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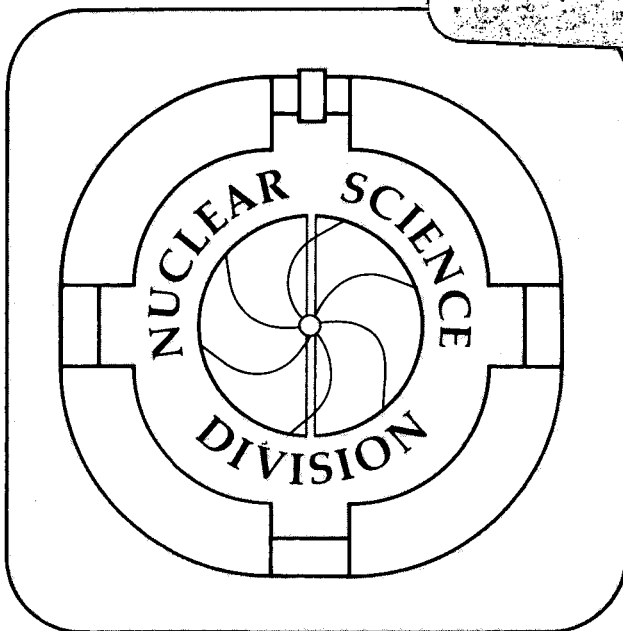
CLASSICAL SIMULATION OF THE FERMI GAS

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December 1986

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Classical Simulation of the Fermi Gas

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Abstract:

We demonstrate that it is possible to approximate the one-particle phase-space distribution of the excited Fermi gas within the framework of classical mechanics by employing a momentum-dependent two-body repulsion, to simulate the Pauli exclusion principle. For a suitable choice of the parameters in this potential, it is possible to achieve a quite good approximation to the momentum distribution over a broad range of temperatures and densities.

¹ On leave from Centro Brasileiro de Pesquisas Física (CNPQ), Rio de Janeiro, Brazil.

1 Introduction

In recent years, there has been steady improvement in the experimental tools for studying nuclear collisions at intermediate energies, *i.e.* bombarding energies from a few tens to a few hundreds of MeV per nucleon. At these energies, the total excitation energy of the collision system is comparable to the total binding energy, so that a disassembly into many nuclear fragments is possible. In concert with the developments on the experimental front, the theoretical descriptions have grown more refined. At the moment, the most sophisticated model of nuclear dynamics at these energies is the Vlasov-Uehling-Uhlenbeck (VUU) model, which describes the system in terms of individual nucleons which move in a common time-dependent one-body field and occasionally scatter with one another.[1] Relative to free collisions, the nucleon-nucleon scatterings are suppressed due to the phase-space Pauli exclusion produced by the presence of other nucleons; this feature is important since the excitation energy is comparable to the Fermi kinetic energy and, consequently, the nucleon gas is still quite degenerate. While the formulation and implementation of this model represents a major step forward in our ability to model nuclear dynamics at intermediate energies, we still have a long way to go before a satisfactory description is at hand. One of the most important limitations of the current VUU-type models is the neglect of dynamical fluctuations: although an entire ensemble of systems are followed, they are all assumed to have the same mean field. This feature strongly limits the utility of the model since fluctuations are very prominent at these energies. Another shortcoming is the fact that fragment formation is not well described in the model, a difficulty shared with most other dynamical models presently in use.

Our goal is to develop an alternative model which may provide a useful supplement to the VUU description, at least until such a time when that model has been further developed to incorporate fluctuations and fragment formation. We seek to develop a model based on the microscopic dynamics of interacting classical particles. A key feature is the introduction of a momentum-dependent potential for the purpose of simulating the Pauli exclusion principle. Such an approach was first taken by Wilets *et al.*[2]. In that work, a repulsive momentum-dependent Pauli potential was postulated and the parameters of an ordinary two-body potential were adjusted to fit certain gross nuclear properties. Although the model met with some success, it was never demonstrated that the phase-space distribution of the nucleons is actually well approximated. Since this property is expected to be important for the dynamical behavior of a colliding system, there is a need for scrutinizing the problem. Therefore, in the present paper, we reconsider the problem of determining an appropriate Pauli potential and we demonstrate that it is in fact possible to obtain a reasonably good reproduction of the important features of the Fermi gas, with a suitable choice of potential parameters. Our thus determined Pauli potential differs in form from that employed in ref. [2]. We see this result as a first step in a program, the next step being the inclusion of a real two-body interaction for the purpose of describing both nuclear matter and finite nuclei. If this proves possible, the foundation is laid for an

interesting dynamical model for the evolution of a highly excited nuclear system far from equilibrium, including its disassembly into multi-fragment final states.

2 General considerations

We consider a system of N structureless identical classical particles in a Euclidian space of dimensionality D . The momentum and position of a given particle i , $i = 1, \dots, N$, are denoted by \mathbf{p}_i and \mathbf{q}_i , respectively. The particles are interacting via a momentum-dependent two-body force, so the total energy of the system is represented by a Hamiltonian of the form

$$H(\mathbf{p}_1, \dots, \mathbf{p}_N, \mathbf{q}_1, \dots, \mathbf{q}_N) = \sum_i T_i + \frac{1}{2} \sum_{ij}' V_{ij}. \quad (1)$$

Here $T_i = p_i^2/2m$ is the kinetic energy of particle i and the two-body interaction energy between particles i and j is $V_{ij} = V(p_{ij}, q_{ij})$, where $p_{ij} = |\mathbf{p}_i - \mathbf{p}_j|$ and $q_{ij} = |\mathbf{q}_i - \mathbf{q}_j|$. The prime on the summation in the interaction term is intended to remind of the convention that the sum over j should exclude the self-interaction term V_{ii} corresponding to $j = i$ (although the inclusion of V_{ii} would be of no dynamical consequence).

