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Why the Salpeter approximation is not valid in the Sun

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Abstract

We review the derivation of the electrostatic screening effect from first principles. We show that under the conditions prevailing in the Sun the number of particles in the Debye sphere is of the order of unity. Consequently, fluctuations play a dominant role in the screening process and lead to an energy exchange between the scattering particles and the surrounding plasma that depends on the energy of the particles. Extensive molecular dynamics calculations show that low-energy particles gain on the average energy from the plasma while high-energy particles lose energy to the plasma, in contrast with the classical Salpeter picture in which all particles gain during the close approach to each other the mean Coulomb energy.

Next, we adopt the Langevin equation for charged particles with the Rosenbluth potential. We show how the two completely independent methods, the molecular dynamics and Langevin equation, yield the same physical results.

We then review the arguments for a static screening based on a static potential and show its basic assumptions and shortcomings. The particular assumptions leading to the Salpeter formula are discussed along with the approximations involved in its derivation. One of the tacit fundamental assumptions in the Salpeter approximation is that the scattering is fully elastic. The inelastic nature of the collisions which are dominant under the solar conditions is clarified.

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1. Introduction

The rates of the nuclear reactions that take place in dense stellar cores are affected by the environment. The effect is known as the screening factor. The Salpeter (1954) theory predicts an enhancement of the rate of all nuclear reactions by a factor which in the limit of weak

screening is given by $\exp(U/kT)$, where $U = Z_1 Z_2 e^2/(R_D kT)$, and where R_D is the Debye radius.

Salpeter (1954) assumed a mean-field theory and stated the approximations involved. Salpeter defined the screening as the extra energy gained by a pair of approaching particles over their relative kinetic energy at large separation. Alastuey and Jancovici (1978) formulated the screening as the enhancement of the population of particles at vanishing separation.

Recently Bahcall *et al* (2001) (hereafter BBGS) have discussed the Salpeter formula and claimed that it should apply to the Sun and that all claims concerning dynamic effects are wrong, including the recent results of Shaviv and Shaviv (2001) (hereafter SS01).

The discussion of BBGS (and implicitly in Alastuey and Jancovici (1978)) is based on the mean-field electrostatic potential. Further, the authors assume that two interacting ions *always* gain energy from the plasma, as the particles approach each other. This additional energy, the screening energy, is taken to be just the mean-field potential of the ions in the plasma, namely, the *long time average* (the thermodynamic time) of the potential felt by an ion in the plasma. As the particles move apart the tacit assumption is that this extra energy is *exactly* returned to the plasma.

The source of the problem in our opinion is the confusion between the statistical and long time averaged behaviour on one hand and the dynamic behaviour of dense plasma on the other. BBGS are of the idea that the screening problem is a static one while we claim that under the conditions in the Sun it is a dynamic one and should be treated as such. When one treats the screening of scattering particles from first principles one finds that not all particles gain the same energy during the close approach. Slow particles gain energy while fast particles lose. Moreover, the energy gain/loss is not a trivial function of the relative kinetic energy, as will be shown later.

In the first part of this paper we present the results of the molecular dynamic (here after MD) method and the agreement between the MD predictions and classical statistical mechanics and (1) infer the critical properties of the collisions between plasma particles, (2) define the screening energy and (3) discuss typical results. Next, we turn to a completely different method to calculate the screening using the Langevin formalism. We show that the qualitative nature of the results does not change. We end with a discussion of the BBGS arguments and show their physical implausibity.

2. *Ab initio* molecular dynamics approach

The advantage of the MD approach is that it is *ab initio*, namely it starts from first principles with no assumptions about mean-field, fluctuations, energy exchange, etc. The disadvantage is the rather long CPU time required for calculations with proper statistics. The MD method used was described in detail by Shaviv and Shaviv (2000) (hereafter SS00).

A critical issue is the boundary conditions. In the classical MD calculations periodic boundary conditions are assumed. The periodicity means that each ion and electron carries with itself as it moves in the calculation box, an infinite series of images in the x, y and z directions.

