Nuclear fusion in dense matter

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The standard theory of nuclear fusion rates in strongly interacting plasmas can be (correctly) derived only when the energy release, Q, is large compared to other energies in the problem. We exhibit a result for rates that provides a basis for calculating the finite Q corrections. Crude estimates indicate a significant defect in the conventional results for some regions of high density and strong plasma coupling. We also lay some groundwork for a path integral calculation of the new effects.

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The calculations of nuclear fusion rates in strongly coupled equilibrium plasmas, as required for some stellar environments, nearly all rely on one simple premise, namely that the rate per unit volume w_s of fusion of ions I_1 and I_2 is given by,

$$w_s = n_1 n_2 \langle \sigma v \rangle K_{1,2}(r=0) / K_{1,2}^{(0)}(r=0),$$
 (1)

where n_1, n_2 are the number densities of the species, σ is the cross-section in vacuum and $K_{1,2}$ is the two body correlator in the presence of the plasma. $K_{1,2}^{(0)}$ is the correlator in the absence of the plasma, and basically cancels out the dependence of the cross-section factor on the Coulomb interaction between I_1 and I_2 . The calculation of $K_{1,2}$ has engendered a big literature, e.g. [1] and references cited therein, in which the correlator is calculated classically in Monte Carlo simulations at larger distances, leading to an effective two-body potential defined as $V_{\text{eff}}(r) = -\log[K_{1,2}(r)]/\beta$, where $\beta = (k_B T)^{-1}$. This is followed by a quantum tunneling calculation using this potential to obtain the overlap at (near) zero separation. This "basically classical" approach has provided the rates that are actually used in stellar calculations in which the plasma is strongly coupled. It has been tested in a very small number of quantum path integral calculations [2],[3] of the correlator under some rather specific conditions (very degenerate electrons, one component plasma). The results appear to be generally supportive of the basically classical approach, at least in some domains [4].

In the present paper we address the fact that the assumption (1) that underlies both of these approaches is not justified in some domains in which it is currently being used. A particular fusion reaction has an energy release Q, and it is only when Q is large that (1) can be established as a valid approximation, as noted in refs.[5][6]. Here we go a step farther both in addressing the question of how big Q must be in order that (1) be usable, and in finding a framework for numerical evaluation in the cases in which it is not. The results are inconsequential for solar physics, but relevant in denser systems.

For the case of two ions in and two ions out, $I_1 + I_2 \rightarrow I_3 + I_4$ we take the nuclear fusion Hamiltonian as a point coupling, describing the idealized case in which

all of the energy dependence of the laboratory crosssection in the relevant energy range is from Coulomb interactions,

$$H_{\rm nf} = ge^{-iQt} \int d\mathbf{r} \psi_3^{\dagger}(\mathbf{r}, t) \psi_4^{\dagger}(\mathbf{r}, t) \psi_1(\mathbf{r}, t) \psi_2(\mathbf{r}, t) + H.C.,$$
(2)

where Q is the energy release in the fusion. Here the ψ_i are nonrelativistic quantum fields that describe creation or annihilation of the respective ions, in a Heisenberg picture with respect to the complete Hamiltonian. The fields could be Fermi or Bose; deviation from Boltzmann statistics for the ions is inconsequential.

The remainder of the complete Hamiltonian is taken as $H = H_{1,2} + H_{3,4} + H_{\rm pl} + H_c$ where $H_{1,2}$ and $H_{3,4}$ are the respective kinetic energies plus Coulomb interactions of the initial and final systems in the absence of the surrounding plasma, $H_{\rm pl}$ contains all of the kinetic energy and Coulomb interactions among themselves of the plasma particles, and H_c is the coupling of the fusing particles and the fusion products to the plasma particles.

