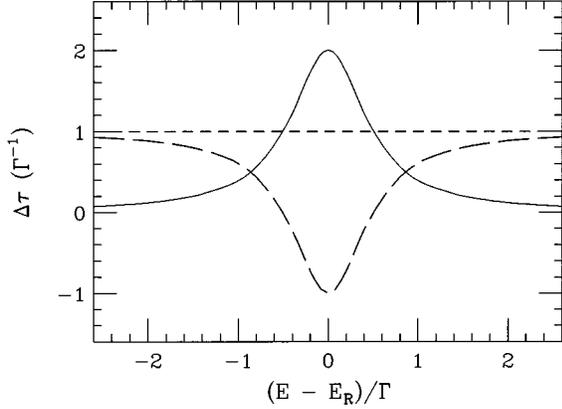


FIG. 1. Time delays in the case of a Breit-Wigner resonance as a function of energy from the resonance divided by the width. The solid line represents the time for the scattered wave $\Delta\tau_s$. The short-dashed line represents the time $\Delta\tau'_s$ which is ergodically consistent when the delay for forward wave or mean field are neglected. Finally, the long-dashed line shows the time delay for the forward wave divided by the fraction of the incoming wave that is scattered, $\Delta\tau'_s - \Delta\tau_s$ [cf. Eq. (5.3)].

This yields the following time delays for the scattered and forward-going waves, respectively,

$$\Delta\tau_s = \frac{d\delta}{dE} = \frac{\Gamma}{2[(E - E_R)^2 + \Gamma^2/4]}, \quad (5.2)$$

and

$$\Delta\tau_f \times \frac{\pi B^2}{\sigma} = \Delta\tau'_s - \Delta\tau_s = \frac{(E - E_R)^2 - \Gamma^2/4}{\Gamma[(E - E_R)^2 + \Gamma^2/4]}, \quad (5.3)$$

where $\Delta\tau_f$ is the time delay of the forward-going wave packet with total cross-sectional area $\pi B^2 = (\pi/k^2) \Sigma_\ell(2\ell + 1)$. Figure 1 illustrates the different times. It is seen that the delay for the forward-going wave turns negative in the vicinity of the resonance. For light in a dielectric medium [27] this corresponds to the increase in group velocity for packets with resonant frequencies.

The energy-averaged delay for the forward-going wave $\Delta\tau_f$ is zero. (This may be expected whenever phase-shift variation is limited to a narrow range in energy.) Weighted with the cross section, the average delay time for scattered waves over energy is equal to the inverse width, coinciding with naive expectations. The actual delay time for scattered waves (5.2) is twice as high at the resonance, see also [28], and it drops rapidly with energy when going away from the vicinity of that resonance.

The result that the time delay equals the inverse width is also obtained when putting all delays into scattering, from (5.2) and (5.3),

$$\Delta\tau'_s = \frac{1}{\Gamma}. \quad (5.4)$$

It is now a common prescription in relativistic simulations to use an energy-independent delay given by the inverse width. Provided that particles are not also propagated through a mean field and resonances are indeed of a Breit-Wigner

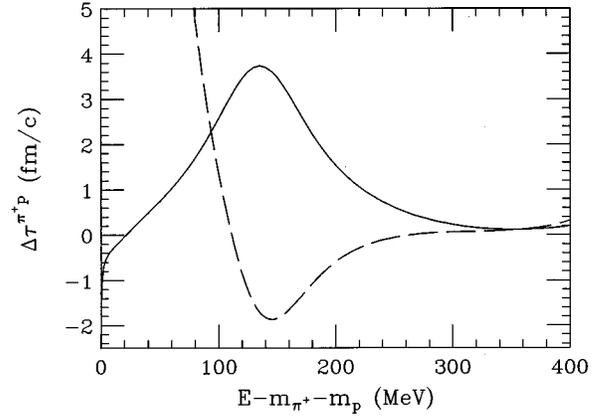


FIG. 2. Time delays for a π^+p system as a function of c.m. kinetic energy. The solid line represents the time delay for the scattered wave averaged over angles and spin directions, $\Delta\tau_s$. The dashed line represents the forward time delay averaged over spin directions and divided by the fraction of the incoming wave that is, on the average, scattered, $\Delta\tau'_s - \Delta\tau_s$.

form, such a prescription would yield correct thermodynamic functions up to the second order in density.

B. $\pi N\Delta$ system

Different resonances in a πN system may be identified as independent particles. For the lowest P_{33} Δ resonance, the width is comparable to the energy of the resonance above the πN threshold and, as such, this width exhibits a significant energy variation. An interacting system of pions, nucleons, and deltas, is of considerable interest for heavy-ion collisions in the beam-energy range from few hundred MeV/nucleon to few GeV/nucleon.

In this section we address three issues. First, by studying πN phase shifts we calculate time delays and indicate differences with the Breit-Wigner case above. Second, we point out that a quantum decomposition of the effective increase of the density of states represented by the time delay would include contributions from *both* the Δ and πN components. Finally, we point out a practical difficulty in separating the Δ and πN components.

Time delays can be calculated given the experimentally determined πN phase shifts [29,30]. The delay of the forward wave [divided by the fraction of particles that scatter as in (5.3)] and the delay of the scattered wave are shown for a π^+p system in Fig. 2. In many prescriptions, time delays are only incorporated into scattering events, which would mean that the combination of the two contributions $\Delta\tau'_s$ is appropriate. One should note that this combination differs significantly from the Breit-Wigner result and is extremely divergent at threshold due to a rapidly declining cross section, cf. Sec. III D. If the mean field is consistently incorporated into a simulation, the appropriate delay is $\Delta\tau_s$ which behaves as the derivative of the phase shift with respect to energy which is approximately the scattering length divided by the velocity in the vicinity of the threshold. This threshold divergence is much weaker than that of $\Delta\tau'_s$.

The imaginary part of a Δ Green's function in a thermal system gives the number of states for the resonance per unit

energy and volume, $\Delta\rho'' = -\text{Im}g_\Delta/\pi$ [31,25]. The requirement then of a consistency with the number of colliding πN pairs gives the time $\Delta\tau_s''$ during which the πN pair should turn into the resonant particle,

$$\frac{\Delta\rho''(E)}{\rho_0(E)} = \frac{\sigma(E)v\Delta\tau_s''}{V}, \quad (5.5)$$

with a result that is the inverse of resonance width [32,33],

$$\Delta\tau_s'' = \frac{1}{\Gamma(E)}. \quad (5.6)$$

This time differs from $\Delta\tau_s'$, such as in Eq. (3.24), that would, in particular, involve the energy derivative of Γ ; likewise $\Delta\rho''$ differs from $\Delta\rho$. Interestingly, within any single spin-isospin channel, either correction to the density of states, $\Delta\rho$ or $\Delta\rho''$, integrates over energy to unity, i.e., one net state is gained. For sharp resonances, with couplings and widths independent of energy, there is no difference between $\Delta\tau_s'$ and $\Delta\tau_s''$, as is apparent from Sec. V A, and there is no difference between $\Delta\rho$ and $\Delta\rho''$.

