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Electron capture rates in a plasma

R. F. Sawyer

Department of Physics, University of California at Santa Barbara, Santa Barbara, California 93106, USA (Received 21 March 2011; published 13 June 2011)

A new general expression is derived for nuclear electron capture rates within dense plasmas. Its qualitative nature leads us to question some widely accepted assumptions about how to calculate the effects of the plasma on the rates. A perturbative evaluation, though not directly applicable to the strongly interacting case, appears to bear out these suspicions.

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I. INTRODUCTION

Calculation of electron capture rates in plasmas is of importance in many astrophysical systems. The influence of the surrounding plasma on the capture rates is completely understood for the case of a weakly coupled plasma in which the electrons are not degenerate, as long as the energy release in the reaction Q is sufficiently large. These conditions are well fulfilled in the solar core, where the capture rate of electrons on ⁷Be has been studied in detail. Here the weak-screening Salpeter factor [1], with a multiplicative factor of $\exp(-e^2 Z \kappa_D/T) \approx (1 - e^2 Z \kappa_D/T)$, gives a 16% rate reduction [2–4]. These calculations of reduction factors are all really just calculations of a screening-induced reduction of the expectation of the electron density at the position of the ion. The methods of the above references are not applicable to cases with (a) strong plasma coupling Γ or (b) small energy release Q in relation to other energies in the problem (or negative O). Indeed, as we explicitly show below, the plasma-induced change of the electron density at the position of the ion is no longer the determining factor in the rate when condition (b) prevails. Also, of the approaches in the above references, only that of Ref. [4] can incorporate high electron degeneracy.²

In the parameter region relevant to explosions and collapse of O-Ne-Mg stellar cores, for example, both conditions (a) and (b) apply, and the electrons are very degenerate. Indeed, Q is here negative for important capture reactions; they become enabled when the Fermi energy increases nearly to the value -Q. In Ref. [5], addressing these systems, we find a simple statement of a procedure that appears to be widely followed [6–9], namely, to calculate the capture rate for an individual electron as in vacuum, except replacing the vacuum Q value for the decay by an effective value $Q + E_1 - E_2$, where E_1 and E_2 are the respective energies of interaction of the initial and final ions in the plasma. There exist more or less standard expressions for these energies derived from classical simulations. For the purpose of our present discussion we designate this correction, with energies calculated as for a classical plasma, as the "ionic energy correction." In applications, it appears that this correction has been applied sometimes with accompanying initial-state Coulomb effects involving the electrons, which we loosely characterize as "screening," and sometimes without them.

The present work begins with the derivation of a new expression for the rate of electron capture, one that we think should be the basis of future calculation of rates in the presence either of strong degeneracy or of strong plasma coupling. Just looking at the form of the result, we believe, should be enough to make one profoundly skeptical about assumptions being made in the literature. We then carry out a systematic perturbative evaluation in the weakly coupled case for cases of arbitrary electron degeneracy, retaining terms of relative order $e^2 Z \kappa_D / T$ in the rates (or of order "Salpeter," as we shall henceforth designate them). The results appear to be in complete disagreement with the assumptions that lead to the ionic energy correction, had they been applied to a weakly coupled problem.

We use the notation κ_D for the screening wave number throughout. In the presence of some degree of degeneracy its square is given by [10]

$$\kappa_D^2 = 4\pi \left[\beta \sum_s e_s^2 n_s + e^2 \frac{\partial}{\partial \mu_e} \int \frac{d\mathbf{p}}{(2\pi)^3} f(E_p) \right], \quad (1)$$

where $e_s = eZ_s$ is the charge of ionic species s, n_s is the number density of that species, and $f(E_p)$ is the Fermi distribution. In the nondegenerate limit this gives the Debye wave number, and in the strongly degenerate limit, the electronic part would give the square of the Thomas-Fermi screening wave number.

II. GENERAL FORMULATION

Our general methods follow those introduced in Ref. [10]. We take the electron capture interaction Hamiltonian for the process of a nonrelativistic electron plus ion I_a going into neutrino plus ion I_b to be given by a zero-range Fermi-type coupling (all the effects of Coulomb interactions in what follows are the same for the Gamow-Teller case),

$$H_W = \int d\mathbf{r} [K(\mathbf{r}, t) + K^{\dagger}(\mathbf{r}, t)], \qquad (2)$$

¹The question of whether or not the exponentiation of the perturbative result is justified is numerically irrelevant in this case.

²However, we know of no very interesting set of conditions that are highly degenerate without also embodying condition (a) or condition (b).

where

$$K(\mathbf{r},t) = ge^{-iQt}\psi_{\nu}^{\dagger}(\mathbf{r},t)\psi_{e}(\mathbf{r},t)\psi_{b}^{\dagger}(\mathbf{r},t)\psi_{a}(\mathbf{r},t)$$
(3)

and Q is the energy release in the reaction. There are suppressed spin indices contracted with each other on the electron and neutrino fields. Here $\psi_{\{a,b\}}$ are nonrelativistic quantum fields that describe creation or annihilation of the respective ions. All fields are in a Heisenberg picture with respect to the complete Hamiltonian. The ionic fields could be Fermi or Bose, but we shall remain in a domain of temperature and density in which deviation from Boltzmann statistics of the ions is inconsequential.

