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Numerical modelling of the quantum-tail effect on fusion rates at low energy☆

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Abstract

Results of numerical simulations of fusion rate d(d,p)t, for low-energy deuteron beam, colliding with deuterated metallic matrix (Phys. Lett. B 547 (2002) 193; Eur. Phys. J. A 13 (2002) 377) confirm analytical estimates given in M. Coraddu et al. (Quantum-tail effect in low energy d+d reaction in deuterated metals, Physica A, this issue), taking into account quantum tails in the momentum distribution function of target particles, and predict an enhanced astrophysical factor in the 1 keV region in qualitative agreement with experiments.

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1. Introduction

Significant divergence from theoretical predictions of non-resonant fusion cross-section at low energies of incident deuteron particles has recently been observed in

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experimental works [1,2]. At energies of the charged deuteron beam less than 5 keV, colliding with deuterated metallic matrix, a great enhancement of the fusion cross-section takes place, compared to theoretical evaluations. The hypothesis of ions interacting via screened potential inside the metallic target was proposed in Ref. [1], but an unrealistically large screening potential was necessary to obtain reasonable agreement with the observed data. It is obvious that problems arising from experimental results need refining the theoretical models actually used.

As it was shown in papers [3,4], the role of quantum corrections to the particle momentum distribution is quite important. A significant deviation from Maxwellian distribution function appears. At large values of momentum, due to quantum corrections, the tail of the distribution has a power-law asymptotic behavior instead of exponential, resulting in modified reaction rates. In particular, this effect leads to non-exponential temperature dependence of inelastic process rates at relatively low temperatures and high densities.

In this paper we present results of numerical calculations of reaction rates for conditions of the interacting particles in the beam and in the target such as those of the experiments [1,2].

2. Numerical modeling of reaction rates for experimental conditions

The state of the system defined by the generalized distribution function over energy and momentum $F(E,\vec{p})$, may be presented in the factorized form: $F(E,\varepsilon)=n(E)a(E-\varepsilon)$, where $\varepsilon = p^2/2m$ is the particle kinetic energy. The reaction-rate constants of the inelastic process between two particles, named "a" and "b", may be presented in a more general form by the integral (see Ref. [5], Starostin et al., this issue)

$$N_a N_b K_{ab} = 8\pi C \int_{-\infty}^{\infty} \mathrm{d}E_a \int \mathrm{d}\vec{p}_a \int_{-\infty}^{\infty} \mathrm{d}E_b \int \mathrm{d}\vec{p} \int \mathrm{d}\vec{q}$$
$$\times\, n(E_a)(1-n(E_a+Q_a-\omega))a_a(E_a-\varepsilon_a)$$
$$\times\, n(E_b)(1-n(E_b+\omega+Q_b))a_b(E_b-\varepsilon_b)$$
$$\times\, a'_a(E_a+Q_a-\omega-\varepsilon_{\vec{p}_a-\vec{q}})a'_b(E_b+\omega+Q_b-\varepsilon_{\vec{p}_b+\vec{q}})\sigma(\varepsilon_p)\sqrt{\frac{2\varepsilon_p}{M}}\,, \quad (1)$$

where E_a, p_a are the energy and momentum of the "a" particle, $\varepsilon_p = p^2/2M$ is the relative kinetic energy in the center of mass, M is the reduced mass of colliding particles, C is a normalization constant, defined from comparison of the expression calculated by (1) and known results at high temperature and low density. We have

$$\vec{p} = \frac{m_b\vec{p}_a - m_a\vec{p}_b}{m_a+m_b}\,.$$

The expression for the population number $n(E)$ depends on the statistical distribution of the system. For the purpose of this work we must consider that deuterons, which are bosons, have the distribution

$$n(E) = (\exp[(E-\mu)/T]-1)^{-1}\,,$$

where μ is chemical potential. For non-ideal plasma, the spectral dependence of the distribution function, defined by Lorentzian profile, is

$$a(E,\vec{p}) = \frac{\gamma_i(E,\vec{p})}{\pi[(E-\varepsilon_p-\Delta(E,\vec{p}))^2+\gamma_i^2(E,\vec{p})]} \; . \tag{2}$$

