Understanding the Screening of Nuclear Reaction in Stellar Cores

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The screening of nuclear reactions in stars takes place under the special conditions that the total number of particles in the screening cloud is of the order of unity. Hence, standard mean field theory is not expected to be valid. We demonstrate by the use of Molecular dynamics that fluctuations dominate the screening and lead to a smaller screening compared with the predictions of the classical mean field theory.

§1. Introduction

The rates of the nuclear reactions in dense stellar cores are affected by the environment. The effect is known as the screening enhancement (Schatzman 1948, Salpeter 1954). Salpeter (1954) assumed a mean field theory for the screening cloud, the Debye theory, and stated the approximations involved.

The mean field theory tacitly assumes that \( N_D = nR_D^3 \gg 1 \), where \( N_D \) is the number of particles in the screening cloud, \( n \) is the number density and \( R_D \) the Debye radius. The conditions in stars along the main sequence are such that \( N_D \approx 1 - 3 \) and the basic condition for the validity of mean field of the screening cloud is not satisfied (cf. Shaviv & Shaviv 2002, hereafter SS02).

A Coulomb plasma contains positive and negative particles both with an infinite range potential giving rise to a finite effective range, the Debye radius. To facilitate the understanding of the effect of the finite effective range on the screening, we experiment with an artificial potential with a finite range and show how the range affects the screening. The results are compared with those obtained using a mean field approximation. The calculation is carried out using Molecular Dynamics (hereafter MD), the advantage being that it is not bound by the validity of the mean field and can be considered as based on first principles.

The structure of the present exposition is as follows: We first define the screening potential and then discuss how to calculate the screening assuming the classical mean field and the dynamic MD method. The differences are then exposed. The results are discussed as a function of the interaction range. Conclusions and implications end the paper.

§2. The definition of the screening potential energy and factor

Let \( V_{6,12}(r_{12}) \) be the binary interaction potential as a function of the radial distance \( r_{12} \) between the particles, namely the potential between two particles in vacuum. When the two particles are part of an N-particles system, all particles may interact with all others and when two particles are separated a distance \( r_{12} \) the effective potential felt by each particle differs from \( V_{6,12}(r_{12}) \).
The total potential energy of the system is given by $E_{\text{pot}} = \sum_{1 \leq i < j \leq N} V_{b,ij}$. The summation is carried out over all particles. Due to the effect of the surrounding particles, the interaction energy between any two particles is written as:

$$H_{\text{int},12}(r_{12}, t) = V_{b,12}(r_{12}) + V_s(r_3(t) \cdots r_N(t)). \quad (2.1)$$

$H_{\text{int}}$ is called the effective interaction between two particles in the system. The screening potential for particles with binary potential $V_{b,12}$ is defined as:

$$V_s(r_3(t) \cdots r_N(t)) = H_{\text{int},12}(r_{12}, t) - V_{b,12}(r_{12}). \quad (2.2)$$

The basic question now is how to calculate $V_s(r_{12}, t)$.

The nuclear rate enhancement is then given by $\exp(-V_s(0)/kT)$ (Clayton p.295).

§3. Calculating the screening potential according to the mean field theory

Mean field theory requires averaging over the potential felt by the interacting particles and tacitly assumes that the mean field is created by many particles so that the charge distribution can be considered as continuous. Hence we write:

$$V_{s,12}(r_{12}, t) = \langle H_{\text{int},12}(r_{12}, t) \rangle - V_{b,12}(r_{12}) = \langle V_s(r_3(t) \cdots r_N(t)) \rangle, \quad (3.1)$$

where the brackets $\langle \rangle$ mean an ensemble average. The frequently made tacit assumption is that $H_{\text{int}}$ is formed by many particles and fluctuations are negligible, so that the ensemble average values can be applied to the screening potential. In this limit ($N_D \to \infty$), the time dependence drops out, namely

$$\langle H_{\text{int}}(r_{12}, t) \rangle \to \langle H_{\text{int}}(r_{12}) \rangle \text{ and } V_s(r_3(t) \cdots r_N(t)) \to \langle V_s(r_{12}) \rangle. \quad (3.2)$$

In the limit of $N_D \to \infty$ (Ichimaru 1994) the radial distribution function $g(r_{12})$ is given by:

$$\langle H_{\text{int}}(r_{12}) \rangle = V_{b,12}(r_{12}) + kT \ln g(r_{12}), \quad (3.3)$$

which is at the base of the Alastuey & Jancovichi (1978) result.