The dynamical evolution of the particles is governed by Hamilton's equations,

$$\dot{\mathbf{p}}_i = -\frac{\partial H}{\partial \mathbf{q}_i}, \quad \dot{\mathbf{q}}_i = \frac{\partial H}{\partial \mathbf{p}_i}. \quad (2)$$

The momentum dependence of V produces a variable effective mass, so that the standard relationship between velocity and momentum, $\mathbf{p}_i = m\dot{\mathbf{q}}_i$, is replaced by the more general form $\mathbf{p}_i = \mathbf{M} \cdot \dot{\mathbf{q}}_i$, where $\mathbf{M}(\mathbf{p}_1, \dots, \mathbf{p}_N, \mathbf{q}_1, \dots, \mathbf{q}_N)$ is the effective mass tensor. The ground state of the system has the minimum energy and it is therefore a solution to the $2D$ coupled equations $\dot{\mathbf{p}}_i = 0$ and $\dot{\mathbf{q}}_i = 0$. Such a state represents a frozen configuration in phase space, with the particles having finite momenta despite their vanishing velocities. Thus the associated effective mass tensor is divergent. This illustrates how the kinematics is strongly affected by the Pauli potential.

When considering an entire ensemble of similar systems, as we shall do, it is convenient to deal with the N -particle distribution function $f^{(N)}(\mathbf{p}_1, \dots, \mathbf{p}_N, \mathbf{q}_1, \dots, \mathbf{q}_N)$. Its form in thermal equilibrium is given by

$$f_{equil}^{(N)} \sim e^{-H/\tau}, \quad (3)$$

where H is given by (1) and τ is the temperature.

Any observable of interest can be expressed in terms of the distribution function $f^{(N)}$. For example, the reduced one-particle phase-space distribution function is given by

$$f^{(1)}(\mathbf{p}, \mathbf{q}) = \langle h^D \sum_i \delta(\mathbf{p}_i - \mathbf{p}) \delta(\mathbf{q}_i - \mathbf{q}) \rangle \quad (4)$$

where $\langle \cdot \rangle$ indicates the $2DN$ -dimensional phase-space integration with $f^{(N)}$ providing the weight function; in practice this is easily accomplished by averaging over the given

ensemble of systems. It is useful in the present context to normalize $f^{(1)}$ such that it measures the phase-space occupancy, *i.e.* the number of particles in an elementary cell of volume h^D around the point (\mathbf{p}, \mathbf{q}) . The spatial density of particles is obtained by performing a momentum integration,

$$\rho(\mathbf{q}) = \int \frac{d\mathbf{p}}{h^D} f(\mathbf{p}, \mathbf{q}) , \quad (5)$$

and the total particle number is recovered by subsequent integration over position,

$$N = \int d\mathbf{q} \rho(\mathbf{q}) = \int \frac{d\mathbf{p}d\mathbf{q}}{h^D} f(\mathbf{p}, \mathbf{q}) . \quad (6)$$

The expression (1) for the energy can be rewritten in terms of the reduced one- and two-particle distribution functions as

$$E = \int \frac{d\mathbf{p}d\mathbf{q}}{h^D} [f^{(1)}(\mathbf{p}, \mathbf{q}) \frac{p^2}{2m} + \frac{1}{2} \int \frac{d\mathbf{p}'d\mathbf{q}'}{h^D} f^{(2)}(\mathbf{p}, \mathbf{p}', \mathbf{q}, \mathbf{q}') V(|\mathbf{p} - \mathbf{p}'|, |\mathbf{q} - \mathbf{q}'|)] \quad (7)$$

$$\approx \int \frac{d\mathbf{p}d\mathbf{q}}{h^D} f^{(1)}(\mathbf{p}, \mathbf{q}) \left[\frac{p^2}{2m} + \frac{1}{2} \int \frac{d\mathbf{p}'d\mathbf{q}'}{h^D} f^{(1)}(\mathbf{p}', \mathbf{q}') V(|\mathbf{p} - \mathbf{p}'|, |\mathbf{q} - \mathbf{q}'|) \right] . \quad (8)$$

Here the second relation is valid when the two-body correlations can be neglected, *i.e.* when $f^{(2)}(\mathbf{p}, \mathbf{p}', \mathbf{q}, \mathbf{q}') \approx f^{(1)}(\mathbf{p}, \mathbf{q}) f^{(1)}(\mathbf{p}', \mathbf{q}')$.

If the ensemble is translationally invariant, then $f^{(1)}$ is independent of position and the spatial dependence of the two-body distribution function $f^{(2)}$ is only via the difference $\Delta\mathbf{q} = \mathbf{q} - \mathbf{q}'$. We then find

$$E = \Omega \int \frac{d\mathbf{p}}{h^D} [f^{(1)}(\mathbf{p}) \frac{p^2}{2m} + \frac{1}{2} \Omega \int \frac{d\mathbf{p}'d\Delta\mathbf{q}}{h^D} f^{(2)}(\mathbf{p}, \mathbf{p}', \Delta\mathbf{q}) V(\Delta\mathbf{p}, \Delta\mathbf{q})] , \quad (9)$$

where $\Omega = \int d\mathbf{q}$ denotes the total volume of the system. Since $\Omega \rightarrow \infty$, it is practical to introduce the energy per particle $\epsilon = E/N$, which is well-defined since $\Omega/N = 1/\rho$. In practice, such a system can be approximated by a periodic system with a sufficiently large periodicity.