When a real particle moves the images move as well. Consequently, as the recoil of a real charge is calculated, an identical recoil is tacitly assumed for all images. The disadvantage of this approach is that only the recoil of the real particles interacting with a single ion is calculated correctly. The images have a vanishing effective mass and the recoil is identical to that of the real charge. In this way, the energy gain/loss by scattering particles from the plasma is poorly approximated.

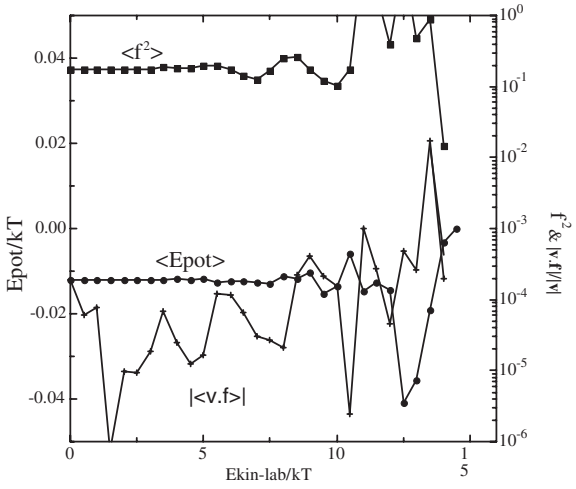

Figure 1. The dependence of the long time average potential energy per particle on the kinetic energy in the laboratory. The filled circles represent the mean potential energy of the protons. The filled squares are the mean of instantaneous force squared acting on the particle averaged over particles in the energy bin and time. The pluses represent the absolute value of the average force.

To prevent the neglect of the recoil, we use a large number of particles (at least $N = 40^3$ and frequently more). For more details see SS00.

2.1. The statistical mechanics results

A fundamental prediction of statistical mechanics is that if the distribution function is separable, then the mean potential energy of a particle does not depend on the kinetic energy. When such a separation exists, if one considers the potential energy of particles in the energy range $(E_{\rm kin}, E_{\rm kin} + \Delta E)$ then the result for the long time average potential should be independent of $E_{\rm kin}$ or ΔE. We have therefore run a calculation in which the long time average potential energy as a function of kinetic energy was carried out as follows:

$$U(E_{\rm kin}, E_{\rm kin} + \Delta E_{\rm kin}) = \lim_{L\to\infty}\left(\frac{1}{NL}\right)\sum_{l=l_0}^{L}\sum_{i=1}^{N} u_i(l\tau)O\left(E_{\rm kin}, E^i_{\rm kin}\right) \tag{1}$$

where $u_i(l\tau)$ is the potential energy of particle i at time $l\tau$. τ is the time step and l is the summation index. The function $O\left(E_{\rm kin}, E^i_{\rm kin}\right)$ is defined by

$$O\left(E_{\rm kin}, E^i_{\rm kin}\right) = \begin{cases} 1 & \text{if} \quad E_{\rm kin} \leqslant E^i_{\rm kin} \leqslant E_{\rm kin} + \Delta E_{\rm kin} \\ 0 & \text{otherwise} \end{cases}. \tag{2}$$

The function O assures that the potential energy of only particles in the right energy bin is summed up in the averaging process. Note that the potential energy of any ion is not constant as a function of time. However, the long time average of all ions should be the same. Here we go one step further and check the long time average when the particles are in a restricted kinetic energy range.

In figure 1 we show the long time average potential energy as a function of the energy bin. The energy bins are 0.05 kT wide. Also shown is the time average of the force and the time average of the force squared.

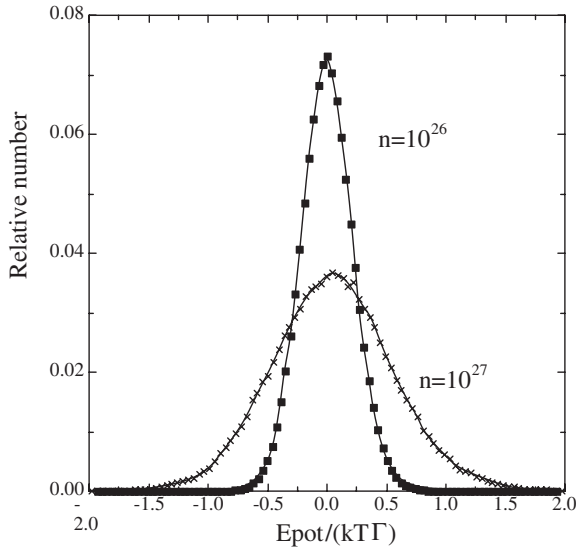

Figure 2. The distribution of the proton potential energy at a given time. The results are shown for $T = 1.5 \times 10^7$ K and $n = 10^{26}\#/cc$ and for $n = 10^{27}\#/cc$. The distributions are normalized to unity and given in units of $kT\Gamma$.