We refer the reader to ref.[5] for the derivation of the basic formal rate expression based on (2),

$$w = g^2 \int_{-\infty}^{\infty} dt \, e^{iQt} \int d\mathbf{r} \left\langle \psi_1^{\dagger}(\mathbf{r}, t) \psi_2^{\dagger}(\mathbf{r}, t) \psi_3(\mathbf{r}, t) \psi_4(\mathbf{r}, t) \right\rangle \times \psi_4^{\dagger}(\mathbf{0}, 0) \psi_3^{\dagger}(\mathbf{0}, 0) \psi_2(\mathbf{0}, 0) \psi_1(\mathbf{0}, 0) \right\rangle_{\mathcal{A}},$$
(3)

where the notation $\langle ... \rangle_{\beta}$ indicates the thermal average in the medium, $\langle O \rangle_{\beta} \equiv Z_P^{-1} \text{Tr}[O \exp(-\beta H)]$ with Z_P the partition function. We take a one component ionic plasma neutralized by degenerate electrons. In this case the plasma coordinates are the ionic positions $\mathbf{R}_1 \mathbf{R}_N$. Then we can transform the result (3) into,

$$w = C \int d\mathbf{r} \int_{-\infty}^{\infty} dt \ e^{iQt} \int d\mathbf{R}_{1}, ..d\mathbf{R}_{N}, ..d\mathbf{R}'_{1}, ..d\mathbf{R}'_{N} \times \langle \mathbf{r}_{1} = \mathbf{r}_{2} = 0, \mathbf{R}_{1}, ..\mathbf{R}_{N} | e^{-(\beta - it)H} | \mathbf{r}_{1} = \mathbf{r}_{2} = \mathbf{r}, \mathbf{R}'_{1}, ..\mathbf{R}'_{N} \rangle_{1,2} \times \langle \mathbf{r}_{3} = \mathbf{r}_{4} = \mathbf{r}, \mathbf{R}'_{1}, ..\mathbf{R}'_{N} | e^{-itH} | \mathbf{r}_{3} = \mathbf{r}_{4} = 0, \mathbf{R}_{1}, ..\mathbf{R}_{N} \rangle_{3,4},$$

$$(4)$$

where the first two arguments in the kets are the coordinates of the reacting ions in the fusion process and the

coordinates \mathbf{R}_i stand for all the other ions in the plasma. The redundant subscripts 1, 2 and 3, 4 on the respective brackets $\langle \rangle$ are a reminder of which of the reacting ions are present in the states within the brackets. The multiplying constant is $C = Z_P^{-1} n_1 n_2 g^2$. The individual steps in going from (3) to (4) are simple: first the expression of the Heisenberg fields in terms of Schrodinger fields, $\psi_S(\mathbf{r}) = \exp[-iHt]\psi_H(\mathbf{r},t) \exp[iHt]$, then introduction of the single particle states for the respective reacting particles, $|\mathbf{r}\rangle = \psi_S^{\dagger}(\mathbf{r})|0\rangle$ and the explicit introduction of the plasma coordinates.

The result (4) is equivalent to the interaction picture result eq. (2.53) of ref. [5]. The latter is better suited to perturbation expansions; the former to our present purposes.

To get w_s of the standard theory as given by (1) we strike the space and time dependence of the first bracket in (4) and take the factor involving the fusion products to be independent of the plasma coordinates,

$$w_{s} = C \int d\mathbf{R}_{1}, ...d\mathbf{R}_{N}$$

$$\times \langle \mathbf{r}_{1} = \mathbf{r}_{2} = \mathbf{0}, \mathbf{R}_{1}, ...\mathbf{R}_{N} | e^{-\beta H} | \mathbf{r}_{1} = \mathbf{r}_{2} = \mathbf{0}, \mathbf{R}_{1}, ...\mathbf{R}_{N} \rangle_{1,2}$$

$$\times \int_{-\infty}^{\infty} dt \, e^{iQt} \int d\mathbf{r} \langle \mathbf{r}_{3} = \mathbf{r}_{4} = \mathbf{r} | e^{-itH_{3,4}} | \mathbf{r}_{3} = \mathbf{r}_{4} = 0 \rangle_{3,4} .$$
(5)