In Eq. (2) γ is the width, Δ stands for the energy shift due to atom–matter interaction. The line width is given by $\gamma_a = N\hbar\sigma_a V_a$; where $\sigma_a = \pi e^4/\varepsilon_a^2$, $V_a = \sqrt{2\varepsilon_a/m_a}$, N is the concentration of scattering centers. For ideal plasma conditions, i.e., when the density decreases, the width $\gamma(E,\varepsilon_p) \to 0$, the function $a(E,\vec{p})$ becomes a delta-function. The cross-section dependence on kinetic energy may be given in the form

$$\sigma_0(\varepsilon_p) = \frac{S(\varepsilon_p)}{\varepsilon_p}\exp(-2\pi\eta(\varepsilon_p)), \qquad \eta(\varepsilon_p) = \frac{Z_1Z_2e^2}{\hbar}\sqrt{\frac{M}{2\varepsilon_p}} \; , \tag{3}$$

where $\eta(\varepsilon_p)$ is the Sommerfeld parameter. The astrophysical factor S is weakly dependent on the kinetic energy.

The influence of the screening potential U_e on the reaction rate, due to the effect of metallic electrons, may be taken into account by adding U_e to the collision energy

$$\sigma(\varepsilon_p) = \sigma_0(\varepsilon_p + U_e) \; . \tag{4}$$

Numerical calculations of the reaction rates were performed in accordance with the above model, for conditions close to the experimental ones: target particles concentration $N_a = 5\times10^{23}\ \mathrm{cm}^{-3}$, and interacting particle masses: $m_a = m_b = 2$ amu. Fusion reactions were considered between target particles of kind "a" and beam particles of kind "b". In the expression of the width we used as concentration N the concentration of the scattering ions in the metallic matrix.

Taking into account high dimension, the computation of the integral (1) can be performed using Monte Carlo method. The kinetic energy distribution of target particles was taken at temperature $T = 2.44\times10^{-2}$ eV, while the "b" particles were taken with the beam energies. It is interesting to note that for the case of a beam of mono-energetic particles the reaction rate computation can be reduced from expression (1) to the more simple integral

$$N_aK' = C\int_0^\infty \mathrm{d}E_a \int \mathrm{d}\vec{p}\, n_a(E_a)a(E_a-\varepsilon_p,\varepsilon_p)\sqrt{\frac{2\varepsilon_p}{M}}\,\sigma(\varepsilon_p)\,\mathrm{d}\varepsilon_p \; . \tag{5}$$

Within the framework of such model, for the case of ideal plasma, when we can neglect the wings of the Lorentzian profile in the integral (5), the expression for the reaction rate can be further simplified:

$$N_aK_2 = N_aK' = C\int_0^\infty \mathrm{d}E_a \int \mathrm{d}\vec{p} \int n_a(E_a)\delta(E_a-\varepsilon_p)\sqrt{\frac{2\varepsilon_p}{M}}\,\sigma(\varepsilon_p)\,\mathrm{d}\varepsilon_p$$
$$\sim \int_0^\infty n_a(\varepsilon_p)\varepsilon_p\sigma(\varepsilon_p)\,\mathrm{d}\varepsilon_p \; . \tag{6}$$

The influence of the distribution wings on the reaction rate value can be obtained by comparison of the computation results of the two expressions (1) and (5). We can also compare such results with the calculated reaction rate $K_1 = \sigma V$, using expression (3). After such comparison it is possible to estimate the astrophysical factor S and the deviation of theoretical predictions from experimental data.