We see that: (a) the mean potential energy does not depend on the kinetic energy; (b) the absolute value of the mean force vanishes; (c) the mean of the square root of the force squared is large.

A few comments: the force acting on a particle in the plasma fluctuates with a large amplitude around a vanishing mean. The vanishing of the mean force agrees with the assumption that the mean potential is spherically symmetric and the ion sits at the centre (at rest). However, the non-vanishing of the instant force implies large fluctuations in the force (the fluctuations are in magnitude and direction). Clearly, assuming a smooth constant in the time potential may lead to large errors in the dynamic problem of screening.

2.2. The distribution of the potential energy of particles

The number of particles in a Debye sphere is given by

$$N_D = (4\pi/3)R_D^3 \qquad \text{where} \quad R_D^2 = kT/4\pi e^2 \sum_j \left(Z_j^2 + Z_j\right)n_j \tag{3}$$

where n_j is the number density of species j with charge Z_j. This expression assumes that both the electrons and the ions contribute to the Debye potential. Assuming pure hydrogen plasma, $n = 10^{26}$ and $T = 1.5 \times 10^7$ K we find that in the core of the Sun $R_D = 0.877\langle r\rangle$ where $\langle r\rangle = n^{-1/3}$ and $N_D = 2.83$.

As the potential part of the distribution function of the particles is $F_N \approx \exp(\varphi_{ij}/kT)$, where φ_{ij} is the Coulomb interaction between two particles, one expects that the potential energy of the single particle will also have a distribution (in contrast to a constant value equal to the mean thermodynamic value).

Namely, not all particles have the same potential energy. Indeed, in figure 2 we show the potential energy distribution in equilibrium found in a snap shot. Two cases are shown: $T = 1.5 \times 10^7$, $n = 10^{26}\#/cc$ and $n = 10^{27}\#/cc$. The potential energy is given in units of

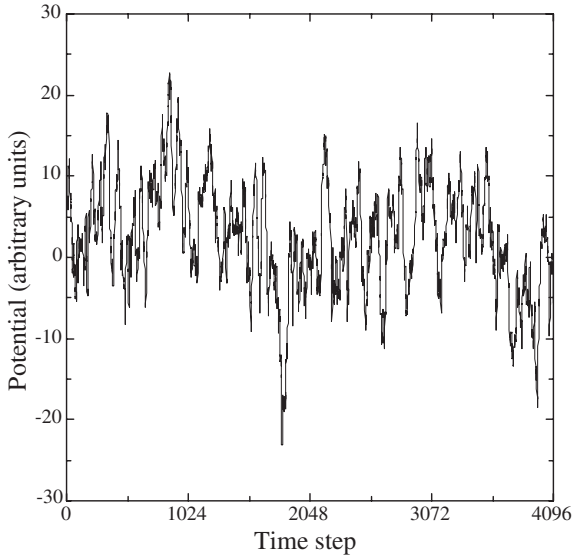

Figure 3. The time dependence of the potential of a single particle. The time steps are constant at 10^{-3} of the time units. The plasma frequency is beyond the range.

$kT\Gamma$ (where $\Gamma = e^2/\langle r\rangle kT$). The width of the distribution is proportional to $1/\sqrt{N_D}$ which in the present case is slightly less than unity. According to Ginzburg (1960), the fact that fluctuations are large implies that the mean-field theory is not a good approximation in this case.

2.3. A stochastic potential

We saw above that the force (and the potential) acting on a given particle in the plasma fluctuates. An example of the potential felt by a certain particle is shown in figure 3 over many time steps. The actual time step is significantly shorter than the fluctuations in the figure.