In order to implement the qualitative concept of closeness, it is desirable to introduce a metric in phase space. This can be accomplished in a convenient manner by defining the dimensionless distance s_{ij} between the two phase-space points $(\mathbf{p}_i, \mathbf{q}_i)$ and $(\mathbf{p}_j, \mathbf{q}_j)$,

$$s_{ij}^2 = p_{ij}^2/p_0^2 + q_{ij}^2/q_0^2 , \quad (10)$$

where $p_{ij} = |\mathbf{p}_i - \mathbf{p}_j|$ and $q_{ij} = |\mathbf{q}_i - \mathbf{q}_j|$. The parameters p_0 and q_0 are suitable characteristic scales for relative momentum and position and are further discussed below.

In the present study, we present results obtained with Pauli potentials of Gaussian form,

$$\begin{aligned} V(\mathbf{p}, \mathbf{q}) &= V_0 (2\pi p_0^2)^{-\frac{D}{2}} e^{-p^2/2p_0^2} (2\pi q_0^2)^{-\frac{D}{2}} e^{-q^2/2q_0^2} h^D \\ &= V_0 \left(\frac{\hbar}{p_0 q_0} \right)^D e^{-s^2/2} . \end{aligned} \quad (11)$$

Here V_0 determines the overall strength, whereas p_0 and q_0 determine the ranges in momentum and position space, respectively. This form has the special advantage that V depends on \mathbf{p} and \mathbf{q} through the dimensionless separation s only, and yet V is separable with respect to momentum and position. In fact, V factorizes totally with respect to all $2D$ dimensions of phase space. The complete separability with respect to position makes the inclusion of neighboring cells in a periodic system especially economical – a distinct calculational advantage. It is useful to define the following reduced potentials,

$$v_p(\mathbf{p}) = \int d\mathbf{q} V(\mathbf{p}, \mathbf{q}) = V_0 (2\pi p_0^2)^{-\frac{D}{2}} e^{-p^2/2p_0^2} h^D, \quad (12)$$

$$v_q(\mathbf{q}) = \int \frac{d\mathbf{p}}{h^D} V(\mathbf{p}, \mathbf{q}) = V_0 (2\pi q_0^2)^{-\frac{D}{2}} e^{-q^2/2q_0^2}. \quad (13)$$

The total strength of the Pauli potential is given by

$$V_0 = \int \frac{d\mathbf{p}d\mathbf{q}}{h^D} v(\mathbf{p}, \mathbf{q}) = \int \frac{d\mathbf{p}}{h^D} v_p(\mathbf{p}) = \int d\mathbf{q} v_q(\mathbf{q}). \quad (14)$$

Roughly speaking, the parameters p_0 and q_0 determine the size of an effectively excluded volume around each particle in phase space. Indeed, they can be thought of as the extensions in position and momentum of a spheroidal excluded volume around each particle. [Note that the range appearing in the two-body Pauli potential is *twice* the radius of the effective excluded volume around each particle, as is easily visualized by considering a system of hard spheres.] In order that each particle block a phase-space volume of magnitude h^D , we would expect p_0 and q_0 to be related by $p_0 q_0 \approx 2\hbar$, a sort of “uncertainty relation”. [In fact, we should expect the product to be slightly smaller than that, with the exact number depending on the dimensionality D , because of the geometric fact that hard spheroids can not be packed to uniformity (as hard cubes can), but always leave a certain fraction of the space empty.]

3 Idealized treatment

In order to gain some familiarity with the model, we consider in this section the idealized situation where the two-body correlations can be neglected, $f^{(2)} \approx f^{(1)} f^{(1)}$. This situation is expected to arise when the spatial range q_0 is large in comparison with the typical spacing between neighboring particles (which is $\sim \rho^{-1/D}$). The expression for the energy then simplifies to

$$\epsilon = \int \frac{d\mathbf{p}}{h^D} f(p) \left[\frac{p^2}{2m} + \frac{1}{2} \int \frac{d\mathbf{p}'}{h^D} f(p') v_p(\Delta p) \right] \quad (15)$$

$$\approx \int \frac{d\mathbf{p}}{h^D} f(p) \left[\frac{p^2}{2m} + \frac{V_0}{2} f(p) \right]. \quad (16)$$

Here $f(p)$ is a short notation for $f^{(1)}(p)$ and the isotropy implies that f only depends on the magnitude $p = |\mathbf{p}|$. The second relation holds when the momentum range p_0 is

small compared with P_F , which represents the characteristic momentum scale for $f(\mathbf{p})$; we have then $v_p(\mathbf{p}) \approx V_0 \delta(\mathbf{p}) h^D$. [For a given density ρ , it is convenient to define the equivalent Fermi momentum P_F through the relation $\rho = \Gamma_D (P_F/h)^D$ pertaining to a standard cold Fermi gas; the relevant geometric coefficients are $\Gamma_1 = 2, \Gamma_2 = \pi, \Gamma_3 = 4\pi/3$.]