We are interested in the time rate of change of the electron density induced by (2). Since the medium is translationally invariant, we can choose to evaluate this time derivative at at point $\mathbf{r} = \mathbf{0}$ and choose time to be zero as well. Directly from the Heisenberg equations, we obtain the rate of change w of the electron density at the origin, $n_e(\mathbf{0}, 0) = \psi_e^{\dagger}(\mathbf{0}, 0)\psi_e(\mathbf{0}, 0)$,

$$w = \langle \dot{n}_e(\mathbf{0}, \mathbf{0}) \rangle_{\beta} = -i \int d\mathbf{r} \langle [n_e(\mathbf{0}, 0), K(\mathbf{r}, 0)] \rangle_{\beta}$$
$$= i \langle [K(\mathbf{0}, 0) - K^{\dagger}(\mathbf{0}, 0)] \rangle_{\beta}. \tag{4}$$

The notation $\langle \cdots \rangle_{\beta}$ indicates the thermal average in the medium, such that for an operator O we have $\langle O \rangle_{\beta} \equiv Z_P^{-1} {\rm Tr} \{O \exp[-\beta (H + H_W - \mu_e N_e)]\}$, where Z_P is the partition function and where $H + H_W$ is the complete Hamiltonian. We wish to calculate the rate to lowest nonvanishing order, i.e., to second order in the weak-coupling parameter g. So it is it clear that one power of g must come from the weak interaction H_W within the statistical factor. Thus we now must consider the linear response [11] of the medium average of the operator $[K(0) - K^{\dagger}(0)]$ to this perturbation,

$$w = -i \int_{-\infty}^{0} dt \int (d\mathbf{r}) \langle [\dot{n}_{e}(0,0), H_{W}(\mathbf{r})] \rangle_{\beta}$$

$$= -\int_{-\infty}^{0} dt \int d\mathbf{r} \langle [K(\mathbf{0},0) - K^{\dagger}(\mathbf{0},0)],$$

$$\times [K(\mathbf{r},t) + K^{\dagger}(\mathbf{r},t)] \rangle_{\beta}, \qquad (5)$$

where now the thermal average in the medium is to be calculated using H alone. H conserves electron number, so that

$$\langle [K(\mathbf{0},0),K(\mathbf{r},t)]\rangle_{\beta} = \langle [K^{\dagger}(\mathbf{0},0),K^{\dagger}(\mathbf{r},t)]\rangle_{\beta} = 0.$$
 (6)

Using in addition the space-time translational invariance of the medium and the antisymmetry of the commutator,

$$\langle [K^{\dagger}(\mathbf{0},0),K(\mathbf{r},t)]\rangle_{\beta} = -\langle [K(\mathbf{0},0),K^{\dagger}(-\mathbf{r},-t)]\rangle_{\beta}, \tag{7}$$

we can write the rate as

$$w = -\int_{-\infty}^{\infty} dt \int d\mathbf{r} \langle [K(\mathbf{0}, 0), K^{\dagger}(\mathbf{r}, t)] \rangle_{\beta}.$$
 (8)

When we take the medium to contain no ions of type b, so that there is no reverse reaction, we can omit the first term in the commutator in (8), which, after inserting (3), gives

$$w = g^{2} \int_{-\infty}^{\infty} dt \int d\mathbf{r} e^{-iQt} \langle \psi_{e}^{\dagger}(\mathbf{r}, t) \psi_{a}^{\dagger}(\mathbf{r}, t)$$

$$\times \psi_{v}(\mathbf{r}, t) \psi_{b}(\mathbf{r}, t) \psi_{b}^{\dagger}(\mathbf{0}, 0) \psi_{v}^{\dagger}(\mathbf{0}, 0) \psi_{a}(\mathbf{0}, 0) \psi_{e}(\mathbf{0}, 0) \rangle_{\beta}$$

$$= g^{2} \int_{-\infty}^{\infty} dt \int d\mathbf{r} e^{iQt} \int \frac{d^{3} p_{\nu}}{(2\pi)^{6}} e^{i\mathbf{p}_{\nu} \cdot \mathbf{r} + iE_{\nu}t}$$

$$\times \langle \psi_{e}^{\dagger}(\mathbf{r}, t) \psi_{a}^{\dagger}(\mathbf{r}, t) \psi_{b}(\mathbf{r}, t) \psi_{b}^{\dagger}(\mathbf{0}, 0) \psi_{a}(\mathbf{0}, 0) \psi_{e}(\mathbf{0}, 0) \rangle_{\beta}.$$
(9)

For almost any purposes the thermal motions and recoil of the reacting ions are ignorable. We distinguish the ion I_a on which an electron is captured and the capture product I_b from the other ions in the plasma, taking a single I_a fixed at the origin, replacing $\mathbf{r} = \mathbf{0}$ in all of the explicit fields in (9) and adding an allover factor of density of ions of type a, n_a . The products of the field operators $\psi_{a,b}$ that occur in (9) now serve only to change one ion into the other. We substitute

$$\psi_a^{\dagger}(\mathbf{0}, t)\psi_b(\mathbf{0}, t) = e^{iHt}|a\rangle\langle b|e^{-iHt}, \tag{10}$$

where the time dependence reflects the fact that the plasma interactions of the two ions are different. We obtain

$$w = \frac{g^2 n_a}{2\pi^2} \int_{-\infty}^{\infty} dt \, e^{-iQt} \int dp_{\nu} \, p_{\nu} e^{iE_{\nu}t} M(t), \qquad (11)$$

where

$$M(t) = Z_P^{-1} \text{Tr}[\langle a|^{-\beta H} e^{iHt} \psi_e^{\dagger}(\mathbf{0}, 0) | a \rangle \langle b| e^{-iHt} | b \rangle$$

$$\times \langle a|\psi_e(\mathbf{0}, 0) | a \rangle]. \tag{12}$$

The ionic states $|a\rangle$, $|b\rangle$ in (12) serve to determine the coupling to the fixed ion in the interaction Hamiltonian. The trace in (12) is over all of the other coordinates. We write

$$M(t) = Z_P^{-1} \text{Tr}[e^{-(\beta - it)H_a} \psi_e^{\dagger}(\mathbf{0}, 0) e^{-iH_b t} \psi_e(\mathbf{0}, 0)], \qquad (13)$$

where

$$Z_P = \text{Tr}\left[e^{-\beta H_a + \beta \mu_e N_e}\right]. \tag{14}$$

Here H_a is the Hamiltonian for the initial system (with H_W turned off since our expressions are already of order g^2) and H_b is that for the final system, not counting the constant Q. The space of states in which the trace in (13) is to be evaluated is just what we have defined as the "plasma"; all electrons and all ions, except ions a and b. To restate the definitions of H_a and H_b , they are the Hamiltonians for the complete plasma in the presence of the respective fixed Coulomb fields of the nuclei a, b.