The physical picture that emerges from the MD calculation is that of protons interacting with a fluctuating cloud of positive and negative charges as well as with the target proton. Under these conditions, we have to see the interaction between the two protons as the effective interaction between two particles in a stochastic fluctuating medium. Hence a static potential cannot provide the entire picture. The stochastic approach can be described with a single particle Hamiltonian of the following form:

$$H_{i,p} = \frac{p^2}{2m} + V_0(r) + V_1(r,t) = H_0 + V_1(r,t) \tag{4}$$

where V_0 is the static potential. H_0 is the Hamiltonian that would lead to the Debye potential. V_1 represents the time-dependent part of the fluctuating environment around the interacting protons.

If $n_p(r,t)$ is the instantaneous number density of the protons then clearly one way to obtain the time-dependent potential is

$$V_1(r,t) = e^2 \int \mathrm{d}r' \frac{\delta n(r',t) - n_D(r')}{|r - r'|} \tag{5}$$

where the fluctuation beyond the local Debye potential is given by $\delta n(r,t)$. In other words, we expect $V_1(r,t)$ to vanish when the fluctuations decay as the number of particles in the Debye

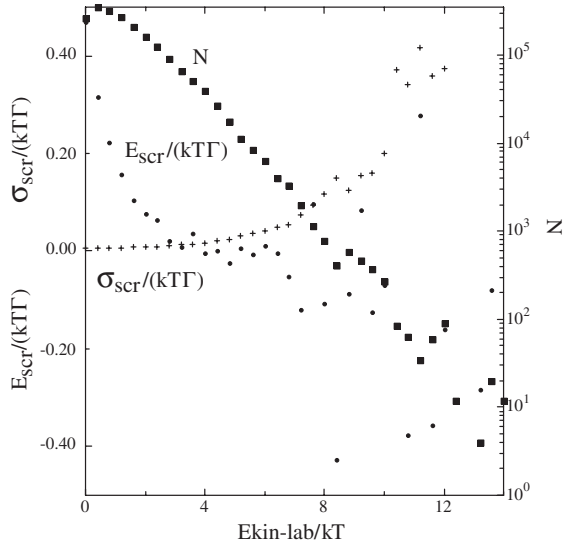

Figure 4. The screening energy as a function of the kinetic energy of the particle in the laboratory. Filled circles are the screening energy in units of kT. Crosses are the Gaussian dispersion given in the same units. Filled squares are the number of particles in the energy bin. The results are for $T = 1.5 \times 10^7$ K and $n = 10^{26}$ pure hydrogen composition.

sphere increases. Once the potential is a function of time the behaviour of particles with different velocities (or kinetic energies) differs unlike the case of a time-independent potential where all particles gain/lose the same energy. Moreover, the time dependence is required to describe the energy exchange between the variable environment and the scattered particle.

2.4. A simple definition of the screening

The MD method allows us to define the screening energy in a simple and clear way. Consider two particles i and j moving in the plasma and scatter one off the other. Let $E_i^{\text{tot}-L,f}$ be the total energy of particle i of the pair when they are far apart and let $E_i^{\text{tot}-L,c}$ be the total energy when they reach the distance of closest approach. The screening energy is given by

$$E_{i,\text{scr}} = E_i^{\text{tot}-L,c} - E_i^{\text{tot}-L,f}. \tag{6}$$

A symmetric expression exists for particle j. The total energy includes kinetic as well as potential parts and is evaluated in the laboratory. The screening energy is the energy gained/lost by a pair of scattering protons as they move from far away to the distance of closest approach. This is very close to the original definition given by Salpeter (1954) to the screening energy (cf ibid equation (2)). In figure 4 we show the results for the screening energy. Clearly, particles with low kinetic energy absorb energy from the plasma during the approach from far away to the distance of closest approach, while particles with high energy lose energy to the plasma. The results can be easily understood in dynamic terms: the plasma contains mainly protons with kinetic energies of the order of kT. When a particle with high kinetic energy penetrates the screening cloud it loses energy to the plasma. On the other hand, a low-energy particle gains energy.