The ground state of the system is determined by the requirement that the energy be a minimum, for the specified density. By performing the variation $\rho \delta \epsilon - \lambda \delta \rho$, it is elementary to show that the solution to this problem is given by a simple parabolic distribution,

$$f(p) = \frac{1}{V_0} \left(\lambda - \frac{p^2}{2m} \right) \theta \left(\frac{p^2}{2m} - \lambda \right). \quad (17)$$

Here the truncation function θ ensures that no particles are found above the "chemical potential" λ . The requirement that f be appropriately normalized yields the relationship

$$\lambda = \left(\frac{D+2}{2} \frac{V_0}{\epsilon_F} \right)^{\frac{2}{D+2}} \epsilon_F. \quad (18)$$

The momentum distribution can be characterized by the mean kinetic energy which is easily found to be

$$\epsilon_{kin} = \frac{1}{\rho h^D} \int d\mathbf{p} f(p) \frac{p^2}{2m} = \frac{D}{D+4} \left(\frac{D+2}{D} \frac{V_0}{\epsilon_F} \right)^{\frac{2}{D+2}} \epsilon_F. \quad (19)$$

For a standard cold Fermi gas the mean kinetic energy is given by

$$\epsilon_{kin}^{FG} = \frac{D}{D+2} \epsilon_F. \quad (20)$$

In order to approximate the momentum distribution for the corresponding Fermi gas, we demand that ϵ_{kin} be equal to ϵ_{kin}^{FG} . This requirement then determines the interaction strength V_0 ,

$$V_0 = \frac{2}{D+2} \left(\frac{D+4}{D+2} \right)^{\frac{D+2}{2}} \epsilon_F. \quad (21)$$

This amounts to $V_0/\epsilon_F = 1.43, 1.13, 0.93$ for $D = 1, 2, 3$, respectively.

This result implies that the "chemical potential" λ is given by

$$\lambda = \frac{D+4}{D+2} \epsilon_F. \quad (22)$$

Furthermore, the maximum occupancy attained is given by

$$f(0) = \frac{\lambda}{V_0} = \frac{D+2}{2} \left(\frac{D+2}{D+4} \right)^{\frac{D}{2}}. \quad (23)$$

This amounts to 1.16, 1.33, 1.51, respectively. Thus, the Pauli potential prevents the particles from assembling at zero momentum, as they would in the absence of the momentum-dependent repulsion, and it actually produces a phase-space occupation that is fairly close to the correct quantum-mechanical one (which is unity up to the

Fermi energy ϵ_F). This result is encouraging, particularly since the present idealized treatment, in which the two-body correlations are neglected, will tend to overestimate the occupancy, so that there is reason to expect that a more refined treatment will produce even better results.

Figure 1 shows the function $f(p)$ for $D = 1$, as calculated with the above determined value of the interaction strength V_0 . It illustrates the effect of a finite temperature τ and a finite momentum range p_0 . These results are obtained by a simple iterative solution method. It is based on the fact that the thermal-equilibrium form of the one-particle distribution function is given by

$$f_{equil}(p) \sim e^{-\epsilon_p[f]/\tau}, \quad (24)$$

where $\epsilon_p[f]$ is the single-particle energy for a particle having the momentum p ; due to the presence of two-body interactions, this quantity depends on the entire one-particle distribution f . Starting from an approximate solution (for example, the analytical zero-range parabolic form (17), or the thermal distribution for non-interacting particles), one can then calculate the associated single-particle energies $\epsilon_p[f]$ and then, using the formula (24) for the equilibrium distribution, generate an improved approximation:

$$\begin{aligned} f'(p) &= c e^{-\epsilon_p[f]/\tau}, \\ f^{new}(p) &= \frac{1}{1+b} (f'(p) + bf(p)). \end{aligned} \quad (25)$$

Here c is the appropriate normalization constant and the “braking coefficient” b is introduced as a tunable quantity whose role is to improve the convergence properties of the iteration procedure. This simple method is very fast and usually works quite well. It can readily be extended to higher dimensions.

It should be noted that there is little effect of increasing the momentum range p_0 from zero to a finite value, as long as it remains small in comparison with P_F , which characterizes the momentum over which $f(p)$ varies significantly. We therefore expect the analytical results obtained above for $p_0 = 0$ to be of relevance also for moderate finite values of p_0 .

4. The Fermi gas

After the above preparations, we now address the three-dimensional Fermi gas. As an approximation to the infinite system, we consider a sample of spatially periodic systems. Each elementary cell is of cubic shape and typically contains 64 particles. The periodicity condition is easily imposed by letting a leaving particle reenter the cell from the corresponding point on the opposite side with the same momentum. The interaction of the explicitly considered particles with particles in neighboring cells is taken into account to sufficiently high order, typically the inclusion of two layers of neighboring cells suffices. [As already noted, this is relatively easy and economical to accomplish, due to the spatial factorization of the interaction.] A thermal sample of states is generated by employing the Metropolis procedure.[3].

The following set of parameters prove to yield quite satisfactory results and they have been adopted as a preliminary set of standard values:

$$\begin{aligned} V_0 &= 34.32 \text{ MeV} , \\ p_0 &= 2.067 \text{ MeV} \cdot 10^{-22} \text{ s/fm} , \\ q_0 &= 6.00 \text{ fm} . \end{aligned} \tag{26}$$

The strength V_0 has the value suggested by the above idealized treatment for $D = 3$, $V_0 = 0.9276 \epsilon_F$.