On studying the density of states for pions or nucleons as in the Appendix, one finds a change, per πN pair, that is equal to $\Delta\rho(E) - \Delta\rho''(E)$, where $\Delta\rho = (1/\pi)(d\delta/dE)$ in any single channel, i.e., one that precisely compensates the discrepancy above. The same type of discrepancy and compensation is found when applying the considerations to a system of pions and rho mesons, where $\pi + \pi \leftrightarrow \rho$ reactions take place. If one were to ask about, in the last system, how many ρ mesons decay into dilepton pairs, the answer would involve the density of rho states within the system, rather than the overall change in the density of states associated with the resonance formation, important for thermodynamic considerations. For certain questions one has to keep in mind that the time delays derived before correspond to the change in the overall density of states and not necessarily to the existence of the resonant particles.

The time for the conversion into a resonant particle in scattering (5.6) may diverge strongly when threshold is approached, which parallels the situation when the overall delay time associated with the interaction is forced onto the scattering. [The conversion time for a spherical wave, that should be identified as $\Delta\tau_{sph} = 2\pi\Delta\rho'' \propto \Gamma(E)$, tends to zero at the threshold.] In practice, manipulations of the conversion time, dividing this time between the scattered and forward waves, may pose more difficulty than the manipulations of the overall delay time, as negative conversion times cannot be simulated.

C. *s*-channel scattering of massless partons

An example, where time delays associated with interaction are relevant, is the collision of partons in ultrarelativistic nuclear reactions. Partons are copiously produced early in reactions and the goal of simulating partonic cascades [34–36] is to determine the equilibration time scale and initial equilibrated energy density. Most partons at midrapidity are produced far off shell and decay via bremsstrahlung. Thus, quantum considerations are necessary to establish the duration of processes.

While we shall not tackle the general problem here, we shall try to gain insight by considering the simplified example of elastic scattering of two massless partons in the *s* channel, assuming that the intermediate particle is massless. This turns out to be quite similar to the case of πN scattering close to the threshold. Since there are no energy scales, to lowest order in perturbation theory the phase shift must depend only on the coupling constant α ,

$$\tan\delta = -c\alpha. \quad (5.7)$$

Then, the overall time delay for a spherical wave from (5.7) is zero. This peculiar result will arise from any theory with no energy scale since phase shifts are dimensionless.

However, QCD acquires a scale Λ through renormalization that gives the coupling constant an energy dependence [37]:

$$\tan\delta = c\alpha(E) = c \frac{4\pi}{\beta_0 \ln(E^2/\Lambda^2)}. \quad (5.8)$$

With this, the time delay for spherical waves becomes

$$\Delta\tau_{sph} = 2 \frac{d\delta}{dE} = \frac{\beta_0}{c\pi E} \sin^2\delta = \frac{\beta_0}{c\pi E} \frac{c^2\alpha(E)^2}{1 + c^2\alpha(E)^2}. \quad (5.9)$$

If all the time delay is put into the scattered wave, as in Sec. III D, then the correct time delay for the scattered wave acquires a particularly simple form

$$\Delta\tau_s' = \frac{\beta_0}{4\pi c E}. \quad (5.10)$$

Note that the time delay does not involve the coupling constant and scales proportional to the inverse energy. If one chose the time delay equal to the inverse width for the intermediate state, then one would certainly have obtained a time proportional to $1/(\alpha E)$, as the width would be proportional to α .

Since an *s*-channel scattering involves an intermediate state very far from being on-shell, the questions involving the time delay for such a process may not be so crucial since these processes are rather rapid. Of greater concern is the formation of partons through bremsstrahlung involving intermediate states which are nearly on shell. Since such processes create the majority of soft particles in an ultrarelativistic *pp* collision, the issue of when and where such particles appear can greatly affect estimates of the initial thermalized energy density. Unfortunately, such two to three or more particle processes are outside the scope of this analysis, but similar problems have been addressed in the context of decaying hadronic resonances [38].

VI. NUCLEON-NUCLEON INTERACTION

The nucleon-nucleon system is one for which the quantum-mechanical scattering-amplitudes have been most carefully measured in physics. It represents the most relevant case of scattering for heavy-ion physics, where semiclassical simulations utilizing single-nucleon degrees of freedom are commonly used to model heavy-ion reactions. At moderate densities and high temperatures, when cluster formation is

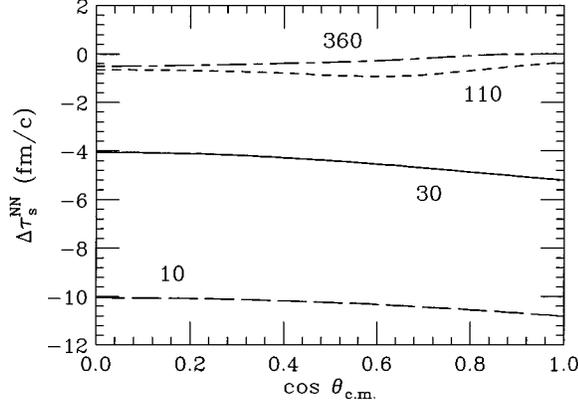


FIG. 3. Spin-isospin averaged time delay for NN scattering as a function of the cosine of c.m. scattering angle, at several values of laboratory kinetic energy indicated in the figure in MeV.

unlikely, it may be reasonable to assume that nucleons interact two at a time. Using phase shifts inferred from scattering data, one can calculate quantum-mechanical scattering amplitudes and determine the appropriate time delays following the prescriptions outlined in the previous sections.