The result (13) for the function M(t), in conjunction with the rate expression (11), is our fundamental result. We show the details of the perturbation evaluation in the Appendix, retaining terms of order Salpeter ($e^2Z\kappa_D$). This calculation appears to be very inefficient, given the simplicity of the result, but we have found no other path to the answer. We state the results in terms of two subsidiary functions, $M_0(t)$ and $M_A(t)$,

$$M_0(t) = \int \frac{d\mathbf{p}_1 d\mathbf{p}}{(2\pi)^3} \langle a_{\mathbf{p}_1}^{\dagger} a_{\mathbf{p}} e^{iE_{\mathbf{p}}t} \rangle = \int \frac{d^3 p}{(2\pi)^3} f(E_p) e^{iE_p t},$$
(15)

$$M_A(t) = \int \frac{d^3 p}{(2\pi)^3} [f(E_p)]^2 e^{iE_p t}, \tag{16}$$

where f(p) is the Fermi distribution,

$$f(E_p) = [1 + e^{\beta(E_p - \mu_e)}]^{-1}.$$
 (17)

The kernel of the rate expression (11) is now given by

$$M(t) = M_0(t) - e \, e_a \kappa_D \beta [M_0(t) - M_A(t)], \tag{18}$$

and the rate is given by

$$w = 2^{3/2} \pi g^2 m^{3/2} \int_{\min(0, -Q)}^{\infty} dE \, E^{1/2} (Q + E)$$

$$\times \{ f(E) - e e_a \kappa_D \beta [f(E) - f^2(E)] \}. \tag{19}$$

We note that to the order that we are working, the result (19) agrees exactly with Eq. (1.21) of Ref. [4] except for the additional term E in the factor Q+E in our result and the inclusion of all vacuum Coulomb effects in Ref. [4]. (In the present work we just stated that vacuum Coulomb effects could be treated additively.) In the vacuum case the extra E term just puts in corrected kinematics. But, as we see more explicitly in the next section, once we make this trivial modification, the rate is no longer determined by the electron density at the location of the ion. References [3] and [4] calculate only the perturbation of the density. Thus it is of some interest that this modification is screened by the same factor (under the E integral) as the Q term, but it is perhaps not unexpected. What is more of note is not what our result contains but what it does not contain. We discuss this at some length in the next section.

III. DISCUSSION

We return to the basic result for the kernel of the capture rate formula,

$$M(t) = Z_P^{-1} \text{Tr}[e^{\beta \mu_e N_e} e^{(-\beta + it)H_a} \psi_e^{\dagger}(\mathbf{0}, 0) e^{-iH_b t} \psi_e(\mathbf{0}, 0)].$$
(20)

If we were to replace both factors $\exp(i H_a t)$ and $\exp(-i H_b t)$ by unity, i.e., evaluate at t = 0, then M would be precisely the electron density at the position of the ion. Then, in accord with the remarks at the end of the last section, we get the standard screening results, where Q + E in (19) is replaced by Q. In our mechanics this replacement comes from the fact that Hamiltonians H_a and H_b both contain electron kinetic energy terms and that there is an electron creation operator standing between the factors containing them, thus producing an $\exp[-iEt]$. But H_a and H_b also contain pieces in which the initial and final ions interact with the plasma. So in parallel fashion, why do we not see another addition to Q in the results, namely, $\Delta Q = \Delta E_a - \Delta E_b$, due to the ionic interaction shifts in the plasma? After all, one can infer energy shifts for the ions at the Salpeter level. For an ion with charge e_a we have $\Delta E_a = e_a^2 \kappa_D/2$ so that the difference between the energy shifts of the initial and final ions in our case would be $ee_a\kappa_D$. But there is no such term in the result (19).

This is our first criticism of the "ionic energy shift" ansatz. It should have manifested itself at our level of approximation, but it did not. A reader might comment, "I look at (19), say, in the nondegenerate limit, and I see just Salpeter screening, an effect that pertains only to physics in the initial state. But we know that the energies of these ions are shifted differently by the plasma interactions, and when these shifts are of order O, they must matter a lot. So the author cannot have put in

all of the physics." But if one wades through the calculations in the Appendix, one finds that such terms come and go; they all cancel in the end. What is left out of the ansatz (initial-state effects + final-state effects) is the fact that many of the individual terms in the development, even to this order, involve one Coulomb interaction with the initial ion and one with the final one. These terms cancel almost all of what comes from the ansatz. We see no valid reason to believe that the ionic energy shift correction by itself, as it is applied in Refs. [6–9], will serve us any better in the strongly coupled case than in our case in which we can really calculate.

In addition to this ionic energy shift, there exists a second plausible correction recommended in some papers dealing with extremely dense and degenerate systems [7,9], namely, an electron energy shift resulting from the screening of the potential seen by the electron. The qualitative description of how this screening should affect the rates is now nothing like the description in weak screening theory; in the latter case the effects are entirely due to the change in electron density at the ionic position and are not directly connected to the energy spectrum of the electrons. But when we address a degenerate case in which Q < 0 and we get captures only as the Fermi energy approaches -Q, it is the energy distribution rather than the electron density that would seem to be the critical feature.