Furthermore, the product of the ranges is $p_0 q_0 = 1.88 \hbar$, which is quite consistent with our expectation of a value somewhat less than two times \hbar . [In applications to nuclear systems, it must be recalled that each nucleon has a four-fold spin-isospin degeneracy, so that ordinary nuclear matter would consist of four separate systems of the type discussed here; nucleons with different spin-isospin components do not interact via the Pauli potential.]

In order to illustrate the effect of this interaction on the particle motion, we show in fig. 2 the phase-space trajectories for the head-on collision of two free particles. As expected, the Pauli potential is only important when the relative momentum is comparable to, or smaller than, the range p_0 . For the smallest relative momenta, the repulsion is so strong that the effective mass becomes temporarily negative. [As already pointed out in ref. [2], this feature makes the relationship between momentum and velocity multivalued and thus precludes a Lagrangian formulation.] These trajectories exhibit a similarity with those resulting from the collision of two particles interacting with a hard-sphere Pauli potential.

In fig. 3 we show the mean kinetic energy per particle as a function of temperature. Three different densities have been considered, corresponding to the standard Fermi energy and both twice and half that. [This corresponds to normal saturation density and densities 2.83 times higher and lower than normal, respectively.] This should cover the range of densities occurring in those nuclear collision processes towards which this work is oriented. It is seen that the mean kinetic energy tracks well the behavior of the Fermi gas as a function of both the temperature and the density.

The more detailed behavior of the momentum distribution is illustrated in fig. 4, which displays the phase-space occupancy $f(p, q)$ as a function of the magnitude of the momentum. [In the present system f does not depend on the position, due to the translational invariance, and only depends on the magnitude of the momentum, due to the isotropy.] For the standard value of the Fermi momentum, a broad range of temperatures is considered, from close to zero to around the Fermi kinetic energy. The agreement with the results for the corresponding Fermi gases is remarkable. The most prominent deviations occur at the lower temperatures, where a peak in f appears at a small finite value of p . This is largely an artifact of the finite cell size employed: at low temperatures the particles prefer to organize themselves into fairly regular structures and this produces pronounced undulations in f . If an additional average were made over an interval in the periodicity of the order of the range q_0 , these undulations would

be reduced. With this in mind, we therefore consider the agreement between the model calculations and the Fermi gas results to be quite satisfactory.

5 Concluding remarks

In the present paper, we have discussed a system of classical particles interacting via a repulsive momentum-dependent two-body potential. We have illustrated some of the general features of such a system and, in particular, we have, for the first time, demonstrated that it is possible to achieve a fairly good imitation of the Fermi gas, with a suitable choice of potential. This result holds promise that it may be possible to develop an interesting model for intermediate-energy nuclear dynamics within the framework of classical equations of motion. We are currently pursuing this next stage of investigation.

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- [3] N. Metropolis, A.W. Rosenblut, M.N. Rosenblut, A.H. Teller, and E. Teller, J. Chem. Phys. 21 (1953) 1087

Figure captions.

Figure 1. Momentum distribution in the idealized system.

For the idealized system ($D=1$, no correlations), the phase-space occupancy $f(p)$ is displayed as a function of the magnitude of the momentum, p . The result (17) for zero temperature, $\tau=0$, and zero momentum range, $p_0=0$, is the parabolic solid curve. The left-hand part shows the effect of increasing the temperature through $\tau=4$ MeV (short dashes) to $\tau=8$ MeV (long dashes). For $\tau=4$ MeV, the right-hand part shows the result of increasing the range from zero (short dashes) through a moderate range, $p_0=3$ MeV $\cdot 10^{-22}$ s/fm (long dashes), to a relatively large range, $p_0=6$ MeV $\cdot 10^{-22}$ s/fm (solid).

Figure 2. Two-body collisions.

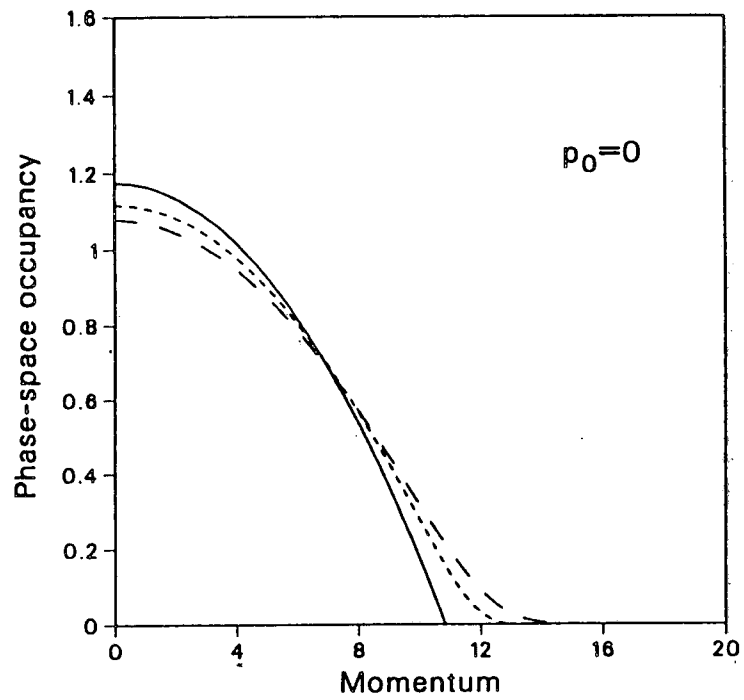
For the interesting part of phase space, the figure shows the trajectories of two particles as they approach each other head on from a large distance, interact via our standard Pauli potential (the Gaussian form (11) with the parameters given in (26)), and ultimately reseparate. The position is in units of fm and the momentum is in units of MeV $\cdot 10^{-22}$ s/fm.