First we present the calculation of the time delay for the scattered wave at a given angle, $\Delta\tau_s(\theta)$, when averaging over the spin and isospin directions. Due to antisymmetrization and the conservation of angular momentum, isospin, and parity, the magnitude of the net nucleon spin is conserved in NN interactions. The $S=0$ amplitude for a given isospin is given by

$$f^{S=0}(\theta) = -\frac{1}{k} \sum_{\ell,j} (2\ell+1) P_{\ell}(\cos\theta) \mathcal{T}_{\ell}, \quad (6.1)$$

where only even or odd values of ℓ are included. That is compensated by the factor before the sum in (6.1) being twice as large as in (2.4). Given the conservation laws, the $S=1$ amplitude is of the general form,

$$\begin{aligned} f_{\mu\mu'}^{S=1}(\theta, \phi) &= -\frac{1}{k} \sum_{\ell} \sqrt{4\pi(2\ell+1)} \langle \ell 0 1 \mu' | j \mu \rangle \\ &\quad \times \langle \ell' (\mu - \mu') 1 \mu' | j \mu \rangle \\ &\quad \times Y_{\ell' \mu - \mu'}(\theta, \phi) \mathcal{T}_{\ell \ell' j}, \end{aligned} \quad (6.2)$$

where $\mathcal{T}_{\ell \ell' j} = i(S_{\ell \ell' j} - \delta_{\ell \ell'})$, and for the coupled waves diagonal matrix elements are $S_{\ell \ell} = \cos 2\bar{\epsilon}_j \exp 2i\bar{\delta}_{j\ell}$, and off-diagonal elements $S_{\ell \ell'} = i \sin 2\bar{\epsilon}_j \exp i(\bar{\delta}_{j\ell} + \bar{\delta}_{j\ell'})$, where $\bar{\epsilon}$ is mixing parameter. In carrying calculations up to a laboratory energy of $E_{\text{lab}} = 400$ MeV, we use all partial waves with both ℓ and j less than 5. The mixing of waves is not very strong in this region. The phase shifts are generated using a potential model that had been carefully fitted to describe the NN data [39].

Using Eq. (2.14), one obtains a delay time $\Delta\tau_s$ that depends on the scattering angle. This time is shown by different lines in Fig. 3 for several values of E_{lab} . Due to the averaging over initial spin and isospin and the amplitude antisymmetrization, the time is symmetric with respect to 90° . The time, averaged over angles, is additionally shown as a func-

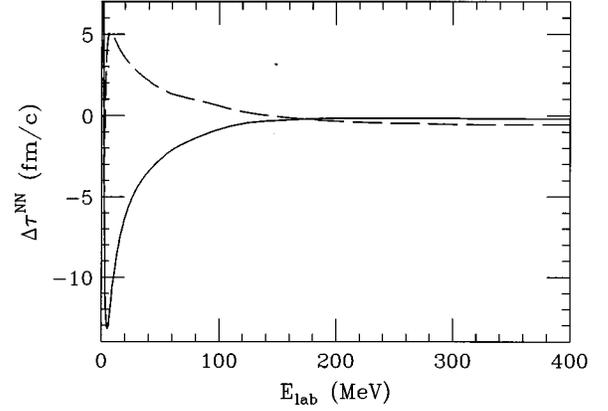


FIG. 4. Time delays for NN system as a function of laboratory kinetic energy. The solid line represents the time for the scattered wave $\Delta\tau_s$ averaged over the scattering angle and the spin and isospin directions. The dashed line represents the time for the forward wave, averaged over spin and isospin directions and divided by the fraction of incident wave scattered, $\Delta\tau'_s - \Delta\tau_s$.

tion of the laboratory energy by a solid line in Fig. 4, together with the forward delay time from Eq. (2.19). The observed negative delay times for scattered waves reflect the negative derivatives of S wave and other phase shifts with respect to energy, weighted in the average time with contributions to the cross section. The falling phase shifts make the interaction, with regard to scattering, effectively repulsive above $E_{\text{lab}} \sim 2.5$ MeV. Notably, the NN interaction is often *only* considered repulsive when phase shifts are predominantly negative, although the energy derivatives of the phase shifts also necessitate consideration. Both the $T=0$ and $T=1$ phase shifts fall with energy, as the Levinson's theorem requires that the deuteron formation in $T=0$ channel and enhancement of the density of states in the d^* region in $T=1$ channel be compensated by a depletion in states at higher energies. In semiclassical considerations, the delay time for scattering should be limited from below by $-2d/v$, where d is interaction range and v is relative velocity. While the negative delay times in Fig. 4 decrease in magnitude with an increasing laboratory energy, their decrease is faster than implied by the above limit. At very low energies, the times for the scattered waves become positive. At $E_{\text{lab}} \lesssim 100$ keV they begin to be governed by the singlet scattering length, $\Delta\tau_s \approx -a_s/v$.

For comparison of the angular dependence, the delay time for a hard-sphere repulsive-scattering (discussed more in the next section) as a function of the scattering angle is

$$\Delta\tau_s(\theta) = -\frac{2d}{v} \sin \frac{\theta}{2}, \quad (6.3)$$

and averaged over forward and backward directions, given the constant scattering cross section,

$$\bar{\Delta}\tau_s(\theta) = \frac{1}{2}(\Delta\tau_s(\theta) + \Delta\tau_s(\pi - \theta)) = -\frac{\sqrt{2}d}{v} \cos\left(\frac{\pi}{4} - \frac{\theta}{2}\right). \quad (6.4)$$

Correspondingly, for repulsive scattering, more negative delay times might be expected at $\theta=90^\circ$ than at $\theta=0$. Indeed, that is observed in NN scattering at the higher laboratory energies. In fact, in the periphery the interaction might be expected attractive and the delay times might be expected to turn to zero or even positive in the forward directions, and not just decline in magnitude as for hard-sphere scattering, and this can be seen for the 360 MeV scattering in Fig. 3. In passing, let us note that to properly isolate forward and backward directions, constructing an amplitude prior to the antisymmetrization, one should continue the phase shifts over the missing partial waves. If one were to identify a hard-sphere radius d for simulations from the delay at 90° , quite low values would have been obtained compared to what was used in simulations [16], declining from $d=0.60\text{--}0.80$ fm for E_{lab} within the range 10–30 MeV to $d=0.15\text{--}0.30$ fm for E_{lab} within the range 100–400 MeV. At low energies, the times become more negative at 0° than at 90° , and this is due to ${}^3S_1\text{--}{}^3D_1$ interference.

The forward delay times are positive in a wide energy range $3 \leq E_{\text{lab}} \leq 150$ MeV, see Fig. 4. In the lower portion of the range, this is due to the fact that, for large S -wave phase shifts, the real forward amplitude, multiplied by a relative momentum, increases, although the S -wave phase shifts decrease. In the higher portion of the above energy range, when S -wave contributions are low, the forward delay times are positive due to the positive energy derivatives of phase shifts for some high partial waves which, unlike in the delays for scattered waves, are not weighted by partial cross sections in the forward direction.