To discuss this suggested effect, we first note that in the derivation of our perturbative results, given in the Appendix, we did need to calculate a change in the electron chemical potential $\delta\mu_e$. Our primary calculation was for fixed chemical potential, and we thereafter made a correction to get the results for fixed electron density. The outcome is that we obtain the Salpeter correction with no explicit $\delta\mu$ appearance, with the stipulation that the chemical potential to be used is obtained from the number density by doing the integral $n_e = \int d\mathbf{p}(2\pi)^{-3} f(E_p)$ and then solving for μ_e as a function of n_e . It appears to us that this gives the statement of results in the best form for applications, and there is no explicit chemical potential shift in the result.

Thus we find reasons to question both of the above corrections; they do not contribute in the weakly coupled case, and we see no reason for them to be the dominant correction in the strongly coupled case. That is not to say that the physical reasoning behind them is incorrect; other corrections are equally important.

Turning to specific applications, we first focus our attention on Ref. [9], which is a comprehensive treatment of electron capture in the infall phase of a type II supernova event, with a full range of nuclear species, temperatures, and densities. Here the screening corrections are a relatively minor feature of the work; still, they give effects ranging from a 25% decrease in rates for a density of $10^{10} gc^{-3}$, temperature of 0.75 MeV (with plasma parameter $\Gamma \approx 1$) to a factor of 2 at a density of 10^{12} , T=1.5 MeV, $\Gamma \approx 3$. Our suggestion here is that these corrections be taken as an estimate of the magnitude of the unknown error *in either direction* due to plasma effects. If this turns out to create important uncertainties in the outcome of the collapse, then it will be time to worry.

In another setting, the accretion of matter onto the surface of a neutron star, the problems could be much more serious. Here, at a depth where nuclear reactions stimulating transient explosive phenomena can occur, it may be that electron capture on a particular nuclear species is the stimulator, and the rates will be extremely density and temperature dependent [12,13]. In this environment, the plasma coupling Γ will be much stronger than those cited in the previous example, and we can expect the effects on rates to be larger, and harder to estimate, even in magnitude. Furthermore, it is the temperature dependence more than the absolute rate that rules in most explosion calculations. Since the plasma corrections, whatever else, will be strongly temperature dependent, we could say that, knowing nothing about them, we equally know nothing about the effective exponent in the temperature dependence of the rate.

There is a body of literature that presents unorthodox results on the effects of the plasma on reaction rates, even in the case of the weakly coupled solar plasma. These results, if correct, would have significant impact on solar models. We wish it to be clear that the work of the present paper does not support any of these claims. One can find a critique in Ref. [14] as well as a list of some of the articles in this category, though there are more recent examples that cover the same topic [15]. There are, in addition, a few papers of the same genre addressing electron capture [16–18]. The last of these engendered a response in Ref. [19], one with which we completely agree. But, that said, the reply in [19] was more in the vein of "We did a correct calculation and had no such terms; therefore your calculation is wrong," rather than tracking down specific mistakes. The same could be said of the arguments given in Ref. [14]. Thus it may be worth adding my own conclusion about one thing that has gone wrong in at least some contributions of this genre. Let me characterize as an "S-matrix approach" one in which one starts the correction of a two-body reaction rate by putting in some more bodies from the plasma in the calculation, working out the multibody reaction rate in some perturbative way, and then doing the thermal average (typically) over the momentum states of the plasma particles. Looking at the actual mechanics in these papers, it appears to me that the assumptions are tantamount to entirely leaving out Coulomb forces in the factor $\exp[-\beta H_a]$ in (13). It is a mistake to do this. We could put the conclusion qualitatively as follows: A treatment strictly from a multiparticle S matrix, followed by averaging over thermal distributions, misses essential physics coming from the fact that the initial particles sit in an interacting medium.

IV. THINKING ABOUT THE STRONGLY COUPLED AND VERY DEGENERATE CASE

A. Ionic energy shift

Returning to the basic equation (20) that determines the kernel of the capture rate formula, we go back and think qualitatively about the ionic energy shift. We first state the case for the shift assumption and then the counter-argument. We take only electron kinetic energies and ionic potential energies in $H_{a,b}$, the electron potential energies not being relevant in the extremely degenerate system, at least not to the effect that we are considering. Now we look first at H_b where there is a term $e_b\phi_I(\mathbf{0})$, the energy of ion b in the fields of all of the other ions. If we forget about where b came

from and when it came into being and consider a problem in which it has been at $\mathbf{r}=0$ all along, we can, in principle, calculate the potential of the plasma ions at the position of b; it is, of course, a function of the charge $e_b=eZ_b$. In classical simulations the energy shift is given by $\Delta E_b=T$ $g(\Gamma_b)$, where g(x) is of order x and $\Gamma_b=Z_b^{5/3}e^23^{-1/3}(4\pi n_e)^{1/3}$. We can calculate the corresponding energy shift for initial ion a. From the time-dependent exponentials in (20) we would infer that these corrections change the effective Q value by an amount $\Delta E_a-\Delta E_b$.