In the expression (5) the first two lines give $n_1n_2g^2K_{1,2}(0)$ as appear in (1). The final line in (5) calculates the phase space, Ω , for the fusion products, and the effects of their mutual Coulomb interaction, in a limit in which their final energy is exactly Q and their total momentum exactly zero. Using $g^2\Omega = \langle \sigma v \rangle [K^{(0)}]^{-1}$ we obtain (1), with the caveat that we have calculated the final phase space neglecting momentum and energy pass-through from the initial state. But this is inconsequential in the large Q limit, which is for other reasons the domain of applicability of (5), as noted in ref. [5] and explicitly demonstrated in an example below.

The best calculation to date of the correlator $K_{1,2}$, implicit in the first factors of (5), appears to be that by Militzer and Pollack [2]. Using $\exp(-\beta H) = [\exp(-\beta H/N_1)]^{N_1}$ in (5), when N_1 is sufficiently large, they use perturbation theory for the individual factors, each effectively now at high temperature, N_1T . This is an expensive calculation because N and N_1 have to be fairly large, and between each of the N_1 factors one must integrate over the full manifold of $\mathbf{r}'_1, \mathbf{r}'_2, \mathbf{R}'_1...\mathbf{R}'_N$.

To apply the same technique to the complete formulation, (4), we would face the additional complications of the time and space integrations, requiring a computation for each point r, t that is the equilivalent of the entire calculation of (5). Furthermore, as it stands, a calculation of (4) at even one point r, t is out of the question because of the oscillating integrands. To make progress, we look at an approximate form of the last bracket $\langle \rangle$ in (4) for

small values of t. For simplicity we take ions I_2 and I_4 to be infinitely massive and to be situated at the origin; we can then eliminate their coordinates altogether, and also eliminate all mention of the center of mass position, r, in (4). In the last bracket $\langle \rangle$ in (4) where the coupling is to the outgoing ions #3 and #4 we make the further simplification in the factor relating to the fusion products,

$$\langle \mathbf{0}|e^{-it(H_{\rm pl}+H_{3,4}+H_c)}|\mathbf{0}\rangle \approx \Lambda \langle \mathbf{0}|e^{-itH_{3,4}}|\mathbf{0}\rangle,$$
 (6)

where

$$\Lambda = 1 - itH_{\rm pl} - it(e_3 + e_4)\phi(\mathbf{0}). \tag{7}$$

Here Λ is an operator in the plasma space, with the R_i indices now suppressed. The label $\mathbf{0}$ in the kets refers only to the position of I_1 . In (7), $\phi(\mathbf{r})$ is the operator for the electric potential of the plasma, which enters in the coupling term of the I_3 , I_4 system to the plasma, $H_C = e_3\phi(\mathbf{r_3}) + e_4\phi(\mathbf{0})$. Commutators that have been neglected in writing (6) in the above form give terms of order t^2 and higher, and would give terms of higher order in Q^{-1} than those that we estimate below.

From (4) the rate is now,

$$w = \int_{-\infty}^{\infty} dt \ e^{iQt} F(t) G(t) \,, \tag{8}$$

where

$$F(t) = C \operatorname{Tr}_{pl} \left[\langle \mathbf{0} | e^{-(\beta - it)H} \Lambda | \mathbf{0} \rangle \right], \tag{9}$$

with the trace performed in the plasma space. G is given by,

$$G(t) = \int \frac{d\mathbf{q}'}{(2\pi)^3} e^{-i\frac{q^2}{2M}(t-i\epsilon)} |\Psi_{\mathbf{q}'}(\mathbf{0})|^2$$

$$\approx i^{-3/2} (t-i\epsilon)^{-3/2} \left(\frac{M}{2\pi}\right)^{3/2}, \tag{10}$$

In (10), $\Psi_{\mathbf{q}'}(\mathbf{0})$ is the Coulomb wave function for asymptotic momentum q', evaluated at the origin. In the second line we have discarded the Coulomb interaction between I_3 and I_4 . The function G(t) is analytic in the upper half t plane except for the branch point at $i\epsilon$; note that this singularity comes from the high q^2 behavior of the integrand in (10) and should have the same form when we restore the Coulomb force between the final particles. A similar analysis of F(t), leaving the plasma out entirely, would give a structure with a singular factor $(t+i\beta)^{-3/2}$. We assume that this analytic structure persists in the presence of the plasma.