Of some interest is the issue of elastic NN interactions at very high energies when amplitudes are primarily diffractive [17]. Schematically, a purely diffractive amplitude may be represented, given $S_\ell=0$ for $\ell \leq \ell_c$ and $S_\ell=1$ for $\ell > \ell_c$, as

$$f(\theta) = \frac{i}{2k} \sum_{\ell=0}^{\ell_c} (2\ell+1) P_\ell(\cos\theta). \quad (6.5)$$

As a diffractive amplitude is purely imaginary, its phase does not depend on energy and the time delays for the elastically scattered waves identically vanish, cf. (2.14). Likewise, the times for the forward waves (2.19) vanish. This is consistent with the concept of particles moving freely around the interaction region.

We conclude this section with a presentation of the pressure in a low density nuclear matter at moderate temperatures, as a function of the density and temperature, such as should be, generally, reproduced in simulations. Within the second order in density the contributions to pressure (beyond the free-gas term $P_0 = n_B T$) come from nucleon antisymmetrization, formation of deuterons, and nucleon-nucleon scattering,

$$P = n_B T \left(1 + a_2(T) n_B \left(\frac{2\pi}{mT} \right)^{3/2} \right), \quad (6.6)$$

where the three respective contributions to the virial coefficient $a_2(T)$ are given by

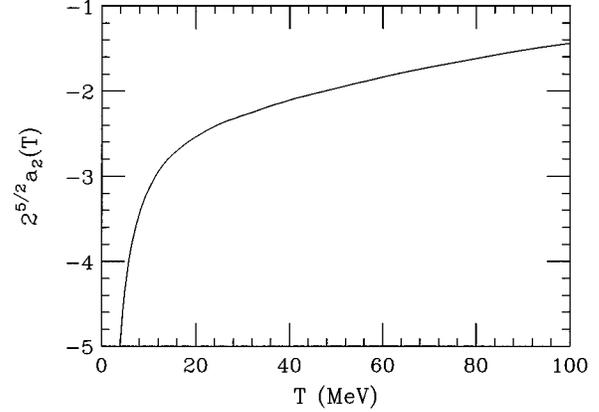


FIG. 5. Second virial coefficient for nuclear matter, multiplied by $2^{5/2}$, from Eq. (6.7), as a function of temperature.

$$2^{5/2} a_2(T) = \frac{1}{4} - 3 e^{B_d/T} - \sum_{Tj/S} (2T+1)(2j+1) \times \int \frac{dE}{2\pi} 2 \frac{d\delta_{j/S}^{TS}}{dE} e^{-E/T}, \quad (6.7)$$

and B_d is the deuteron binding energy. Antisymmetrization increases the pressure, deuteron formation lowers the pressure, while at most temperatures, scattering increases the pressure. The overall effect of interactions, following Levinson's theorem, declines with the increase of temperature. The second virial coefficient (6.7) is shown as a function of temperature in Fig. 5.

VII. DELAYS IN SIMULATIONS

A. Effect of scattering prescriptions

Without explicitly delaying or advancing particles as they pass near each other within a simulation, the time spent by particles in the vicinity of one another can be affected by the scattering prescription. The prescription can make $\Delta\tau_s$ positive or negative. Effects of scattering prescriptions on macroscopic features of reaction dynamics at Bevalac energies have been investigated in Refs. [13–16], see also [40]. We analyze two examples, hard sphere scattering and scattering at the point of closest approach.

Our first example is that of hard-sphere two-particle scattering. Given a volume in relative coordinates of radius R , and a hard-sphere potential that rises as particles are a distance d away, the expected reduction in the density of two-particle states within the relative volume, due to scattering, becomes $\Delta\rho/\rho_0 = \Delta\tau^{\text{coll}}/\tau_0 = -d^3/R^3$. Particles that make contact along a line at an angle α to the direction of original relative motion, get deflected by an angle $\theta = \pi - 2\alpha$. When reaching the boundary of the relative volume defined with the radius R , the particles traverse a relative distance that is altered by the scattering. The alteration divided by the relative velocity, gives the change in the time spent in the vicinity of the other particle, $\Delta\tau_s(b)$, that depends on impact parameter and can be worked out from geometry,

$$\Delta \tau_s(b) = -\frac{2\sqrt{d^2-b^2}}{v} = -\frac{2d \cos\alpha}{v} = -\frac{2d}{v} \sin \frac{\theta}{2}. \quad (7.1)$$

The average change in time due to scattering is then given by an integral over the product of the probability density that a specific scattering occurred, times the change in time in that scattering,

$$\Delta \tau^{\text{coll}} = \frac{\int db b \Delta \tau_s(b)}{\int db b} = -\frac{d^2}{R^2} \frac{4}{3} \frac{d}{v}. \quad (7.2)$$

In the last expression, the factors d^2/R^2 and $(4/3)d/v$ represent, respectively, the probability that a collision occurs and the average time lost then in a collision. The average time spent within the volume of radius R follows from dividing the volume by cross-sectional area and velocity $\tau_0 = (4\pi/3)R^3/\pi R^2 v = (4/3)R/v$, and we find that $\Delta \tau^{\text{coll}}/\tau_0 = -d^3/R^3$, as we expected. The pressure corresponding to (6.3), (7.1), and (7.2), in the absence of statistical effects, from (3.17) and (3.18), is

$$P = nT + n^2 T \frac{2\pi d^3}{3}. \quad (7.3)$$

Positive delay times are obtained when scattering the particles as if off a thin spherical shell of size d open in the direction of motion (the case of a concave rather than convex mirror). Then expressions (7.1) and (7.2) remain valid but with changed signs.

Within the most common prescription for scattering in a simulation, it is assumed that particles scatter when they come abreast of each other, at a distance $b < d = \sqrt{\sigma/\pi}$. When deflected in a direction making an angle θ relative to the original direction, within a plane at an azimuthal angle ϕ with respect to the original reaction plane, the particles reach a distance $R \gg d$ after a time longer by

$$\Delta \tau_s(b, \Omega) = -\frac{b}{v} \sin\theta \cos\phi, \quad (7.4)$$

than in the absence of scattering. If the scattering is repulsive ($\phi=0$) and isotropic, i.e., $\cos\theta$ distribution is flat, then the average delay time for a given impact parameter becomes equal to

$$\Delta \tau_s(b) = -\frac{\pi b}{2v}. \quad (7.5)$$

By averaging over all impact parameters one further gets

$$\Delta \tau^{\text{coll}} = -\frac{d^2}{R^2} \frac{\pi}{3} \frac{d}{v}. \quad (7.6)$$

Notably, the time lost in any one collision is reduced here by only a factor $\pi/4$ compared to hard-sphere scattering. By choosing $\phi = \pi$ in collisions, one can produce positive delay times.