The screening potential as given by eq. (3.1) is supposed to be the mean potential felt by the colliding particles and is meaningful when the fluctuations are negligible. As stated by Ichimaru (ibid) this potential has no dynamic role. However, the actual enhancement is $\exp(-V_s/kT)$ and when there are fluctuations one has to take the mean $\langle \exp(-V_s/kT) \rangle$. In the weak screening limit, when $V_s/kT \ll 1$ the difference is expected to be negligible. However, if the fluctuations are large, the non linearity of the exponential comes into play and the effect may be large.

§4. The dynamic method to calculate the screening

The Molecular Dynamic method allowed us to define the screening energy from first principles in a simple and clear way.
Consider two particles 1 and 2 scattering off each other inside the N-body system. Let $E_{12}^{rel-kin-CM,f}$ be the relative kinetic energy when the pair is far apart and let $E_{12}^{rel-kin-CM,c}$ be the relative kinetic energy when the pair reaches the distance of closest approach. The screening energy is then given by:

$$V_s = E_{12}^{rel-kin-CM,c} - E_{12}^{rel-kin-CM,f} - V_{b,12}(r_{tp}), \quad (4.1)$$

where $V_{b,12}(r_{tp})$ is the binary potential interaction at the moment of closest approach. Here all energies are evaluated in the Center of Mass system. The screening energy is the energy gained/lost (from or to the particles around) by the scattered protons as they move from far away to the distance of closest approach. The potential energy of each of the the particles due to the interaction between each one and the rest of the particles is ignored when the particles are far away. This definition is very close to the original definition given by Salpeter (1954) to the screening energy.

§5. The basic difference between the two types of methods to evaluate the screening

The standard definition of the screening applies ensemble averages of the interaction and its potential between particles. The effective potential used between any two particles is obtained by continuously averaging over all particles.

The present definition is dynamic, namely the potential energy is calculated only when the two scattering particles are at the distance of closest approach so that they have converted their kinetic energy into a potential one and the radial velocity vanishes.

It is expected that the two methods will converge to the same value for $N_D \to \infty$ and will deviate from one another when $N_D \to 0$.

§6. The short range repulsive potential

The basic idea of the short range repulsive potential is to be able to control or parametrize the number of particles in the screening/neutralizing cloud. Also, the finite interaction range releases us from the complications of the infinite Coulomb force and the need to neutralize the positive ions, hence the calculation includes only one kind of particles which mass $m_p$, equal to the mass of the proton.

It is well known that the effective Coulomb interaction in plasmas is short range. However, this phenomenon is not to be confused with the present approach to demonstrate the effect of the number of particles on the screening and how the statistical limit is reached. In the case of the Coulomb force, it is the play between the positive and negative charges that creates the effective short range. Here we do not discuss this effect but assume that we have imaginative particles with hypothesized short range potential.

We assume a single component system and that the effective binary potential to be given by:

$$V_b(r) = C \left( \frac{1}{r} + \frac{r}{R_{n}^2} - \frac{2}{R_{n}} \right) \text{ for } r < R_{n}$$
where $R_n$ and $C_f$ are free parameters. Clearly, when $R_n \to 0$ we get a short range force and in principle, no screening is expected.