Figure 3. Mean kinetic energy.

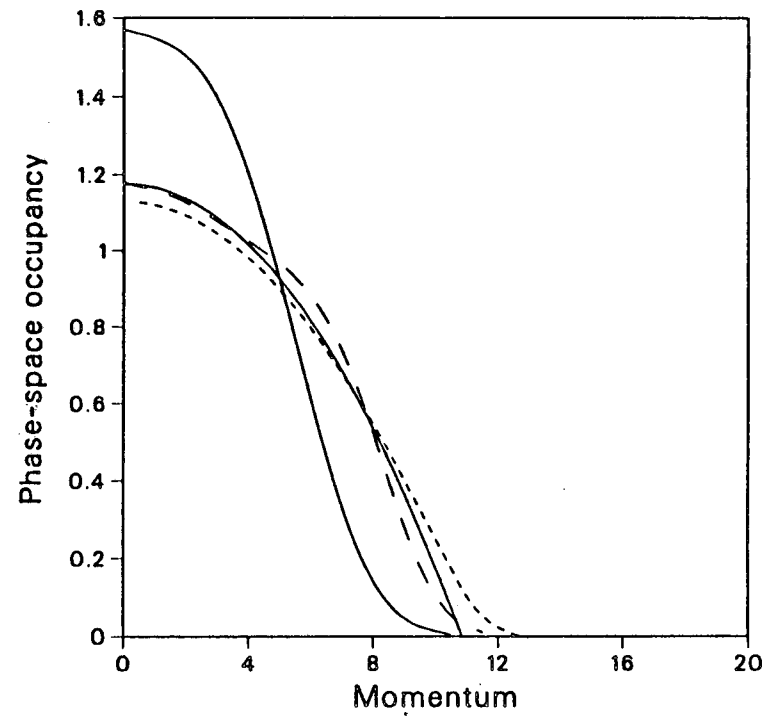
The figure shows the mean kinetic energy as a function of the temperature, for three different densities characterized by the Fermi kinetic energies $T_F = 18.5, 37, 74$ MeV. The dashed curves are the exact Fermi-gas values. The results obtained from the Metropolis calculation with our standard Pauli potential (11) are shown as shaded bands whose widths correspond to the associated statistical error.

Phase-space occupancy.

The figure displays the phase-space occupancy $f^{(1)}$ as a function of the magnitude of the momentum (in units of MeV $\cdot 10^{-22}$ s/fm), for four different values of the temperature. The dashed curve is the exact Fermi-gas values, while the histograms are calculated with our standard Pauli potential (11).

