Classical Lagrangian Model of the Pauli Principle

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ABSTRACT

A classical Lagrangian model of the Pauli potential is introduced. It is shown that the kinematic kinetic energy ($\sum \frac{1}{2}mv^2$) in the model approximately reproduces the energy of a free Fermi gas at low temperatures and at densities relevant in nuclear collisions with moderate beam energies. Differences between canonical and kinematic quantities are pointed out. The Pauli potential can be used in transport simulations.
Nuclear collisions at beam energies on the order of 100 MeV/nucleon offer a unique testing ground for the dynamics of many-fermion systems. After pioneering studies at the Berkeley Bevalac, the SIS-18 accelerator in Darmstadt has now become the main theater for the experimental investigation of the rich variety of phenomena displayed in these collisions.

Semiclassical approximations proved to be useful in modeling nuclear collisions at these energies. The resulting transport codes, which are based on the Boltzmann equation, are at present the main tools used to extract physical information from the data. Although these models are popular and successful, most of them make a large number of simplifying assumptions and face difficulties with some aspects of the physics as well as with the numerical implementation. Many of the difficulties can be traced back to the problem of enforcing the restrictions on the occupancy of states implied by the Fermi statistics of the nucleons.

An alternative approach is to seek a classical many-body description simulating the effect of the Pauli principle. This can be accomplished by a potential that keeps the nucleons apart in phase space (‘Pauli potential’). Such a classical model was first proposed by Wilets and collaborators.\[1\] It has been demonstrated that many features of the Fermi gas can approximately be reproduced with a suitably chosen Pauli potential.\[2\] The Pauli potential has been incorporated in computational simulations of nuclear collisions.\[3, 4, 5\] One major advantage of classical dynamical models is that once the model is defined, no further approximations are necessary.

An important consequence of the introduction of the Pauli potential is that differences appear between the canonical and the kinematic quantities. This complication can be ignored as long as attention is focused only on the canonical momenta. Here we argue that one needs to keep track of the differences between canonical and kinematic quantities, and that the latter determine several physical observables of interest. In particular, thermodynamic quantities will be sensitive to the kinematic momenta. (Note that there are analogous differences between the canonical and kinematic momenta in the fermionic molecular dynamics model developed by Feldmeier.\[6\]) The classical simulations mentioned above have all been carried out in the Hamiltonian framework, where the natural variables are the canonical rather than the kinematic momenta.

Motivated by the above arguments, we study a classical Lagrangian model of the ‘Pauli potential,’ which can be used in collision simulations. The fermion nature of the nucleons, which is the most important quantum feature in nuclear collisions, should be retained in these simulations even if other quantum corrections are neglected. In common with earlier work, we aim at a model which implements the ‘Pauli principle’ in a classical framework (by this we mean that identical nucleons must be kept apart in the phase space). However, we depart from earlier studies by presenting calculations in the Lagrangian formalism.

Formally, the Hamiltonian for any physical problem must be constructed via the Lagrangian.\[7\] The Lagrangian is a function of \( n \) generalized coordinates \( q_i \), their time-derivatives, \( \dot{q}_i \), and possibly the time. (We will only deal with Lagrangians \( L(\ldots, q_i, \dot{q}_i, \ldots) \) without explicit time-dependence in the following.) The Hamiltonian \( H \) is obtained by introducing the canonical momenta, \( p_i = \partial L/\partial \dot{q}_i \), then constructing...
$H = \sum \dot{q}_i p_i - L$, and expressing it as a function of $q_i$ and $p_i$ only.

Pauli potentials have been defined in the past as (canonical) momentum-dependent potentials for inclusion in the Hamiltonian formalism.\cite{1, 3, 2, 4} We call this class of potentials Hamiltonian Pauli potentials. As an example, consider the Hamiltonian Pauli potential between two nucleons of relative separation $x$ and relative canonical momentum $p$ (in one dimension),

$$V(x, p) = V_0 \exp(-s^2/2), \quad (1)$$

where $V_0$ is a constant ($V_0 > 0$), and the phase-space separation $s$ is given as

$$s = \sqrt{(x/x_0)^2 + (p/p_0)^2}, \quad (2)$$

with appropriate length- and momentum-scales $x_0$ and $p_0$, respectively.\cite{2} To see to what extent $p$ is different from the kinematic momentum, $\mu \dot{x}$, one may use the canonical equation

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{\mu} \left( 1 - \frac{V_0}{p_0^2} e^{-s^2/2} \right), \quad (3)$$

where $\mu$ is the reduced mass. In other words, the velocity is decreased by the presence of the Pauli potential. The effect is negligible for nucleons far apart in phase space, but leads to a ‘crystallized’ ground state if the same potential is used in the many-body problem representing a nucleus.\cite{2} In the many-body ground state the nucleons have finite (canonical) momenta, but vanishing velocities.