3. Self-consistent Langevin simulation of Coulomb collisions in plasma

We consider a head-on collision between two protons immersed in a fully ionized hydrogen plasma. We write the equations of motion as

$$\begin{aligned} m_{p,1}\frac{\mathrm{d}\mathbf{v}_1}{\mathrm{d}t} &= e^2\frac{\mathbf{r}_{12}}{|r_{12}|^3} + e^2\sum_{i\neq 1,2}^{N}\frac{\mathbf{r}_{1i}}{|r_{1i}|^3} \\ m_{p,2}\frac{\mathrm{d}\mathbf{v}_2}{\mathrm{d}t} &= e^2\frac{\mathbf{r}_{21}}{|r_{21}|^3} + e^2\sum_{i\neq 1,2}^{N}\frac{\mathbf{r}_{2i}}{|r_{2i}|^3} \end{aligned} \tag{7}$$

where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ and we separate the direct interaction between the two scattering particles and the interaction between each one of them and the rest of the particles in the plasma. The summation is carried over all particles. At this point the electrons are treated like protons with opposite charge so that the sum runs over all particles in the plasma. The two scattering protons have indices p_1 and p_2 while the field ions (which can be electrons, protons or heavier ions) are marked with index β.

The idea now is to replace the potential due to all other particles by dynamic friction and a stochastic force and obtain the corresponding Langevin equations for the two protons moving in the plasma (cf Qiang *et al* 2000, Riskin 1997, Bobylev and Nanbu 2000), namely

$$\begin{aligned} m_{p,1}\frac{\mathrm{d}\mathbf{v}_1}{\mathrm{d}t} &= e^2\frac{\mathbf{r}_{12}}{|r_{12}|^3} + m_{p,1}\mathbf{F}_d(\mathbf{v}_1) + m_{p,1}\mathbf{Q}_1(\mathbf{v}_1)\cdot\mathbf{S}(t) \\ m_{p,2}\frac{\mathrm{d}\mathbf{v}_2}{\mathrm{d}t} &= e^2\frac{\mathbf{r}_{21}}{|r_{21}|^3} + m_{p,2}\mathbf{F}_d(\mathbf{v}_2) + m_{p,2}\mathbf{Q}_2(\mathbf{v}_2)\cdot\mathbf{S}(t) \end{aligned} \tag{8}$$

where $\mathbf{F}_d$ is a deterministic dynamic friction force and the vector $\mathbf{S}$ is a random vector with the following properties:

$$\langle S(t)\rangle = 0 \qquad \text{and} \qquad \langle S_i(t)S_j(t)\rangle = \delta_{ij}\delta_D(t-t') \qquad i,j = 1,2,3,\ldots \tag{9}$$

namely completely stochastic. Here δ_D is the Dirac δ function. The force term Q_i is known as the Langevin force (i is the index of the particle. $\mathbf{Q}$ is a tensor).

Rosenbluth *et al* (1957) have shown that in the case of a plasma, the dynamic friction can be described as a generalized potential now known as the Rosenbluth potential. Assume a particle moves through a plasma composed of ions β, then the dynamic friction force exerted by the β particles on particle α, $\mathbf{F}_\alpha$, is given as

$$\mathbf{F}_\alpha(\mathbf{v}) = -\lambda\frac{m_\alpha + m_\beta}{m_\alpha m_\beta}(4\pi e_\alpha e_\beta)^2\nabla_v\varphi_\beta(\mathbf{v}). \tag{10}$$

When different species β exist, the force is the sum over the force exerted by each species separately. $\lambda = \ln\Gamma$ is the classical Coulomb cutoff . The first Rosenbluth potential φ is given by

$$\varphi_\beta(\mathbf{v}) = -\frac{1}{4\pi}\int\frac{f_\beta(v')\,\mathrm{d}v'}{|v-v'|} \tag{11}$$

where the integration is carried over the velocity distribution of the scattering particles $f_\beta(v)$. The tensor $\mathbf{Q}$ is derived from the diffusion tensor via the relation $D_{ij} = Q_{ik}Q_{jk}$ where

$$D_{ij} = C\frac{\partial^2\mathbf{G}(\mathbf{v})}{\partial\mathbf{v}_i\partial\mathbf{v}_j} \qquad \text{where} \quad \mathbf{G}(\mathbf{v}) = \int f(\mathbf{v}_\beta)|\mathbf{v}-\mathbf{v}_\beta|\mathrm{d}\mathbf{v}_\beta \tag{12}$$

$\mathbf{G}(\mathbf{v})$ is the second Rosenbluth potential and it is related to the first one (Qiang *et al* 2000).