Generally, given required delay times such that $|\Delta \tau_s| < (2/3)d \langle \sin\theta \rangle = (\Delta \tau_s)_{\text{max}}$, these times may be generated making a fraction ν of all scatterings repulsive and a fraction $1 - \nu$ attractive. This fraction is given by

$$\nu = \frac{1}{2} \left(1 - \frac{\Delta \tau_s}{(\Delta \tau_s)_{\text{max}}} \right). \quad (7.7)$$

B. Numerical determination of equations of state and transport coefficients

While we have limited ourselves to the discussion of effects of two-particle interactions on thermodynamic properties, many-body calculations can provide information accounting for interactions of a few particles at a time [10,12]. The prescriptions for interactions in simulations may affect microscopic thermodynamic quantities within a higher order than the second in density and they can also affect transport coefficients. Given the prescriptions, thermodynamic quantities, and transport coefficients for simulations can be determined numerically and confronted with those from fundamental calculations.

All thermodynamic quantities can be derived once one knows the pressure as a function of the chemical potential and temperature, $P(\mu, T)$. To determine the pressure, the system may be enclosed in a box of macroscopic volume V , in contact with a free noninteracting gas with of chemical potential μ and temperature T , possibly only within some external potential lower than μ . The contact with the gas can be made through the walls in one direction, and in two remaining directions periodic conditions may be used. If clusters are produced within the simulation, then the interfaces to the free gas can be made impermeable to those. Nucleons not in a cluster, on the other hand, getting into the free zone, would never return. At the same time, nucleons from the free zone with equilibrium phase-space distribution for given μ and T with the inclusion of statistics, would pour in into the box. The pressure within the box could be then computed using the following virial-type expression with terms for different possible ways of accounting for interactions in a simulation:

$$P = \frac{1}{\tau V} \left\{ \frac{1}{3} \left(\int dt \sum_j \mathbf{p}_j \cdot \mathbf{v}_j - \sum_{i < j} \mathbf{p}_{ij} \cdot \mathbf{v}_{ij} \Delta \tau_{ij}^{jj} \right) + \int dt \sum_{i < j} \mathbf{F}_{ij} \cdot \mathbf{r}_{ij} + \sum_{i < j} \Delta \mathbf{p}_{ij} \cdot \mathbf{r}_{ij} \right) + \int dt \int dV \left(\rho U - \int_0^{\rho(t)} d\rho' U \right) \right\}. \quad (7.8)$$

The above equation is limited to the mean field being momentum independent.

With regard to (7.8), pressure is recognized as the density of momentum flux in equilibrium, in any one direction. In (7.8) the pressure is evaluated by taking a trace of the momentum flux tensor and dividing it by 3 for the three directions; τ is the time over which the system is investigated. The first term on the rhs of (7.8), with a sum over particles in a box, accounts for the transport of momentum when particles move. The second term, with a sum over particle encounters, accounts for the situations when particles pass in the vicinity of one another and their relative motion is delayed in a simulation by $\Delta \tau_f$. The vector $\mathbf{p}_{ij} = (\mathbf{p}_i - \mathbf{p}_j)/2$ is relative momentum and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ is relative velocity. The third term on the rhs of (7.8) accounts for transport of mo-

mentum with two-particle interactions treated explicitly. The force $\mathbf{F}_{ij} = \dot{\mathbf{p}}_{ij}$ is that due to particle j on particle i . Due to the interaction, the relative momentum changes as particles are separated by \mathbf{r}_{ij} . The fourth term accounts for instantaneous changes of relative momentum in collisions, and the final term accounts for the effects of interactions treated in the mean-field approximation. It is apparent in (7.8) that positive (negative) forward delay times, for a given particle number, reduce (enhance) the pressure. Further, the attractive scattering style, $\Delta \mathbf{p}_{ij} \cdot \mathbf{r}_{ij} < 0$, reduces the pressure, while the repulsive style, $\Delta \mathbf{p}_{ij} \cdot \mathbf{r}_{ij} > 0$, enhances it.

Transport coefficients such as shear viscosity or heat conductivity may be determined within a simulation by imposing different conditions within the free gas beyond the two walls of the box in contact with that gas. Provided that the walls are perpendicular to the x axis and at $x = \pm \Delta x$, the viscosity coefficient may be determined by giving collective velocities to the free gas in the y direction equal to $\pm \Delta v$ in the two separated regions. The coefficient then follows from an off-diagonal term of the momentum flux tensor in the box

$$\eta = -\frac{1}{\tau V \Delta v / \Delta x} \left(\int dt \sum_j p_j^y v_j^x - \sum_{i < j} p_{ij}^y v_{ij}^x \Delta \tau_f^{ij} + \int dt \sum_{i < j} F_{ij}^y x_{ij} + \sum_{i < j} \Delta p_{ij}^y x_{ij} \right). \quad (7.9)$$

To gain an insight into (7.9), one may consider a simple assessment of the viscosity in a medium when ignoring the effects of the finite range and duration of interactions, i.e., investigating, in particular, only the effects associated with the first term in (7.9). Provided that particles propagate freely between collisions for an average time $\tau_F \approx 1/n\sigma\langle v \rangle$, a particle at a position x_i of velocity v_i^x would have, on the average, a momentum in the y direction such as characteristic for a position this particle had a time τ_F earlier. With this, Eq. (7.9) gives

$$\begin{aligned} \eta &\approx -\frac{1}{V \Delta v / \Delta x} \sum_i m \langle v^y \rangle (x_i - v_i^x \tau_F) v_i^x \\ &= -\frac{1}{V \Delta v / \Delta x} \sum_i m (x_i - v_i^x \tau_F) (\Delta v / \Delta x) v_i^x \\ &\approx mn \langle (v^x)^2 \rangle \tau_F = \frac{mn \langle v^2 \rangle \tau_F}{3} \approx \frac{m \langle v \rangle}{3\sigma}. \end{aligned} \quad (7.10)$$

The hard-sphere scattering is known to enhance viscosity to within the lowest order in density, but the enhancement factor for viscosity is smaller than that for pressure. For a given shear the medium with hard-sphere scattering, to lowest order, behaves as less viscous compared to one where effects of interaction range and duration may be ignored. For the numerical determination of a heat conduction coefficient, given assumptions of a simulation, the temperature should be set different in the two regions with free gas adjacent to the box where interactions take place.