But the actual term in the interaction, say, H_a , that induces an energy shift for ion a is $e_a\phi(\mathbf{0})$. First, through this term, the plasma redistributes itself around the ion, creating a potential, which then shifts the energy of the ion through another action of H_a . In a perturbative calculation the plasma is thereupon returned to its original state. If we let H_a act only once, it will transfer a bit of momentum from ion a to the plasma. Of course, the whole expression is a trace, so everything has to be returned to its initial value. But that bit of momentum can be returned to the plasma particles after the electron capture, through the interaction H_b . In the weakly coupled case there is substantial cancellation between these categories of effects. We cannot argue that in the strongly coupled case they would cancel in any particular way. But we would not trust a result that takes one part and discards the other

B. Ab initio numerical calculations?

We take a box containing N_I ions, not including a or b, and N_e electrons. The initial and final ions a and b that participate in the capture process are at the point $\mathbf{r} = \mathbf{0}$ and manifest themselves only in the potentials H_a and H_b . In one respect we are at an advantage here, in comparison with a parallel treatment of the nuclear fusion problem, because we probably do not care about regions in the space of the ions $\mathbf{R_i}$ that are classically inaccessible or nearly unaccessible at the temperature of the medium. Thus we can plausibly take the ions to be absolutely classical and entirely omit the ionic kinetic energy terms from H_a and H_b . We take a basis set of N_e electrons at positions $\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_{N_e}}$ and N_I ions at positions $\mathbf{R_1}, \mathbf{R_2}, \ldots, \mathbf{R_{N_I}}$. Using the cyclic invariance of the trace in (20) to move $\psi(0, 0)$ from the last position to the first and putting in the position basis, we have

$$M(t) = Z_P^{-1} \int d\mathbf{R}_1, \dots, d\mathbf{R}_{N_I}, \dots, d\mathbf{r}_2, \dots, d\mathbf{r}_{N_e}$$

$$\times \int d\mathbf{r}'_2, \dots, d\mathbf{r}'_{N_e} \langle \{\mathbf{0}, \mathbf{r}_2, \dots, \mathbf{r}_{N_e}\}, \mathbf{R}_1, \dots, \mathbf{R}_{N_I} \rangle$$

$$\times |e^{-(\beta - it)H_a}| \{\mathbf{0}, \mathbf{r}'_2, \dots, \mathbf{r}'_{N_e}\} \mathbf{R}_1, \dots, \mathbf{R}_{N_I} \rangle$$

$$\times \langle \{\mathbf{r}'_2, \dots, \mathbf{r}'_{N_e}\}, \mathbf{R}_1, \dots, \mathbf{R}_{N_I} | e^{-itH_b} | \{\mathbf{r}_2, \dots, \mathbf{r}_{N_e}\},$$

$$\times \mathbf{R}_1, \dots, \mathbf{R}_{N_I} \rangle. \tag{21}$$

We have here shifted from the grand canonical ensemble to the canonical ensemble, with a definite number of electrons. The $\{\cdots\}$ around the electron basis states signify a total antisymmetrization. The ionic part requires no symmetrization. Note that the intermediate integration is over electronic positions only. We have taken the classical limit for the ions, in which the

ionic kinetic energy term is omitted and the ionic coordinates within H_a and H_b remain at their external values.

Could we in principle use the trick of Ref. [20], $\exp(-\beta H) = [\exp(-\beta H/N_S)]^{N_S}$, taking N_S to be sufficiently large so that we can make a lowest-order perturbative expansion in the Coulomb potentials in each individual factor? Each factor would then be at a sufficiently high temperature N_ST to validate this lowest-order expansion. This would be at best an expensive calculation because N_1 , N_e , and N_I all have to be fairly large, and between each of the N_1 factors in the product one must integrate over the full manifold of some $\mathbf{r}'_1, \ldots, \mathbf{r}'_{N_e}$, not to mention the enormous antisymmetrizations required. And the final blow to this suggestion is probably that, because of the real-time exponentials, we would have rapidly oscillating integrands.

Perhaps instead, we could start by taking a very degenerate plasma. The electron sea is so stiff that it does nothing, except that one electron gets captured, creating an electron hole in the final state. Should we be worried about the effects of the (ionically) irregular plasma on what that hole does? Perhaps somewhat symbolically, we can write a much simpler equation,

$$M(t) = Z_P^{-1} \int d\mathbf{R}_1, \dots, d\mathbf{R}_{N_I} \langle \mathbf{R}_1, \dots, \mathbf{R}_{N_I} | e^{-(\beta - it)H_a}$$

$$\times |\mathbf{R}_1, \dots, \mathbf{R}_{N_I} \rangle \langle \bar{\mathbf{r}} = \mathbf{0}, \mathbf{R}_1, \dots, \mathbf{R}_{N_I} | e^{-itH_b}$$

$$\times |\bar{\mathbf{r}} = \mathbf{0}, \mathbf{R}_1, \dots, \mathbf{R}_{N_I} \rangle. \tag{22}$$

Is it possible to calculate the matrix elements for the hole to go from the origin back to the origin in time t under the action of H_b for a big set of irregular distributions of ions? If one had to know the answer, the eikonal method might serve.

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APPENDIX: PERTURBATION CALCULATIONS

To demonstrate the methods we divide the respective Hamiltonians as $H_{a,b} = H_0 + H_{a,b}^I$, in which the interaction term contains all Coulomb interactions of the electrons in the plasma and the interactions of the distinguished ions I_a and I_b with both electrons and plasma ions. Coulomb interactions among the ions in the plasma are retained in H_0 . We denote the charges of the electron and two ions, respectively, as e, e_a , and e_b , where $e_b = e_a - 1$, obtaining

$$H_a^I = \int d\mathbf{r} \{-e[\phi_I(\mathbf{r}) + \frac{1}{2}\phi_e(\mathbf{r})]n_e(\mathbf{r}) + e_I n_I(\mathbf{r})\phi(\mathbf{r})\} + e_a \phi(\mathbf{0}), \tag{A1}$$

$$H_b^I = \int d\mathbf{r} \{-e[\phi_I(\mathbf{r}) + \frac{1}{2}\phi_e(\mathbf{r})]n_e(\mathbf{r}) + e_I n_I(\mathbf{r})\phi(\mathbf{r})\} + e_b \phi(\mathbf{0}). \tag{A2}$$