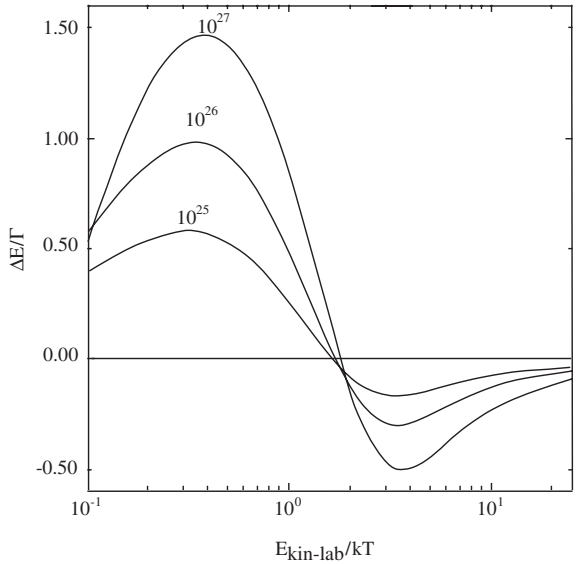

Figure 5. The solution to the Langevin equation for three plasma densities. The energy gain/loss by two protons scattering off each other in a head-on collision is shown as a function of the relative kinetic energy at large separation.

The above Langevin equation relates the states of the particles before and after the collision. We are interested in the relation between the state of the particles before the collision and the state of the particles at the classical turning point (Qiang *et al* 2000, Lampe *et al* 2000, Manheimer *et al* 1997, Fang 1978).

Next, we assume the plasma to be in equilibrium and hence assume the Maxwellian distribution so that the Rosenbluth potential becomes (see Shohet 1971, Sturrock 1994):

$$\varphi_\beta(v_z) = n_\beta \left(\frac{m_\beta}{2\pi kT}\right)^{3/2} \frac{4\pi}{v_z} \int_0^{v_z} \exp\left(-\frac{m_\beta v_\beta^2}{2kT}\right) v_\beta^2 \, \mathrm{d}v_\beta. \tag{13}$$

To simplify the physics we consider the two particles to move along the z axis and calculate the energy change due to the dynamic force.

In figure 5 we show the solution of the Langevin equation for particles arriving from far away and undergoing a head-on collision with one another. The results are given in terms of the absolute energy. The results for the energy gain/loss are given in units of Γ. We see the anticipated behaviour, namely, when the energy is low relative to kT, the particle gains energy from the plasma and vice versa when the energy is high. These results, which are based on simplified analytical potentials, confirm the basic results of the MD calculations.

The stochastic term **Q** gives rise to a distribution around the mean results shown in figure 5. Detailed results will be reported elsewhere.

4. The arguments justifying the Salpeter approximation

BBGS attempt to explain why the Salpeter formula is the correct and accurate one under the conditions prevailing in the core of the Sun. In doing so they misquote Salpeter (1954). As a matter of fact, the argument given by BBGS is not the one given by Salpeter (1954). In principle, our definition of the screening energy conforms with Salpeter's definition (except

for the fact that Salpeter defines the screening energy in the centre of mass system while we use the laboratory system).

Salpeter argues about the validity of the approximations he implemented in his derivation: 'We have used a continuous (average) charge density $\bar{\rho}(r)$ and in its evaluation have used the statistical Boltzmann factor $\exp[-U(r)/kT]$ for particles at the point r. For this procedure to be strictly valid many nuclei and electrons should be contained in a volume small enough so that $\bar{\rho}(r)$ and $U(r)$ do not vary appreciably over this volume'. In other words, Salpeter (1954) discusses density fluctuations and states that he ignores them in his approximation. The Salpeter (1954) approximation boils down to assuming negligible density spatial fluctuations.