VIII. CONCLUSIONS

The principal goal of simulating heavy-ion collisions is to infer the equation of state of nuclear matter. The effective equation of state for a simulation depends on several aspects: treatment of the mean field in simulation, time delays for interactions and scattering prescriptions, inclusion of various resonances. In this paper we have carried out a detailed investigation of the time delays and of scattering prescriptions, and have shown that they should be incorporated in coordination with the mean field. If that is not followed, the effective equation of state may be inconsistent with two-body scattering which constrains thermodynamic quantities to within the second order in the virial expansion.

In Sec. II expressions were derived for the average delay of an outgoing scattered wave as a function of the scattering angle. In Sec. III, such delays in dynamics were shown to be consistent with the two-body density of states if a forward delay or mean field were included and calculated in terms of the forward scattering amplitude. Other ergodically consistent prescriptions were presented where all the effective time delays were incorporated either entirely into the scattering or into the mean field. Alterations to these considerations for a Fermi-degenerate system were shown to be nontrivial in Sec. IV. Sections V and VI illustrated the time-delay considerations with the examples of resonance and NN scattering. In Sec. VII it was shown that repulsive and attractive scattering schemes can be interpreted in terms of time delays, and that equations of state associated with these schemes may be understood quantitatively at a two-body level. The implications of scattering prescriptions for transport coefficients were also discussed and a practical method of determining the equation of state and coefficients for a simulation was presented.

We conclude by giving some perspective to the considerations discussed here. Most of the flow in high-energy $\lesssim 1$ GeV/nucleon heavy-ion collisions stems from the one-body free-gas pressure. The interactions of particles affect the pressure and can increase the observed flow of a collision by $\approx 50\%$ compared to a free gas. As experiments are now able to measure sideways flow and squeeze out flow differences to better than 20%, a detailed and careful understanding of the simulations becomes crucial. Demonstrating that a simulation reproduces experimental results to within 10–20% has little meaning unless thermodynamic properties of the simulation are understood to within 10–20% as well. Simulations are becoming more sophisticated. Important aspects, such as the change of the dispersion relation for pions, are being incorporated through energy-dependent mean fields. At very relativistic energy, simulations must incorporate a large number of resonances which can be very broad compared to the temperature. It is hoped that the prescriptions and constraints presented here will contribute to both the development of improved codes and to a better understanding of existing approaches.

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APPENDIX

In this appendix we investigate changes in two-particle scattering rates induced by the presence of other particles, within the lowest order in density, in the context of the ergodic theorem. To reach directly essential results we adopt simplifying assumptions. First, we concentrate on a subsystem of one of the particles engaged in scattering, denoted as 1, and the spectator particle denoted as 2. We assume that these two particles interact only perturbatively with all other particles within the system, but not necessarily with one another. If the system has many particles confined to a finite volume and sampling is done over a long time τ , then we may write an ergodic theorem for the subsystem of particles 1 and 2 alone:

$$\frac{1}{\tau} \frac{d\tau}{d\mathbf{p} dE} = \left(\int dE' \frac{dn}{dE'} e^{-E'/T} \right)^{-1} \frac{dn}{d\mathbf{p} dE} e^{-E/T}. \quad (\text{A1})$$

In the above $d\tau/d\mathbf{p} dE$ denotes time spent in a given set of internal states, per unit volume of energy-momentum space, $dn/d\mathbf{p} dE$ denotes the number of states, and $e^{-E/T}$ is relative probability that any single internal state is occupied at any instant. An equivalent formulation of the ergodic theorem (A1) is that for any two states (\mathbf{p}, E) and (\mathbf{p}', E') :

$$\left(\frac{d\tau}{d\mathbf{p} dE} \right)^{-1} \frac{dn}{d\mathbf{p} dE} e^{-E/T} = \left(\frac{d\tau}{d\mathbf{p}' dE'} \right)^{-1} \frac{dn}{d\mathbf{p}' dE'} e^{-E'/T}. \quad (\text{A2})$$

For simplification, we next assume that 2 is much heavier than 1, whereupon we can make no distinction between relative states of 1 and 2 and single-particle states of 1. Equation (A2) then may be also written as

$$\begin{aligned} & \left(\frac{d\tau}{d\mathbf{p}_1 dE_1} \right)^{-1} \frac{dn_1}{d\mathbf{p}_1 dE_1} e^{-E_1/T} \\ &= \left(\frac{d\tau}{d\mathbf{p}'_1 dE'_1} \right)^{-1} \frac{dn_1}{d\mathbf{p}'_1 dE'_1} e^{-E'_1/T}. \end{aligned} \quad (\text{A3})$$

We are now set to address the scattering of a particle 3, representing the remainder of the system, with particle 1, in the presence of 2. Transition or scattering rate within the system are given by a transition matrix element squared multiplied by the density of final states in energy, times 2π . When sampling is carried out over a long time, the number of transitions within the system from one set of states to some other should be the same as from the other set to the first. On multiplying both sides of Eq. (A3) by common factors and after manipulations, we can demonstrate an equivalence of the ergodic condition (A3) with the general condition of the equality of the number of transitions in the different directions. Specifically, we multiply both sides of (A3) by a product of average number densities of 3,

$dN_3/d\mathbf{p}_3 dE_3 = dn_3/d\mathbf{p}_3 dE_3 \times e^{-E_3/T}$, in the vicinity of two different states (\mathbf{p}_3, E_3) and (\mathbf{p}'_3, E'_3) , such that $\mathbf{p}_1 + \mathbf{p}_3 = \mathbf{p}'_1 + \mathbf{p}'_3$ and $E_1 + E_3 = E'_1 + E'_3$, and by a matrix element squared in the momentum representation, same for direct and inverse transitions, $|\mathcal{M}_{13 \rightarrow 1'3'}|^2 = |\mathcal{M}_{1'3' \rightarrow 13}|^2 \equiv |\mathcal{M}|^2$. After manipulations we get

$$\begin{aligned} & \frac{d\tau}{d\mathbf{p}_1 dE_1} \frac{dN_3}{d\mathbf{p}_3 dE_3} \frac{(2\pi)^4}{V^3} |\mathcal{M}|^2 \frac{dn_1}{d\mathbf{p}'_1 dE'_1} \frac{dn_3}{d\mathbf{p}'_3 dE'_3} \\ &= \frac{d\tau}{d\mathbf{p}'_1 dE'_1} \frac{dN_3}{d\mathbf{p}'_3 dE'_3} \frac{(2\pi)^4}{V^3} |\mathcal{M}|^2 \frac{dn_1}{d\mathbf{p}_1 dE_1} \frac{dn_3}{d\mathbf{p}_3 dE_3}. \end{aligned} \quad (\text{A4})$$