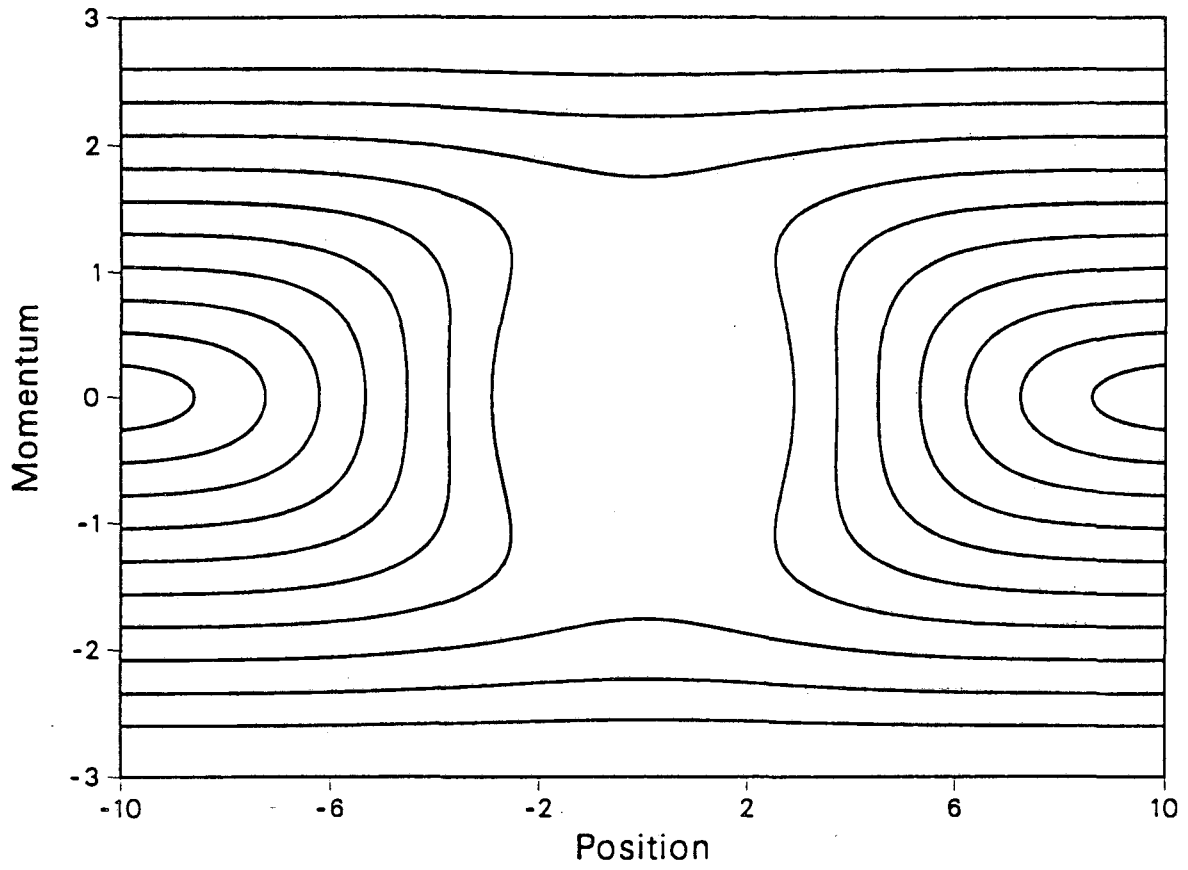


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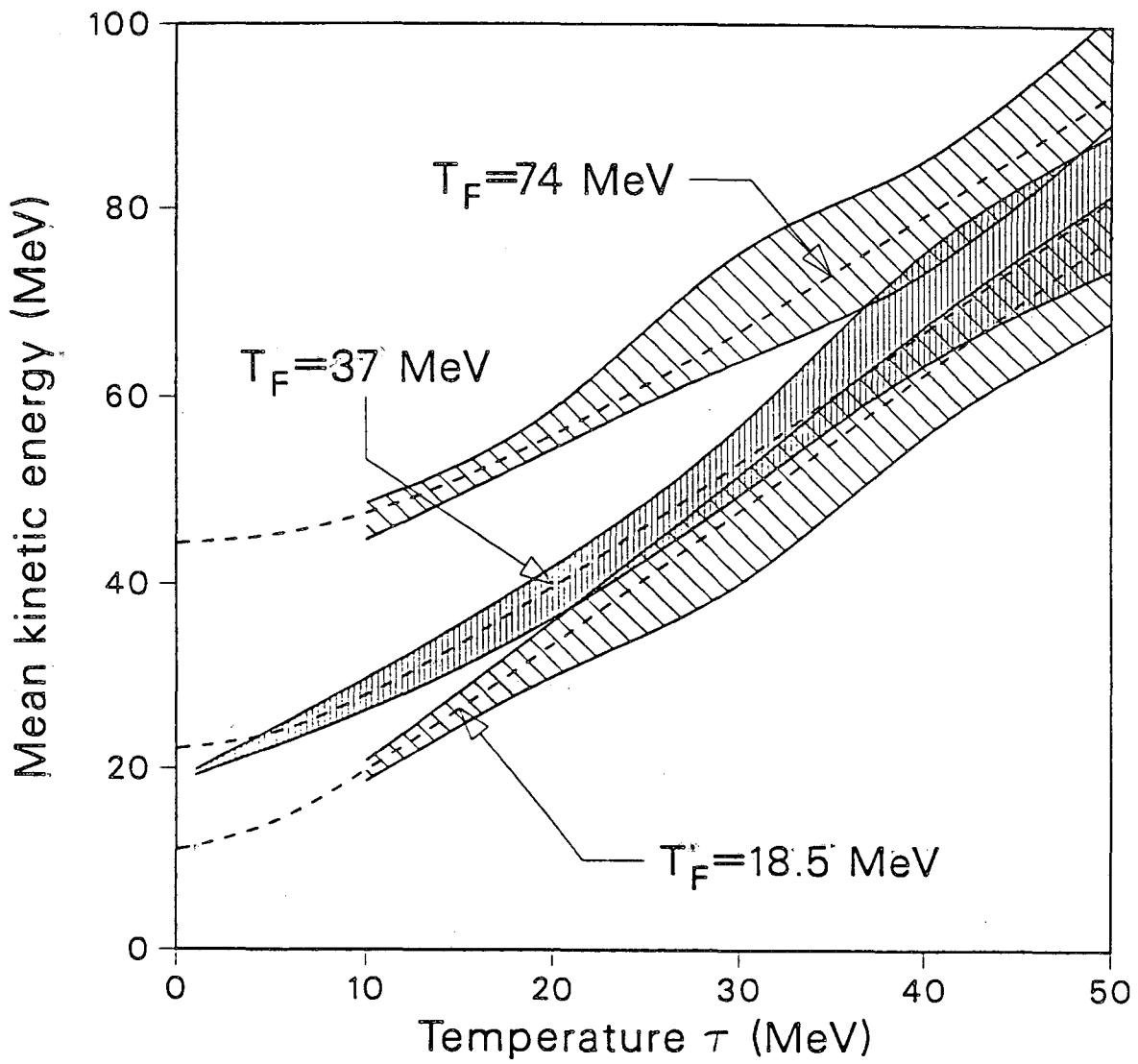
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Figure 1.



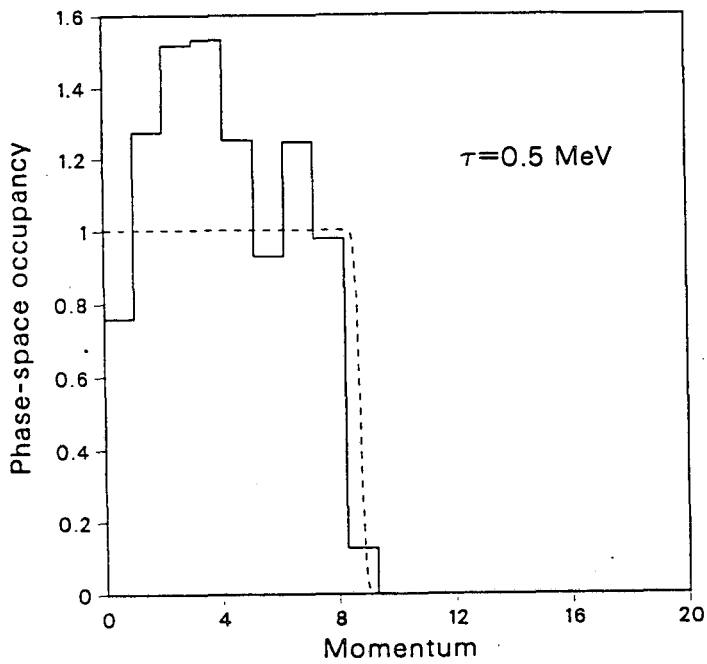
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Figure 2.