§7. The method of collecting the dynamic data

For each particle the program searches for nearest particle which moves towards it. There may be other particles in the vicinity and even closer to the particle examined. However, only the particle moving towards the selected particle is chosen. Once the close particle is identified, the motion of the pair is followed through the approach to the distance of closest approach and separation. The complete dynamic properties like kinetic and potential energies, the kinetic energy of the center of mass system, etc., are registered for later reduction. The pair is followed until their separation distance is larger then $R_n$. The dynamic quantities are registered upon separation and compared with those found when the particles were at the distance of closest approach. In this way the dynamics of the binary collision in the presence of many other particles is pursued in detailed. Questions like polarization of the surrounding by the approaching particles are automatically taken care off.

§8. Results

We carried out a series of calculations in which the range for the force $R_n$ was changed. The thermodynamic conditions are $n = 10^{26}$ and $T = 1.5 \times 10^7$. We calculated all the dynamic properties of the collisions and obtained the effective potential felt by the scattering particles as a function of the relative kinetic energy at $-\infty$. In all cases the initial conditions were random positions and Maxwellian velocities. The results for the first 20 dynamics times were neglected. In the present case, a dynamic time is the time it takes a particle with energy $kT$ to cross the mean interparticle distance $\langle r \rangle$.

8.1. The mean screening potential energy during the close approach

The mean screening potential energy at the moment the particles are at the classical turning point $r_{tp}$ is given in fig. (1). The figure shows the mean screening potential energy contribution to the

![Figure 1](image-url)
total interaction potential between the two scattering particles at the classical turning point as a function of the relative kinetic energy at large separation (the relative kinetic energy in the CM system). The results are for several different ranges $R_n$. We see that as the interaction range increases the mean potential energy (for a given relative kinetic energy) becomes more independent of the relative kinetic energy, namely the curves become flatter. On the other hand, as $R_n$ becomes of the order of unity or less, we see that the potential energy felt by slow particles increases by up to a factor of two relative to the potential felt by the fast particles at $r = r_{tp}$. The low kinetic energy limit is essentially the adiabatic limit, however it is not quite equal to the *ensemble mean* potential energy of a particle in the system for low $R_n$ but approaches it as $R_n$ increases. This result demonstrates the expected, namely, when the scattering particles are fast, the mostly thermal particles in the surrounding respond differently from the case in which the approaching particles move very slowly and have ample time to polarize the surrounding. The numerical statistical errors shown in the figure increases with decreasing $R_n$ because the numerical difficulties in getting a proper statistics increase with decreasing $R_n$. Note, the ensemble mean potential energy of a particle, when sampled at random, is found to be independent of the kinetic energy in the laboratory exactly as predicted by the mean field theory (see SS01 & SS02).

8.2. *The distribution of the potential energy*

Of particular interest is the distribution of the potential energy among the particles because it demonstrates the changes that take place when $R_n$ becomes smaller than unity. If $V_{b,12}$ is the binary potential then the distribution should be $\exp(-\sum V_{b,ij}/kT)$, times a phase space factor, where the summation is carried over all particles. The distribution is then symmetric around the mean field value. We expect in the limit $N_D \gg 1$ a narrow distribution, the width of which is negligible for practical purposes. Indeed, we see from fig. (2) that as the interaction range increases the distribution approaches a symmetric distribution with a decreasing relative width. In principle, this distribution should approach in the limit of a large number of particles in the screening radius to the one found in a snap shot. The situation changes when $R_n \leq 1$, as is seen in fig. (3). The striking feature is that the distribution in the latter case is not symmetric at all. Furthermore, the relative width of the distribution is very large. The deviations from a symmetric distribution is another symptom of the breakdown of the mean field assumption for the problem at hand ($N_D \leq 1$).
8.3. A stochastic potential at $N_D \leq 1$

The distribution in the potential energy among particles was shown previously. Now we turn to the time dependence of the force. We find that the force (and the potential) acting on a given particle in the system fluctuates. As expected, the small number of particles with in the sphere of the interaction causes temporal fluctuations in the potential felt by every particle. Note that the potential calculated is the potential felt by the particle, namely the Lagrangian potential and not the Eulerian one (the potential at a given location in space).