The volume V is assumed here to be large compared to the range of interactions. The lhs of (A4) represents number of transitions that take place, per element of energy-momentum space $d\mathbf{p}_1 dE_1 d\mathbf{p}_3 dE_3 d\mathbf{p}'_1 dE'_1$, from states 13 to 1'3'. The rhs represents number of inverse transitions per energy-momentum element $d\mathbf{p}'_1 dE'_1 d\mathbf{p}'_3 dE'_3 d\mathbf{p}_1 dE_1$. By virtue of energy-momentum conservation the energy-momentum elements involving any three out of the four states in the above are actually identical. The number of transitions in (A4), e.g., on the lhs, is represented in terms of the time spent by particle 1 in the region (\mathbf{p}_1, E_1) times the probability of finding particle 3 in the region (\mathbf{p}_3, E_3) , times the transition rate into (\mathbf{p}'_1, E'_1) and (\mathbf{p}'_3, E'_3) .

Equation (A4) is fully equivalent to (A3) or (A1). Given that interaction of particle 3 with any other particles is perturbative, the perturbative scattering of 1 and 3 is modified in the presence of 2, compared to free space, by a changed final density of states. From (A4) it follows that, to comply with ergodicity, it is necessary to allow particles to participate in transitions at any time when in a given relative state. In the transition rate and in the cross section, it is necessary to account for the changed final-state density.

Within many-body theory, a final-state density for scattering is typically described in terms of single-particle spectral functions [31,25] equal, up to a factor, to the imaginary part of single-particle Green's function (3.8), $A = -2\text{Im}g$. For example, for the case above, the number of transitions in which particles from (\mathbf{p}_1, E_1) and (\mathbf{p}_3, E_3) interact and populate (\mathbf{p}'_1, E'_1) and (\mathbf{p}'_3, E'_3) , per unit time and per momentum volume $d\mathbf{p}_3 d\mathbf{p}'_1$, given well-defined energies of 3, would be represented as

$$\frac{V}{(2\pi)^6} f(\mathbf{p}_3) |\mathcal{M}|^2 A(\mathbf{p}'_1, E'_1). \quad (\text{A5})$$

On comparing the previous expression for transitions with the one in terms of A , one can conclude that, in the discussed case,

$$\frac{V}{(2\pi)^4} A(p_1, E_1) = \frac{dn_1}{d\mathbf{p}_1 dE_1} = \frac{dn}{d\mathbf{p}_1 dE_1}. \quad (\text{A6})$$

This implies an integral relation between the density of relative states ρ and A ,

$$\frac{dn}{dE_1} \equiv \rho(E_1) = \frac{V}{(2\pi)^4} \int d\mathbf{p}_1 A(p_1, E_1). \quad (\text{A7})$$

We now proceed to examine an explicit form of A in the \mathcal{F} -matrix approximation in which interactions within a two-particle system, such as that of 1 and 2 in the above, are fully accounted for. With an explicit form of A , we shall further examine the validity of (A7), establishing a correspondence between different terms in A and in ρ . We shall then discuss in-medium scattering rates.

From (3.8) we find

$$\begin{aligned} A(\mathbf{p}_1, E_1) &= -2 \operatorname{Im}g(\mathbf{p}_1, E_1) \\ &= \frac{\gamma(\mathbf{p}_1, E_1)}{[E_1 - e(p_1) - u(\mathbf{p}_1, E_1)]^2 + [\gamma(\mathbf{p}_1, E_1)]^2/4}. \end{aligned} \quad (\text{A8})$$

Here the real and imaginary parts of self-energy separately depend on energy and momentum. In the \mathcal{F} matrix approximation, this dependence corresponds to a separate dependence of the \mathcal{F} -matrix on energy and momentum as in the Lippman-Schwinger equation. On expanding A for low scattering rate γ , in the discussed case rate for scattering of 1 off 2 given large V , we obtain

$$\begin{aligned} A(\mathbf{p}_1, E_1) &\approx \left(1 - \frac{\partial u(\mathbf{p}_1, E_1)}{\partial E_1} \Big|_{E_1 = \mathcal{E}(\mathbf{p}_1)}\right)^{-1} 2\pi\delta[E_1 - \mathcal{E}(\mathbf{p}_1)] \\ &\quad - \gamma(\mathbf{p}_1, E_1) \frac{\mathcal{P}}{E_1 - \mathcal{E}(\mathbf{p}_1)} \quad (\text{A9a}) \\ &\approx 2\pi\delta[E_1 - \mathcal{E}(\mathbf{p}_1)] + \frac{\partial u(\mathbf{p}_1, E_1)}{\partial E_1} \Big|_{E_1 = \mathcal{E}(\mathbf{p}_1)} \\ &\quad \times 2\pi\delta[E_1 - \mathcal{E}(\mathbf{p}_1)] - \gamma(\mathbf{p}_1, E_1) \frac{\mathcal{P}}{E_1 - \mathcal{E}(\mathbf{p}_1)}. \end{aligned} \quad (\text{A9b})$$