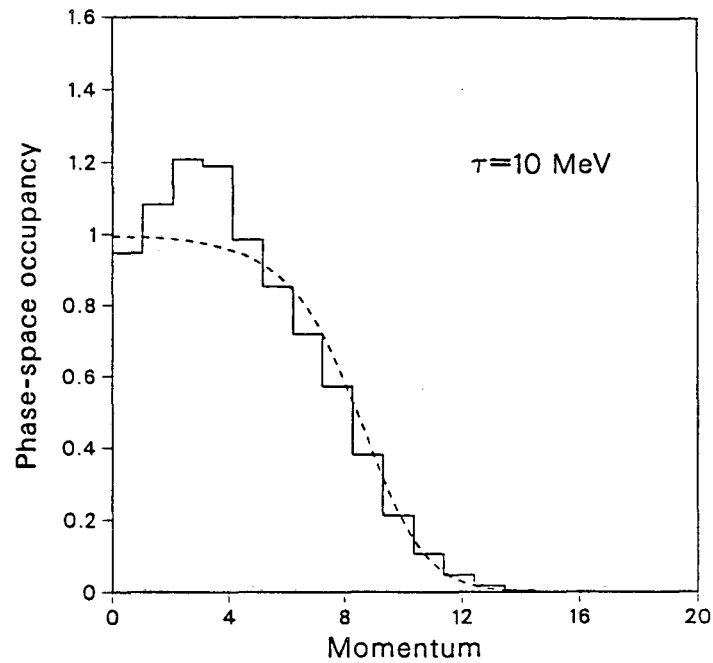


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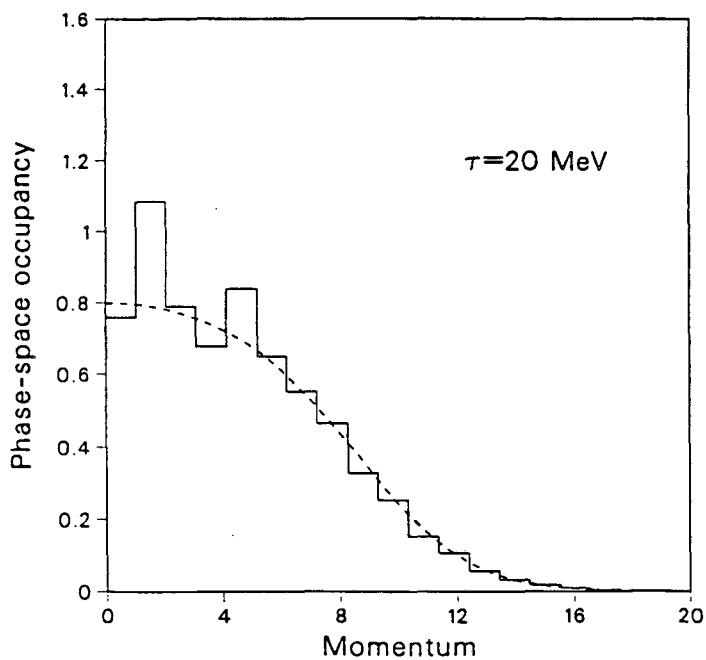
Figure 3:



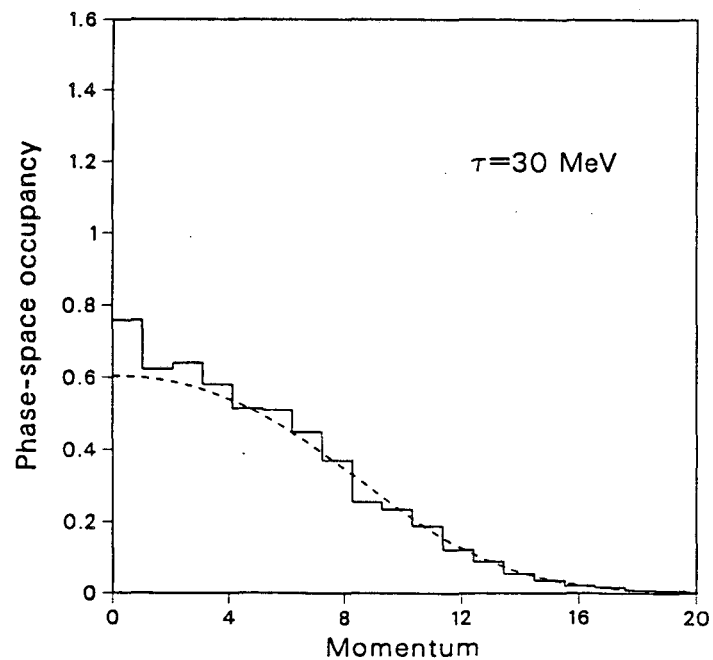
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XBL 8611-4687



XBL 8611-4688

Figure 4.

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