The emerging physical picture from the MD calculations is that of a particle interacting with a fluctuating cloud of neighboring particles (when $R_n \approx 1$). The stochastic approach can be described with a single particle Hamiltonian of the following form:

$$H_{i,p} = \frac{p^2}{2m} + V_0(r) + V_1(r, t) = H_0 + V_1(r, t), \quad (8.1)$$

where $V_0$ is the static limit to the true potential. $V_1$ represents the time-dependent part of the fluctuating environment around the interacting protons. A possible way to obtain the time dependent potential is:

$$V_1(r, t) = e^2 \int dr |r - r'| \frac{\delta n(r, t)}{|r - r'|}, \quad (8.2)$$

where the fluctuation beyond the local two body potential is given by $\delta n(r, t)$. *Once the potential is a function of time, the distribution function is not separable any longer and the effect of the screening on the scattering particles depends on the momentum of the particle.* The time dependence is required to describe the energy exchange between the variable environment and the scattered particle (see Murillo & Weisheit 1998). We expect that $V_1(r, t) \to 0$ in the limit of $R_n \to \infty$ when the number of interacting particles tends to $\infty$.

The time dependency of the potential explains the shortcoming of using the pair distribution function to calculate the screening when $N_D \leq 1$. The tacit assumption in the usage of $g(r)$ to calculate the screening is that the potential is defined as a function of $r$ only, which is not the case when fluctuations are important. One can of course find $g(r)$ by averaging over the fluctuations. However, the results for $R_n \approx 1$ are found to depend on the relative kinetic energy.
§9. The results for the screening as a function of $R_n$

The screening correction for the tunnelling through the potential was calculated as a function of the relative kinetic energy at large separation and compared with the classical expression calculated from the mean potential energy per particle in the system.

In fig. (5) we give the ratio of the new screening factor to the old one for two values of the potential strength ($C_f = 1$ & $C_f = 10$). We see that as the range increases the ratio approaches unity from below. Namely, (a) the effect of the fluctuations decreases with increasing $R_n$ and (b) the fluctuations usually reduce the screening. On the other hand, as the range decreases to below unity marked deviations take place. The positive contributions of the fluctuations are unable to overcome the negative ones. The mean potential energy decreases but the effect of the fluctuations decreases slower.

§10. Conclusions

We have carried out a numerical experiment in which the finite range of the interaction and its strength are varied. The variation went from the region of short range, even smaller than the mean inter particle distance, to a high range of up to 10 mean inter particle distances. Thus the behavior of the system could be followed as the number of particles in the neutralizing domain is changed from very few to many. The numerical experiment allows us to single out the peculiarities of systems with a short range (effective) potential and obtain the limit of a large number of particles in the neutralization domain. In particular, we find that

- The screening deviates significantly from the classical value as soon as the neutralization radius approaches unity from above (the density increases at a constant temperature).
The standard mean field results for the screening deviate from the values obtained for a small numbers of particles.

- The effects are not linear in the strength of interaction and vary with relative kinetic energy.
- The screening potential energy $V_s$ must be derived from dynamic considerations when $R_n = O(1)$. As the particles approach each other their potential polarization effect cause a deviation of the screening energy from the ensemble averaged potential energy.
- The present results are a numerical experiment in the behavior of an hypothetical gas. However, a plasma composed of positive and negative charges possess an affective neutralizing radius - the Debye radius. We expect that a plasma will show the same effects when the Debye radius replaces $R_n$.

§11. Acknowledgements

The author is happy to acknowledge a discussion with M. Fisher about fluctuations. This research was partly supported by the Foundation for the Promotion of Research at the Technion and by the Asher Foundation at the Asher Space Research Institute.

References

8) Schatzman, E., J. Phys. Rad. 9,46,(1948)