A Pauli potential similar to the one given in eq. (1) has been arrived at based on a consideration of the evolution of two Gaussian wave packets,\cite{4} while a Hamiltonian Pauli potential with quite different scaling properties is used by Wilets and collaborators (also in atomic processes).\cite{8}

The one-dimensional two-body problem has recently been examined with a simplified version of the Pauli potential, where it was possible to carry out all calculations in both the Lagrangian and Hamiltonian formalisms.\cite{9} The difference between the canonical and the kinematic quantities has been demonstrated in this simplified framework.

Here we employ a more realistic Lagrangian Pauli potential inspired by the Hamiltonian form (1). We take

$$V(x, \dot{x}) = V_0 \exp(-t^2/2), \quad (4)$$

where the separation $t$ in $(x, \dot{x})$ space is given by

$$t = \sqrt{(x/x_0)^2 + (\dot{x}/v_0)^2}, \quad (5)$$

with scale parameters $x_0$ and $v_0$. For the two-body problem defined by this Lagrangian Pauli potential,

$$p = \frac{\partial L}{\partial \dot{x}} = \left( 1 + \frac{V_0}{\mu v_0^2} e^{-t^2/2} \right) \mu \dot{x}. \quad (6)$$
It is worth noting that $\mu \dot{x}$ is the relevant quantity in nucleon-nucleon collisions, cross sections, and with respect to the thermodynamics of the system.

We wish to investigate the finite-temperature behavior of a system of particles interacting via the Lagrangian Pauli potential \((4)\). The three-dimensional many-body Lagrangian takes the form

$$L = \frac{mN}{2} \sum_i (\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2) - \frac{V_0}{2} \sum_{i \neq j} \exp \left[ -\frac{\left\{ \left( \frac{r_{ij}}{r} \right)^2 + \left( \frac{v_{ij}}{v} \right)^2 \right\}}{2} \right],$$

with relative coordinates $r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$, and relative velocities $v_{ij} = \sqrt{(\dot{x}_i - \dot{x}_j)^2 + (\dot{y}_i - \dot{y}_j)^2 + (\dot{z}_i - \dot{z}_j)^2}$. As before, $V_0$ is the overall strength, $r$ and $v$ are scale parameters, and $m_N$ stands for the nucleon mass.

In what follows, we focus on the behavior of the many-body system at low temperatures (up to $\approx 5$ MeV) and densities corresponding to deviations from standard nuclear matter density that are not too large. The latter requirement means that densities around $0.04$ fm$^{-3}$ will be considered for a given type of nucleon with a given spin orientation.

Thermal averaging is carried out in the phase space defined by canonically conjugate variables. Schematically, for an observable $A(x, p)$,

$$\overline{A} = \frac{\int dx dp e^{-\beta H} A(x, p)}{\int dx dp e^{-\beta H}},$$

where the integrals are over the phase space, and $\beta$ is the inverse temperature. We emphasize that $p$ in eq. \((8)\) stands for the canonical momentum. It is therefore necessary to first map the $(x, \dot{x})$ space to the $(x, p)$ space in the present formalism before applying the Metropolis algorithm \([10]\) to calculate averages. The mapping in the $\dot{x} \rightarrow p$ direction poses no technical problem with our Lagrangian Pauli potential, so each trial step is made first in $(x, \dot{x})$ space and then the corresponding step in $(x, p)$ space is measured. This measurement is used to rescale the $(x, \dot{x})$ step so that we get a uniform walk through $(x, p)$ space. In order to maintain full control over the resulting step size in the $p$ subspace, it is necessary to hold the $x$’s constant while changing the $\dot{x}$’s. For this reason we split the calculation into two parts: a standard Monte Carlo sampling of $x$-configurations, and a Metropolis sampling over the $p$-subspace (“$p$-Metropolis procedure”) for each $x$-configuration.

Several (typically ten) $x$-configurations are chosen for each temperature by filling a specified volume (periodic boundary conditions) with $N$ nucleons at random. We have chosen $N = 60$ for the illustrative results presented here. We examined the dependence of our calculations on the number of nucleons and found small surface effects to be still present for $N = 60$. However, since the required CPU time is approximately quadratic in $N$, we carried out most of our calculations with this value. The surface effects can be decreased by decreasing the range of the Pauli potential in coordinate space.