We turn now to discuss the plausibility of the physical dynamic argument. Let $\langle \delta E_{\rm in}(E_{\rm kin}^{-\infty})\rangle$ be the average energy gain/loss by two approaching particles, the energy of which at large separation is $E_{\rm kin}^{-\infty}$. Note that the energy gain/loss $\delta E_{\rm in}(E_{\rm kin}^{-\infty})$ may have a distribution and we here use the average over this distribution.

We assume here that the average energy gain/loss by the particles depends on the relative kinetic energy at large separation. Similarly, let $\langle \delta E_{\rm out}(E_{\rm kin}^{\infty})\rangle$ be the average energy gain/loss by two particles as they move from the distance of closest approach to a large separation. Again, we assume dependence on the relative kinetic energy at large separation. Define by $\Delta E_{\rm coll}(E_{\rm kin}^{-\infty})$ the energy change in a collision by a pair of particles that have before the scattering a relative kinetic energy $E_{\rm kin}^{-\infty}$ and after the collision they have a relative kinetic energy of $E_{\rm kin}^{\infty} = E_{\rm kin}^{-\infty} + \Delta E_{\rm coll}(E_{\rm kin}^{-\infty})$. In the general case (when the energy change depends on the relative kinetic energy at large separation) the total change in the relative energy during a collision of the two particles is given by

$$\Delta E_{\rm coll}(E_{\rm kin}^{-\infty}) = \int \delta E_{\rm in}(E_{\rm kin}^{-\infty} - E)\delta E_{\rm out}(E_{\rm kin}^{-\infty} + E)\,{\rm d}E \tag{14}$$

where the integration is carried out over all energies E. Let now $f(E_{\rm kin})$ be the distribution function of kinetic energies at equilibrium. Clearly, at equilibrium the following condition must hold

$$\langle \Delta E_{\rm coll}(E_{\rm kin}^{-\infty})\rangle = \int_0^{\infty} {\rm d}E_{\rm kin}^{-\infty} f(E_{\rm kin}^{-\infty})\Delta E_{\rm coll}(E_{\rm kin}^{-\infty}) = 0. \tag{15}$$

As the distribution is a positive definite function, it follows that either $\Delta E_{\rm coll}(E_{\rm kin}^{-\infty})$ changes sign at least once at some relative kinetic energy or $\Delta E_{\rm coll}(E_{\rm kin}^{-\infty}) \equiv 0$. The first possibility about the change of sign does not depend on the particular interaction but on the condition of equilibrium. This is exactly what the MD result shows. The Salpeter approximation corresponds to the second case, namely,

$$\begin{aligned} &\Delta E_{\rm coll}(E_{\rm kin}^{-\infty}) \equiv 0 \\ &\delta E_{\rm in}(E_{\rm kin}^{-\infty}) = \delta_D(\delta E_{\rm in} - U) \\ &\delta E_{\rm out}(E_{\rm kin}^{\infty}) = \delta_D(\delta E_{\rm out} + U). \end{aligned} \tag{16}$$

The first condition implies no change of energy in a collision irrespective of the relative energy at large separation. The second condition means that the energy gained by the two particles from the plasma upon approaching each other is constant and equal to the mean potential energy per particle. The third condition means that as the particles separate they always lose the same energy, namely the energy gained upon approach. Another way to put it is as follows: in the Salpeter approximation all proton–proton collisions are fully elastic, no energy is lost/gained to the plasma. The SS01 results are the extension to inelastic collisions.

The screening energy is $\delta E_{\rm in}(E_{\rm kin}^{-\infty})$ and the MD calculations as well as the Langevin equations show that it is positive for low $E_{\rm kin}^{-\infty}$ and negative for high kinetic energies.

5. Conclusions

The screening energy is associated with the relaxation processes in the plasma. Thermodynamic averages are long time averages and hence not relevant to the details of the scattering and the relaxation which takes place during single scatterings and collisions.

Fluctuations become important when $N_D \approx 1$ and as a consequence the scatterings take place under a time-dependent effective potential. The interaction with the fluctuations is such that on average low-energy particles gain energy and vice versa.

When a totally different method is used to calculate the classical screening, the same basic results are found, supporting the detailed results of the MD method.

Acknowledgment

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