Here ϕ_e and ϕ_I are the respective electric potentials produced by the electrons, and $\phi = \phi_I + \phi_e$ is the total potential of the plasma. We have not included the basic Coulomb interactions between electrons and I_a and I_b . But if we repeated the calculations to come using Coulomb wave functions instead of plane waves, we would not find any medium-dependent terms that are of leading order $e^2\kappa_D$. There is, of course, a conventional Coulomb correction in the absence of the plasma; perturbatively, it begins at order $e^2\kappa_D$ screening corrections. At the level of the present paper this vacuum contribution can just be added to the answer; Coulomb wave functions are not needed for calculating the rest of the corrections.

We introduce the interaction picture through the identities

$$e^{-H_a(\beta-it)} = e^{-H_0(\beta-it)}\Omega_+(-i\beta, t),$$
 (A3)

$$e^{-iH_bt} = \Omega_-(0, t)e^{-iH_0t},$$
 (A4)

where

$$\Omega_a^{(+)}(-i\beta, t) = \exp\left[i\int_{-i\beta}^t dt' \hat{H}_a^I(t')\right]_{\perp}, \quad (A5)$$

$$\hat{H}_{a}^{I}(t) = e^{iH_{0}(t+i\beta)}H_{a}^{I}e^{-iH_{0}(t+i\beta)}.$$
 (A6)

In (A5) the subscript + stands for time ordering of the integrals. Similarly, we have

$$\Omega_b^{(-)}(0,t) = \exp\left[-i\int_0^t dt' \hat{H}_b^I(t')\right],$$
 (A7)

where

$$\hat{H}_b^I(t) = e^{iH_0t} H_b^I e^{-iH_0t}, \tag{A8}$$

and now the integral is anti-time-ordered. Substituting in (13), we obtain

$$\begin{split} M(t) &= Z_{P}^{-1} \text{Tr}[e^{-H_{a}(\beta - it)} \psi_{e}^{\dagger}(\mathbf{0}, 0) e^{-iH_{b}t} \psi_{e}(\mathbf{0}, 0)] \\ &= Z_{P}^{-1} \text{Tr}[e^{-H_{0}(\beta - it)} \Omega_{a}^{(+)}(-i\beta, t) \psi_{e}^{\dagger}(\mathbf{0}, 0) \Omega_{b}^{(-)} \\ &\times (0, t) e^{-iH_{0}t} \psi_{e}(\mathbf{0}, 0)] \\ &= Z_{P}^{-1} \text{Tr}[e^{-H_{0}\beta} \Omega_{a}^{(+)}(-i\beta, t) \psi_{e}^{\dagger}(\mathbf{0}, 0) \\ &\times \Omega_{b}^{(-)}(0, t) e^{-iH_{0}t} \psi_{e}(\mathbf{0}, 0) e^{iH_{0}t}]. \end{split}$$
(A9)

We expand the Ω factors in powers of the coupling, retaining only terms of order e^2 (or e_a^2 , ee_a , e_a^2 , etc.). Schematically, each will have powers of e coming from the thermal expectation of a product of two ion-electric-potential $\phi(\mathbf{r})$ operators; these are determined by the Hamiltonian H_0 . If this potential-potential correlator is itself expanded in powers of e, the expansion begins with terms of order e^2 , so that the rate corrections would be of order e^4 , but the terms have an infrared singularity from the long-range Coulomb force, and when that is properly

³In our terminology, the distinguished ions I_a and I_b are not part of the "plasma." Since Fermi statistics prevents us from distinguishing an electron, we include all electrons in the "plasma."

regulated, the entire correction to the rate will be of order e^3 . In the present paper we pursue only these e^3 terms; the neglected terms will go as power e^4 or higher. For this purpose we shall need the part of the field correlation function that is the most singular as κ_D goes to zero,

$$\langle \phi(\mathbf{k}, t')\phi(-\mathbf{k}', t'')\rangle_{IR} \approx 4\pi\delta(\mathbf{k} - \mathbf{k}')\beta^{-1}\kappa_D^2 \frac{1}{(k^2 + \kappa_D^2)k^2},$$
(A10)

which is time independent.

We now expand $\Omega_a^{(+)}$,

$$\Omega_a^{(+)}(-i\beta, t) = 1 - i \int_{-i\beta}^t dt_1 \hat{H}_a^I(t_1) - \int_{-i\beta}^t dt_1 \hat{H}_a^I(t_1) \times \int_{-i\beta}^{t_1} dt_2 \hat{H}_a^I(t_2), \tag{A11}$$

and $\Omega_h^{(-)}$,

$$\Omega_b^{(-)}(0,t) = 1 + i \int_0^t dt_1 \hat{H}_b^I(t_1) - \int_0^t dt_1 \hat{H}_b^I(t_1) \times \int_0^{t_1} dt_2 \hat{H}_b^I(t_2).$$
(A12)

Before getting bogged down in the evaluation of a multiplicity of terms we think for a moment about the general form of the expressions generated by the expansion. Leaving out most of the arguments of the functions and not concerning ourselves with orders of factors, we note that the form is the expectation value,

$$\left\langle \left\{ -e \int n_e \left[\phi_I + \frac{1}{2} \phi_e \right] + e_{\{a,b\}} \phi(0) \right\} \right.$$

$$\times \left. \left\{ -e \int n_e \left[\phi_I + \frac{1}{2} \phi_e \right] + e_{\{a,b\}} \phi(0) \right\} \psi_e^{\dagger} \psi_e \right\rangle. \tag{A13}$$