Then defining the cut in the $t^{-1/2}$ function in (9) to run from $i\epsilon$ to $i\infty$, and that in $(t+i\beta)^{-3/2}$ in F to run from $-i\beta$ to $-i\infty$, we deform the t integration contour to run from $i\infty - \epsilon$ to 0 to $i\infty + \epsilon$ and replace it with a simple integral of the discontinuity and a real integration variable, τ , ending with,

$$w = i^{-3/2} \int_{-\infty}^{\infty} dt \, F(t) e^{iQt} (2\pi M)^{3/2} (t - i\epsilon)^{-3/2}$$

$$= 2i^{-3/2} \int_{-\infty}^{\infty} dt \, \frac{d}{dt} [e^{iQt} F(t)] (2\pi M)^{3/2} (t - i\epsilon)^{-1/2}$$

$$= -2^{1/2} \left(\frac{M}{\pi}\right)^{3/2} \int_{0}^{\infty} d\tau \, \tau^{-1/2} \, \frac{d}{d\tau} \left[e^{-Q\tau} F(i\tau)\right], \quad (11)$$

the integration by parts before transforming the contour being required in order to avoid a non-integrable singularity at t=0 in the final form.

The rate corrections of order Q^{-1} are now calculated from the linear term in the expansion of of F(t) in powers of t. From (9) and (7) we obtain just,

$$F(t) = C \operatorname{Tr}_{pl} \left[\langle \mathbf{0} | e^{-\beta H} [1 + it H_{1,2}] | \mathbf{0} \rangle_{1,2} \right], \qquad (12)$$

the terms with $t\phi(0)$ having cancelled through conservation of charge, and the terms with $tH_{\rm pl}$ having cancelled as well. The term with unity in the final bracket gives the rate w_s of (5). We estimate the contribution δF of the linear term in t the "basically classical" approximation, in which plasma coordinates are eliminated in favor of an effective Hamiltonian $H_{\rm eff}={\rm KE}+V_{\rm eff},$

$$\delta F(i\tau) = n_1 n_2 g^2 \zeta^{-1} \tau \langle \mathbf{0} | e^{-\beta H_{\text{eff}}} H_{1,2} | \mathbf{0} \rangle, \qquad (13)$$

where $\zeta = \int d\mathbf{r} \langle \mathbf{r} | e^{-\beta H_{\text{eff}}} | \mathbf{r} \rangle$. We evaluate (13) taking a minimal modification of the potential due to the plasma, following ref. [7],

$$\delta H \equiv H_{\text{eff}} - H_{1,2} \approx -\Gamma \beta^{-1} [1 - (r/2a)^2],$$
 (14)

where a is the average interparticle spacing and Γ the classical plasma coupling strength. We evaluate using

$$\langle \mathbf{0}|H_{1,2}e^{-\beta H_{\text{eff}}}|\mathbf{0}\rangle = -\langle \mathbf{0}|[\frac{\partial}{\partial\beta} + \delta H]e^{-\beta H_{\text{eff}}}|\mathbf{0}\rangle.$$
 (15)

and

$$e^{-\beta H_{\text{eff}}} \approx e^{-S_0} e^{\xi} \,, \tag{16}$$

where $S_0=[27\pi^2\beta M(Ze)^4/4\hbar^2]^{1/3}$ and $\xi=[\Gamma-(45\Gamma^3)/(32S_0^2)]$, as in eq.28 of ref.[7]. Here $\Gamma=Ze^2\beta/a$ where $a=(3/4\pi n_I)^{1/3}$. In the second term in (15) we take δH at the time averaged (imaginary) time \bar{r} , eq.13 in ref.[7]. We obtain,

$$\frac{\delta w}{w_s} = -\frac{\partial S_0}{\partial \beta} Q^{-1} - \frac{129}{64} \frac{\Gamma^3}{S_0^2 \beta Q} \,. \tag{17}$$