To estimate the influence of momentum distribution tails on the reaction rate and the difference with the Maxwellian case, it is necessary to take into account the finite width of the Lorentzian profile (2). As was shown in Refs. [4,5], the main result of quantum corrections is that the momentum distribution function has asymptotically a power-law tail

$$f(\varepsilon_p) = C' \int_0^\infty \mathrm{d}E_a a(E_a - \varepsilon_p, \varepsilon_p) \sim \exp(-\varepsilon_p/T) + C_a(T)/\varepsilon_p^4 . \quad (7)$$

Using such decomposition in Eq. (5), it is possible to calculate the reaction rate, taking into account non-Maxwellian distribution function

$$K_3 = C_3 \int_0^\infty \mathrm{d}\varepsilon_a f(\varepsilon_a) \sqrt{\frac{\varepsilon_p \varepsilon_a}{M}}\, \sigma(\varepsilon_p) . \quad (8)$$

The results of such calculations are shown in the Table 1.

The reaction rate constants, calculated by different models, agree among themselves at beam energies above 2 keV. Decreasing energy in the range between 2 and 1 keV, we have found that K_1 and K_2 have still close values, while the rate constant K is much larger. It is interesting to note that the constants K_3 and K have relatively close values. Thus, it is possible to conclude, that, for correct estimations of the rate constants, it is quite possible to use the expressions shown in Eq. (5). The results of these calculations show that the wings of the momentum distribution are very important for a correct evaluations of the reaction rates. In the last column of Table 1 we presented the factor which characterizes the deviation of the rate in cause of non-ideal plasmas.

It is interesting also to estimate the role of the screening effect on the reaction rate and to compare it to the considered mechanisms. For that purpose the calculations were performed within the framework of the proposed model, but with addition of a screening potential $U_e = 28$ eV. Its influence was taken into account in accordance with expression (4). Such value of the potential seems realistic for the experimental conditions [1]. The results of calculations are presented in the Table 2.

Table 1
Comparison of the reaction rates $\langle \sigma v \rangle$ as function of the energy of the beam using the general expression of Eq. (1), K, and the three models in Eq. (3), K_1, in Eq. (5), K_2, and in Eq. (8), K_3

E_a (keV)	K_1	K_2	K_3	K	K/K_1
15	4.381E+04	4.045E+04	7.393E+04	4.38E+04	1.00E+00
10	4.073E+03	3.762E+03	6.877E+03	4.11E+03	1.01E+00
5	1.711E+01	1.580E+01	2.892E+01	1.77E+01	1.03E+00
2	2.615E − 04	2.421E − 04	4.487E − 04	2.85E − 04	1.09E+00
1.8	5.038E − 05	7.223E − 05	1.344E − 04	5.62E − 05	1.12E+00
1.5	2.339E − 06	3.850E − 06	7.343E − 06	3.34E − 06	1.43E+00
1.2	3.613E − 08	7.474E − 08	2.265E − 07	7.84E − 07	2.17E+01
1	8.252E − 10	7.711E − 10	5.678E − 08	2.82E − 07	3.42E+02

Table 2
Same as Table 1 taking into account the screening effect according to Eq. (4) with $U_e = 28$ eV

E_a (keV)	K_1	K_2	K_3	K_3/K_1
15	4.474E+04	4.133E+04	7.552E+04	1.6879937
10	4.237E+03	3.914E+03	7.152E+03	1.6880552
5	1.911E+01	1.766E+01	3.232E+01	1.69143
2	4.059E − 04	5.370E − 04	9.931E − 04	2.4466201
1.8	8.433E − 05	1.184E − 04	2.197E − 04	2.6056397
1.5	4.605E − 06	7.336E − 06	1.383E − 05	3.0034846
1.2	9.315E − 08	1.819E − 07	4.320E − 07	4.638S3085
1	2.863E − 09	6.951E − 09	7.386E − 08	25.801192

Here we have not presented the results of the more general computations using Eq. (1), because we have obtained rather correct estimates using model (5). We find a weak influence of the screening effect, using the reasonable value of the potential, which agrees with the results of [1,2]. Taking into account quantum corrections, the theoretical evaluations of the rates increase, in the low-energy range at 1–2 keV and less, if compared to the rates evaluated without the quantum effect.

3. Uncited reference

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