Now we state some results of peering into the term-by-term outcome:

- (1) The electron operators within ψ_e , ψ_e^{\dagger} each get paired with an electron operator in an n_e or ϕ_e term earlier in the expression. The terms in which they eat each other are "disconnected"; i.e., their contribution gets canceled by a perturbation in the partition function in the denominator of (A9), in conjunction with an unperturbed numerator.
- (2) Terms where both ψ and ψ^{\dagger} pair with the operators from the same curly braces in (A13) are not infrared divergent in the absence of screening and will therefore not contribute in leading order.
- (3) Bearing in mind point (2) above, when a single ψ or ψ^{\dagger} is to be paired with an operator from the product

$$\frac{1}{2} \int d\mathbf{r} \phi_e(\mathbf{r}) n_e(\mathbf{r}) = \int d\mathbf{r} \int d\mathbf{r}' |\mathbf{r} - \mathbf{r}'|^{-1} n_e(\mathbf{r}) n_e(\mathbf{r}'),$$
(A14)

then the pairing will be, in effect, the same when it is with an operator in n_e or when it is with one in ϕ_e . Thus, if we add

a stipulation to the calculation of (A13) that the explicit ψ_e and ψ^{\dagger} are never to be paired with ϕ_e in this kind of term, we can compensate by multiplying the ϕ_e in (A13) by 2. To put it more simply, we can replace $H_{a,b}$ of (A1) and (A2) by

$$\begin{split} H_a^I &= \int d\mathbf{r} [-e\phi(\mathbf{r})n_e(\mathbf{r})] + e_a\phi(\mathbf{0}), \\ H_b^I &= \int d\mathbf{r} [-e\phi(\mathbf{r})n_e(\mathbf{r})] + e_b\phi(\mathbf{0}), \end{split} \tag{A15}$$

with the above stipulation on computation. These operators $\hat{H}_{a,b}^{I}(t)$ in the interaction picture are now given in terms of the electron creation and annihilation operators $a^{\dagger}(p)$ and a(p) by

$$\hat{H}_{a,b}^{I}(t) = \int \frac{d^3k}{(2\pi)^3} \phi(k,\tau) \left[e_{a,b} - e \int \frac{d^3p}{(2\pi)^3} \right] \times a_{\mathbf{p}+\mathbf{k}}^{\dagger} a_{\mathbf{p}} e^{i(E_{p+k} - E_p)\tau} , \tag{A16}$$

where $\tau = t + i\beta$ for the incoming system a and $\tau = t$ for the final system. In the the small \mathbf{k} limit we can set $\tau = 0$ in the final bracket in (A16). We do keep an infinitesimal \mathbf{k} in the indices of the operators $a_{\mathbf{p}+\mathbf{k}}$, as we shall see below. Since the infrared part of the correlator is also time independent, there is, in effect, no time dependence. Putting (A16) into (A11) and (A12) and then putting the results into (A9) and using (A10), we obtain

$$M(t) = M_0(t) - 4\pi \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\beta^{-1} \kappa_D^2}{k^2 (k^2 + \kappa_D^2)} \left[\left(\frac{t^2}{2} + i\beta t - \frac{\beta^2}{2} \right) \times M_1(t) - (t + i\beta)t M_2(t) + \frac{t^2}{2} M_3(t) \right],$$
 (A17)

where

$$M_{1}(t) = \lim_{k \to 0} \left\langle \left[e_{a} - e \int d\mathbf{p}_{3} \, a_{\mathbf{p}_{3} + \mathbf{k}}^{\dagger} a_{\mathbf{p}_{3}} \right] \right.$$

$$\times \left[e_{a} - e \int d\mathbf{p}_{4} \, a_{\mathbf{p}_{4} - \mathbf{k}}^{\dagger} a_{\mathbf{p}_{4}} \right] \int d\mathbf{p}_{1} d\mathbf{p} e^{iE_{p}t} a_{\mathbf{p}_{1}}^{\dagger} a_{\mathbf{p}} \right\rangle, \tag{A18}$$

$$M_{2}(t) = \lim_{k \to 0} \left\langle \left[e_{a} - e \int d\mathbf{p}_{3} \, a_{\mathbf{p}_{3} + \mathbf{k}}^{\dagger} a_{\mathbf{p}_{3}} \right] \right.$$

$$\times \int d\mathbf{p}_{1} a_{\mathbf{p}_{1}}^{\dagger} \left[e_{b} - e \int d\mathbf{p}_{4} \, a_{\mathbf{p}_{4} - \mathbf{k}}^{\dagger} a_{\mathbf{p}_{4}} \right] \int d\mathbf{p} e^{iE_{p}t} a_{\mathbf{p}} \right\rangle, \tag{A19}$$

$$M_{3}(t) = \lim_{k \to 0} \left\langle \int d\mathbf{p}_{1} a_{\mathbf{p}_{1}}^{\dagger} \left[e_{b} - e \int d\mathbf{p}_{3} a_{\mathbf{p}_{3} + \mathbf{k}}^{\dagger} a_{\mathbf{p}_{3}} \right] \right.$$

$$\times \left[e_{b} - e \int d\mathbf{p}_{4} a_{\mathbf{p}_{4} - \mathbf{k}}^{\dagger} a_{\mathbf{p}_{4}} \right] \int d\mathbf{p} e^{iE_{p}t} a_{\mathbf{p}} \right\rangle, \tag{A20}$$

and M_0 is the unperturbed part,

$$M_0(t) = \int d\mathbf{p}_1 d\mathbf{p} \langle a_{\mathbf{p}_1}^{\dagger} a_{\mathbf{p}} e^{iE_{\mathbf{p}}t} \rangle = \int d^3 p f(p) e^{iE_{p}t}.$$
(A21)

Here f(p) is the Fermi distribution, $f(E_p) = (1 + e^{\beta(E_p - \mu_e)})^{-1}$, and the electron chemical potential is determined from the electron density to zeroth order in e by $n_e = \int d\mathbf{p}(2\pi)^{-3} f(p)$. When we calculate perturbative corrections, we must explicitly include a correction that readjusts the relation between chemical potential and density, which we shall do below.