The energy $\mathcal{E}(\mathbf{p}_1)$ in the above is a solution of the equation $E_1 - e(\mathbf{p}_1) - u(\mathbf{p}_1, E_1) = 0$. The factor multiplying the $2\pi\delta$ in (A9a) is termed a wave-function renormalization factor, and

$$\begin{aligned} \frac{\mathcal{P}}{x} &= \frac{d}{dx} \frac{\mathcal{P}}{x} = \frac{d}{dx} \lim_{\epsilon \rightarrow 0} \frac{1}{2} \left(\frac{1}{x+i\epsilon} + \frac{1}{x-i\epsilon} \right) \\ &= \lim_{\epsilon \rightarrow 0} \frac{d}{d\epsilon} \frac{1}{2i} \left(\frac{1}{x+i\epsilon} - \frac{1}{x-i\epsilon} \right), \end{aligned} \quad (\text{A10})$$

see also [41,42]. Equation (A9b) follows from (A9a) on recognizing that, according to a dispersion relation, the energy derivative of the mean field is proportional to the off-shell scattering rate. Thus, it is expected to be small when the rate is small. If V is large enough, then the mean field itself is small, and we can further expand A in terms of u ,

$$\begin{aligned} A(\mathbf{p}_1, E_1) &\approx 2\pi\delta[E_1 - e(p_1)] - u[\mathbf{p}_1, e(p_1)] \\ &\quad \times 2\pi\delta'[E_1 - e(p_1)] + \frac{\partial u(\mathbf{p}_1, E_1)}{\partial E_1} \Big|_{E_1 = e(p_1)} \\ &\quad \times 2\pi\delta[E_1 - e(p_1)] - \gamma(\mathbf{p}_1, E_1) \frac{\mathcal{P}}{E_1 - e(p_1)} \end{aligned} \quad (\text{A11a})$$

$$\begin{aligned} &= 2\pi[\delta[E_1 - e(p_1)] - u(\mathbf{p}_1, E_1)\delta'[E_1 - e(p_1)] \\ &\quad - \gamma(\mathbf{p}_1, E_1) \frac{\mathcal{P}}{E_1 - e(p_1)}]. \end{aligned} \quad (\text{A11b})$$

Within the \mathcal{F} -matrix approximation, the mean field and scattering rate due to 2 are

$$\begin{aligned} u(\mathbf{p}_1, E_1) &= \int \frac{d\mathbf{p}_2}{(2\pi)^3} f(\mathbf{p}_2) \operatorname{Re}\langle p | \mathcal{F}(E) | p \rangle \\ &= \operatorname{Re}\langle p_1 | \mathcal{F}(E_1) | p_1 \rangle / V, \end{aligned} \quad (\text{A12})$$

and

$$\begin{aligned} \gamma(\mathbf{p}_1, E_1) &= -2 \int \frac{d\mathbf{p}_2}{(2\pi)^3} f(\mathbf{p}_2) \operatorname{Im}\langle p | \mathcal{F}(E) | p \rangle \\ &= -2 \operatorname{Im}\langle p_1 | \mathcal{F}(E_1) | p_1 \rangle / V, \end{aligned} \quad (\text{A13})$$

with the center expressions following under assumption of well-defined energies of 2, and rhs expressions representing results for the specific case under discussion.

On inserting A in the form (A11a) into the rhs of (A7), we find that the leading term in (A11a) produces ρ_0 from Eq. (3.1). The second term in (A11a), with a derivative of the δ function, gives a complete contribution to $\Delta\rho$ associated with the forward delay time,

$$\frac{d}{dE} \left(\rho_0 \frac{1}{V} \langle p | \operatorname{Re}\mathcal{F}(E) | p \rangle \right) = \frac{1}{\pi} \sum_{\mathcal{L}} (\mathcal{L} + 1) \cos 2\delta_{\mathcal{L}} \frac{d\delta_{\mathcal{L}}}{dE}, \quad (\text{A14})$$

compare Eq. (3.11). The derivative from the δ function acting on ρ_0 gives a contribution associated with $\Delta\tau_1^{\text{clas}}$, cf. Eq. (3.4), and the derivative acting on u gives a contribution associated with $\Delta\tau_2^{\text{clas}}$, cf. Eq. (3.5). Finally, the remaining wave-function renormalization and off-shell terms in (A11a) yield *jointly*, on insertion into the rhs of (A7) and after lengthy manipulations, a scattering contribution to ρ of the form $\rho_0\sigma v\Delta\tau_s/V$, where $\Delta\tau_s$ is given by (3.12), compare (3.2) and (3.7), indeed confirming the equality in (A7). The manipulations involve, in particular, expressing the δ function and principal value in (A11) in terms of the imaginary and real parts of the free two-particle Green's function, and an extensive use of the relations between the imaginary and real parts of the free two-particle Green's function and the \mathcal{F} matrix, following from the Lippman-Schwinger equation, Eq. (4.8) with $N=1$ in G_0 . Presence of the momenta p_1 in the last term in (A11a) and in (A13), far from the shell defined by $e(p_1) = E_1$, indicate the effects of near zone in the interaction of 1 and 2.

Generally, in a scattering rate a single-particle spectral function A would be used for each of final-state particles. On the basis of the example above, one would conclude that use of such function leads to the population of states consistent with two-particle density. A more general relation between A and ρ , than (A7), is

$$\frac{V}{2\pi} \int d\mathbf{p} \frac{\delta}{\delta f(\mathbf{p}_2)} A(\mathbf{p}_1, E + P^2/2M - e(p_2)) = \Delta\rho(E), \quad (\text{A15})$$

where integration is carried out over relative momentum at fixed total momentum $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$. Use of the distribution $f(\mathbf{p}_2)$ in (A12) and (A13) allows for various momentum values of 2. As f is not normalized to yield one particle within a given volume, there is a possibility for 2 being absent from V , giving a reduction in the relative weight of the correction to the density of states due to the interaction, cf. (A11).

In practical applications, the incorporation of the first correction term in A in (A11a), associated with the forward delay time, amounts to correcting single-particle energies in the scattering rates by the mean field. The incorporation of the scattering delays in the final states in scattering rates can be much more cumbersome given the form of terms in (A11a). One possible solution to get consistency with ergodicity is to multiply rates or cross sections by factors of the form

$$1 + \int d\mathbf{p}_2 f(\mathbf{p}_2) \sigma v \Delta\tau_s, \quad (\text{A16})$$

for each of final-state particles. That would be analogous to putting all delays into the forward delay time in the particle propagation, discussed in Sec. III D. A weakness of an approach where just final-state densities in two-particle scattering are modified on account of scattering with other particles, is the disregard of correlations that may persist throughout the interaction process. Effects of correlations become even apparent in a more detailed analysis of the discussed simple example with perturbative scattering. Thus a careful reader might notice that the matrix elements in (A4) for transitions should not be, generally, taken between plane waves but rather between eigenstates of an internal Hamiltonian of 1 and 2. Separation of the wave functions for these states into incident and scattered portions would, generally, yield two-particle and three-particle scattering terms in the transition rate. Interference of the forward and scattered waves for 1 and 2 would yield shadowing corrections in the matrix element for the scattering of 1 and 3. The genuine three-particle scattering term would be characterized by the lack of momentum conservation within the subsystem of 1 and 3 alone. However, such effects are beyond the scope of present paper.

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