The first term on the RHS of (17) simply adjusts the phase space for the outgoing particles by adding an energy on the order of the Gamow energy to the final state, note the discussion of energetics above, after (5). The remaining term comes specifically from the r^2 term in the effective potential. (The contributions from the r independent modification canceled, using $(\partial/\partial\beta)\Gamma = \Gamma/\beta$.)

This r^2 term gives a fractional correction $\approx .4\,\mathrm{MeV}/Q$ for the case of the extreme conditions of $^{12}\mathrm{C}$ + $^{12}\mathrm{C}$ at a temperature of $10^8\mathrm{K}$ and a density of $10^{10}\mathrm{gc}^{-3}$.

A correction of the above magnitude does not necessarily create a problem for, say, the conventional calculation of $^{12}\mathrm{C} + ^{12}\mathrm{C} \to ^{23}\mathrm{Na} + \mathrm{p}$ where the Q value is about 2 MeV, and where the applications care about factors of ten and not about 20% corrections. But the fractional correction is much larger than T/Q. The next logical step would be to expand of the right hand $\langle \rangle$ in (4) in an infinite series of operators in the plasma space, of which (12) displays the first two terms. Our conjecture is that the contour distortion can then be applied to give individual terms each of which could be calculated with the path integral method.

We can get complementary information from perturbative calculations in a system in which the expansion in powers of Q^{-1} is not applicable. We consider a reaction $I_1+I_2 \rightarrow I_3$, where I_3 is a narrow resonance, and where the decay of the resonance is nearly all into channels other than the entrance channel. The formalism above is applicable simply by eliminating every reference to ion #4 in every equation. The local interaction, (2), removing the ψ_{4}^{\dagger} factor, perfectly describes the limit in which the Breit-Wigner formula, with Coulomb removed, becomes a constant times a delta function in energy. As context we mention the possible application to ${}^{12}C + {}^{12}C$ fusion at temperatures in the range of a few times 10⁸ K, where the magnitude of Q, which is negative in this case, is chosen to be close to the Gamow peak for the fusion reaction, resulting in enhancements to the rate [8]- [10].

We consider only the order in which there are two interactions of the distinguished ions I_1, I_2, I_3 with the plasma; the superficial order of w in the coupling parameter is e^4 but the long range part of the Coulomb force reduces the order of the leading term to e^3 . For these terms the dimensionless strength parameter is $\lambda_1 = e^2 Z^2 \kappa_D$ with $\kappa_D^2 = 4\pi n_I Z^2 \beta$. To calculate we introduce an interaction representation in which the "interaction" Hamiltonian is H_c , the coupling of I_1, I_2, I_3 to the plasma particles, and the unperturbed Hamiltonian, $H_0 = H - H_c$. The calculations are fairly standard, with the replacement, e.g. within the first $\langle \rangle$ in (4),

$$e^{-H(\beta - it)} = e^{-H_0(\beta - it)} \exp\left[i \int_{-i\beta}^t dt' H_c^I(t')\right]_+, \quad (18)$$

where the final subscript indicates time ordering along the path $-i\beta$ to 0 to t. The perturbation terms will come from the first and second terms in the expansions of the final exponentials of (18) and its (anti-time-ordered) counterpart for the second $\langle \rangle$ in (4). To distinguish the source of the terms that follow we introduce independent charges of the fusing particles and the fusion products, e_1, e_2, e_3 , taking $e_1 = e_2 = eZ = e_3/2$ at the end of the calculation. When we calculate just the terms of order