The thermal averages in (A18)–(A20) are readily calculated. A number of terms are disconnected and canceled by perturbative corrections to the partition function: (a) all terms of order e^2 in which $p = p_1$, i.e., in which operators in $\psi(\mathbf{0})$ are paired with those in $\psi^{\dagger}(\mathbf{0})$, and (b) some more that are discussed below. The rest of the terms can be expressed in terms of M_0 in (15), the function M_A ,

$$M_A(t) = \int \frac{d^3 p}{(2\pi)^3} [f(p)]^2 e^{iE_p t}, \qquad (A22)$$

and a time-independent constant R,

$$M_1(t) = M_2(t) = M_3(t)$$

= $(e_a - e)^2 M_0(t) + (2e_a e - e^2) M_A(t) + e^2 R M_0(t)$,
(A23)

where *R* is a time-independent constant that is proportional to the system volume and that will be canceled by a corresponding perturbation of the partition function.

We reconstitute the complete time-dependent function M(t), which, when inserted in (11), gives the rate:

$$M(t) = \left[1 + \frac{1}{2}(e_a - e)^2 \kappa_D \beta\right] M_0(t) + \frac{1}{2}(2ee_a - e^2)\kappa_D \times \beta M_A(t) - \frac{1}{2}\kappa_D \beta e^2 R M_0(t).$$
 (A24)

Now we calculate the changes of the same order to the partition function, where the system is governed by H_a ,

$$Z_{P} = \langle e^{-\beta H_{0}} \Omega_{a}^{+}(-i\beta, 0) \rangle_{\beta} = \left\langle e^{-\beta H_{0}} \left\{ 1 + \int_{-i\beta}^{0} dt_{1} \int_{-i\beta}^{t_{2}} dt_{2} \left[e_{a} \phi(\mathbf{0}, t_{1}) + e \int d\mathbf{r} \phi(\mathbf{r}, t_{1}) n_{e}(\mathbf{r}, t_{1}) \right] \right.$$

$$\times \left[e_{a} \phi(\mathbf{0}, t_{2}) + e \int d\mathbf{r}' \phi(\mathbf{r}', t_{2}) n_{e}(\mathbf{r}', t_{2}) \right] \right\}_{\beta}. \quad (A25)$$

The calculation follows the lines outlined above, but it is simpler. We obtain a contribution of order e_a^2 that is the same as the order e_a^2 term in (A24), but without the factor of $M_0(t)$. Therefore, in conjunction with the $1M_0(t)$ term in (A9), we see that the partition function perturbation removes the

 $e_a^2 \kappa_D \beta M_0(t)$ term from (A24). The other nonvanishing term coming from (A25) is of order e^2 , and it exactly removes the final term, proportional to R, from (A24).

Next we must recognize that in our calculation the chemical potentials were held fixed while we calculated perturbations to the rates. But the relation between number density and chemical potential has corrections of exactly the same order as the rates. In the next section we calculate the changes in this relation, and we find that the reexpression of the results in terms of the corrected densities removes the remaining terms of order e^2 from (A24),⁴ leaving the final result for the corrections of leading order as simply

$$M(t) = M_0(t) - e e_a \kappa_D \beta [M_0(t) - M_A(t)].$$
 (A26)

C. Keeping n_e fixed

In Sec. IV we used a relation between the change in the electron number density δn_e when we turn on Coulomb interactions in the medium while keeping the chemical potential fixed and the chemical potential change $\delta \mu_e$ that is then required to restore the original electron density. Then this $\delta \mu_e$, inserted as a correction into the Fermi distribution in the unperturbed rate function $F_0(t)$, generates a change that must be added to the terms shown in (A24) so that the complete result gives the change in rate induced by the Coulomb forces while keeping the number density, rather than the chemical potential, constant. We have

$$n_e = Z^{-1} \text{Tr}[e^{\beta H} \psi^{\dagger}(\mathbf{0}) \psi(\mathbf{0})]$$

= $Z^{-1} \text{Tr}[e^{\beta H_0} \Omega_e^{\dagger}(0, -i\beta) \psi^{\dagger}(\mathbf{0}) \psi(\mathbf{0})], \quad (A27)$

where the operator $\Omega_e^+(0, -i\beta)$ is expanded in exactly the form shown in (A11), except that we omit the interaction of the ion with the plasma in the calculation; that is, we take $e_a = e_b = 0$. Only the second order in the expansion contributes, and we see that the answer is given in terms of functions that we have already exhibited, now evaluated at t = 0,

$$n_e = n_e^{(0)} + \frac{1}{2}e^2\kappa_D\beta[M_0(0) - M_A(0)].$$
 (A28)

This gives a density shift that is compensated by a chemical potential shift,

$$\delta\mu_e = \frac{1}{2}e^2\kappa_D. \tag{A29}$$

We must compensate with a shift $\delta \mu_e$ in the function $M_0(t)$. Expanding, this gives a shift in the function that determines the rate,

$$\delta_e M(t) = -\frac{1}{2} e^2 \beta \kappa_D [M_0(t) - M_A(t)].$$
 (A30)

⁴This mirrors the situation in the case of a perturbative calculation of plasma corrections to fusion rates, as discussed in Ref. [10].

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