The nucleons are held at fixed positions while their momenta are changed during the $p$-Metropolis procedure. The results for the different $x$-configurations are then
averaged with equal weights, and their spread around the average divided by the square root of the number of $x$-configurations provides an estimate of the statistical uncertainty in the result for the given temperature.

To achieve fast equilibration, the step size is continually adjusted at the beginning of the $p$-Metropolis procedure, so that about half of the attempted steps are accepted (or rejected). We assume that equilibrium has been sufficiently approached when the procedure yields the first extremum of $\mathbf{\Pi}$. Averaging is started at this point with a constant step size in momentum space.

Specifically, we put $A = E_{\text{kin}}/N$ in eq. (8), where by $E_{\text{kin}}$ we mean the kinematic kinetic energy,

$$E_{\text{kin}} = \sum_i \frac{1}{2} m_N v_i^2 = \frac{m_N}{2} \sum_i (\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2).$$

We study the dependence of this quantity on the temperature and density, since (as mentioned above) the kinematic quantities are most important for the purposes of simulations and thermodynamics. We therefore wish to judge the success of our model by the extent to which (9) reproduces the kinetic energy of a Fermi gas (which, in the case of a free Fermi gas, is identical to the total energy).

The temperature dependence of the results is displayed on Fig. 1 for the parameters $V_0 = 1.17$ GeV, $r = 1.5$ fm, and $v = 0.163c$. The density has been fixed at the value corresponding to standard nuclear matter density. The calculations are represented by the points with their statistical uncertainties at different temperatures. The dashed line corresponds to a quadratic least-square fit through these points with reduced $\chi^2 \approx 0.81$. (A linear least-square fit would yield reduced $\chi^2 \approx 1.23$.) Also shown (solid line) is the temperature dependence of the energy per particle of an ideal Fermi gas in the low-temperature approximation (through second order in the ratio of the temperature to the Fermi energy, $T/\epsilon_F$). The three parameters of the Pauli potential can be used to approximately reproduce the ground-state energy of the Fermi gas, $\frac{3}{2} \epsilon_F$, and can be traded against each other to some extent to obtain fits of similar quality. We chose a strong Pauli potential with relatively small ranges. The calculated results are not inconsistent with the desired behavior in the temperature range of interest, but the fit overestimates the specific heat.

Fig. 2 shows the dependence of the kinematic kinetic energy per nucleon on the density at a temperature of 0.5 MeV for the same values of the parameters. It is seen that the desired Fermi-gas behavior (solid curve) is approximately reproduced. Numerically, the agreement can be judged sufficiently close up to densities corresponding to about 1.5 standard nuclear matter density.

Fig. 3 displays an example of the distribution function in the kinematic kinetic energy, $\sum \frac{1}{2} m v^2$ at a temperature $T = 5$ MeV in our model. While the histogram (model) reproduces the Fermi gas (dashed line) only approximately, we can see that the occupation of the low energies is limited, in contrast to the expectation for a classical system without the Pauli potential. The distributions at other temperatures have qualitatively similar features.

In the present work we have calculated the temperature and density dependence of the kinematic kinetic energy of a classical system of particles under the influence
of a Pauli potential. The precise meaning of the Pauli principle in the classical framework used here and in standard Hamiltonian simulations is of course open to interpretation to some degree. It is physically clear, however, that the Pauli principle keeps identical nucleons apart in phase space. Such a requirement can be satisfied with both Lagrangian and Hamiltonian Pauli potentials. Here we used this freedom of implementation to introduce a Lagrangian Pauli potential. The kinematic kinetic energy in the model approximately reproduces the energy of a free Fermi gas at low temperature and at densities relevant in nuclear collisions with moderate beam energies. We emphasized the role of the kinematic quantities (as opposed to canonical momenta) for thermodynamic purposes. These kinematic quantities can be calculated in the model. We foresee applications of this Pauli potential to situations wherein fragmentation or evaporation at low temperatures plays an important role.

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Figure Captions

**Fig. 1:** The average kinematic kinetic energy per nucleon as a function of the temperature at the density $\rho = 0.04 \text{ fm}^{-3}$. The dashed line corresponds to a quadratic least-square fit as explained in the text. The solid line represents an ideal Fermi gas in the low-temperature approximation.

**Fig. 2:** The average kinematic kinetic energy per nucleon as a function of the density at temperature $T = 0.5 \text{ MeV}$. The dashed line is a fit through the data. The solid line displays the Fermi-gas result.

**Fig. 3:** The distribution function in terms of the kinematic kinetic energy at temperature $T = 5 \text{ MeV}$. The histogram represents the model, the dashed line corresponds to an ideal Fermi gas.
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