 e^3 in (4) we obtain,

$$w = g^{2} n_{1} n_{2} \zeta^{-1} \int_{-\infty}^{\infty} dt [1 - \beta^{-1} \kappa_{D} J(t)] e^{iQt} \int d\mathbf{r}$$
$$\times \langle \mathbf{0}, \mathbf{0} | e^{-H_{1,2}(\beta - it)} | \mathbf{r}, \mathbf{r} \rangle_{1,2} \langle \mathbf{r} | e^{-iH_{3}t} | \mathbf{0}, \mathbf{0} \rangle_{3}, \quad (19)$$

where

$$J(t) = (e_1 + e_2)^2 \left(\frac{t^2}{2} - \frac{\beta^2}{2} + i\beta t\right) + e_3^2 \frac{t^2}{2} - (e_1 + e_2)e_3(t^2 + i\beta t),$$
 (20)

When charge conservation is imposed, the individually time dependent terms in (20) add up to $-(e_1+e_2)^2\beta^2/2$, and we obtain the perturbative change in rate,

$$\delta w = (1/2)(e_1 + e_2)^2 \kappa_D \beta w^{(0)}, \qquad (21)$$

where however the e_1^2 and e_2^2 terms are to be dropped because they are exactly compensated by the changes in chemical potential required to keep the number densities of the respective species constant, as shown explicitly in ref [5]. In the end we obtain just the Salpeter [11] correction (for $Z_1 = Z_2 = Z$), $\delta w = \lambda_1 w^{(0)}$. Using instead just the term in (20) in which the plasma couples only to the incoming ions would produce a spurious addition of relative order $(\beta Q)^{-1}$ to our earlier large Q expansion, and more damaging spurious effects in a resonance case (where we cannot use the Q^{-1} expansion).

Deriving the correct Salpeter result from a wrong equation, (5), can lead one to believe that there exist further corrections of order λ_1 coming from the coupling of the fusion products to the plasma. Other works, e.g. refs.[9] [12], have combined a standard screening enhancement, of order e^{Γ} , with an resonance energy shift, of order Γ/β . In our weak coupling framework, including the latter would be incorrect, since the fractional correction to order λ_1 is given completely by (21). Thus it appears to be incorrect in the strongly coupled case as well, though the issue deserves further scrutiny.

We have calculated the residual, non-infrared divergent, terms of order e^4 in the perturbation expansion for the resonance production case coming from two interactions of the plasma with the final resonance. We find a fractional correction of a few times $\lambda_2 L[Q/E_{\rm Gamow}]$ where $\lambda_2 = e^4 Z^3 \hbar \beta^{5/2} n_I M^{-1/2}$ and the function L is of order unity when Q is of order E_{Gamow} . Thus the correction is superficially of order \hbar while the order λ_1 correction of (21) is classical. However, there is also implicit \hbar dependence in $E_{\rm Gamow}$. For example in $^{12}{\rm C}+^{12}{\rm C}$ at a temperature of $10^8 K$, this correction would be 100%for densities greater than about $10^8 \mathrm{gc}^{-3}$. The classical coupling Γ (or $\lambda_1^{2/3}$) has become strong for even lower density, so this perturbative estimate of a quantum effect must be regarded with suspicion, and is of no value to phenomenology. But it is worrisome that the usual picture does not in any way include the physics of these terms, especially when applied at one hundred times the density at which they appear to become important.

The most important new results in this paper are the presentation of the basic governing equation (4) and the demonstration that the real time dependence therein can lead to big changes when Q is not sufficiently large. It is noteworthy that, even when we evaluated the correction using the classical potential, the time dependence in the framework combines with the quantum effects in the short distance tunneling region to produce significant changes. The last, perturbative, parts of the paper serve as a further caveat with respect to using the existing lore when Q is not large.

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