QUANTUM EFFECT ON ENHANCEMENT FACTOR OF NUCLEAR FUSION REACTION RATE

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ABSTRACT

In this paper, we study the enhancement of fusion reaction between two identical nuclei under influence of ultradense environment adopting classical and quantum approach.

After verifying the high accuracy of the analytical expression for the screening potential (SP) using the short range order effect for the classical One-Component-Plasmas (OCP), we proceed to obtain a new formula for the enhancement factor of the pycnonuclear reaction rate by combining the above solution and the path integral Monte Carlo data. This approach, considering at the same time the classical point of vue and the quantum effect, will allows us to have a more accurate result comparing with other works.

Keywords: OCP (One-Component Plasmas), SP (screening potential), path integral Monte Carlo (MC) data, analytical formula, pycnonulear reaction rate, quantum effect.

TÓM TẮT

Hiệu ứng lượng tử lên hệ số khuếch đại của tốc độ phản ứng tổng hợp hạt nhân

Trong bài báo này, chúng tôi khảo sát sự khuếch đại của phản ứng hạt nhân xảy ra giữa hai hạt nhân đồng nhất dưới tác dụng của môi trường đậm đặc trong khi bằng cách tiếp cận cổ điển và lượng tử.

Sau khi kiểm chứng độ chính xác cao của biểu thức giải tích cho thế màn chắn có được do sử dụng hiệu ứng tương tác ngắn cho hệ plasma một thành phần cổ điển (OCP), chúng tôi thực hiện các tính toán để thu được công thức mới tính hệ số khuếch đại của tốc độ phản ứng áp suất hạt nhân bằng cách phối hợp nghiệm ở trên và số liệu Monte Carlo tích phân lộ trình. Cách tiếp cận xem xét đồng thời quan điểm cổ điển và tác dụng lượng tử này sẽ cho phép chúng ta có được kết quả chính xác hơn khi so sánh với các công trình khác.

Từ khóa: OCP (Plasma một thành phần), thế màn chắn, số liệu Monte Carlo tích phân lộ trình, công thức giải tích, tốc độ phản ứng áp suất hạt nhân, tác dụng lượng tử.

1. Introduction

The terminology "thermonuclear reaction", which indicates the fusion of two nuclei under the condition of very high temperature, is widely used. But beside this category of reaction, as pointed out in many works, there exist also fusions which can occur when the density of the environment attains to some high enough value at low

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temperature (see, for example, [1]). Contrary to “thermonuclear”, this should be named “pycnonuclear” reaction as proposed by one pioneer work [2].

There are several theoretical works for the enhancement of nuclear fusion rate under high pressure using the classical OCP (One-Component-Plasma) model and the results show satisfactory accuracy comparing with the non quantum Monte Carlo (MC) simulations [3, 4, 5].

However, in order to obtain a more realistic result, one can not ignore the quantum influence when the distance between two nuclei is near to the De Broglie wavelength. In fact, when two particles are close together enough, the fusion process is affected by the probability of passing through the Coulomb barrier.

The aim of this paper is, after showing the accuracy of the results established in previous works for classical calculations, to present a new formula for the coefficient of enhancement of pycnonuclear fusion by combining the classical and quantum formalisms; This must show the small enough error with respect to the path integral MC data.

2. Overview of the model and basic classical results

In the first stage, we determine the quantities which characterize model OCP widely used in most works to compute the enhancement factor of a nuclear fusion process. The coupling parameter

$$\Gamma = \frac{(Ze)^2}{akT}$$

helps us to compare the magnitude of Coulomb interaction $\frac{(Ze)^2}{a}$ and the range of thermal motion energy kT, where a is ion sphere radius. From now on, we will use all quantities in units of a.

With $H(r)$ indicating the screening potential (SP) of the environment, the radial distribution function, which expresses the contact probability of two ions, is given by

$$g(\mathrm{r}) = \exp\left[-\Gamma\left(\frac{1}{r} - H(\mathrm{r})\right)\right].$$

Note that numerical values of this function $g(r)$ are provided by Monte Carlo (MC) simulations, but at too small range of the distance r between two nuclei, this MC method can not give any results, so that, one must apply the Widom polynomial of twelfth degree [4]:

$$H(r) = h_0 - h_1 r^2 + h_2 r^4 - h_3 r^6 + h_4 r^8 - h_5 r^{10} + h_6 r^{12}, \tag{1}$$

where the coefficient h_1 has the exact value $\frac{1}{4}$ as demonstrated rigorously in some theoretical calculations, and h_0 corresponds to the fusion process of two particles, on which we will focus in this work.

The coefficients h_i in (1), especially h_0, for the classical case, have been computed in several works. The agreement between the MC data and the analytical formula is highly adequate [4].

In this paper, we shall use the expression of h_0 proposed in [5] for classical model:

$$h_{0\Gamma} = h_0(lm) - \frac{\Phi}{100\Gamma} \tag{2a}$$

where

$$h_0(lm) = 1.056299 + \frac{1.039957}{\Gamma^{0.676936}} - \frac{1}{\Gamma}\left(0.274823\ln\Gamma + 1.084319\right) \tag{2b}$$

and

$$\Phi = \sum_{k=0}^{5} a_k (\ln\Gamma)^k , \tag{2c}$$

Table 1. *Coefficients in (2c)*

a_0	a_1	a_2	a_3	a_4	a_5
6.69370	–0.69922	–2.80549	1.95369	–0.43372	0.03298

The advantage of (2a, b, c) is that the formalism used is compatible with the Binary Ionic Mixture (BIM) and the linear mixing rule in thermodynamics. The error of these formulae is the same as the one which committed in MC computations.

3. Enhancement factor and path integral MC data

As mentioned above, one must consider the quantum effect at value of the internuclear distance r comparing with the thermal De Broglie wavelength $\lambda_d = \frac{h}{\sqrt{2\pi mkT}}$ where h is the Planck constant and m, mass of the particle. In fact, in addition to the coupling factor Γ, are to be considered the parameters $\eta = 2\pi\frac{\lambda_d^2}{a^2}$ or $\zeta = \left(\frac{4\Gamma^2}{\pi^2 r_s}\right)^{\frac{1}{3}} = \left(\frac{4}{\pi^2}\Gamma\eta\right)^{\frac{1}{3}}$, representing the correlation between classical model and the length from which there exists the overlap of the two wave packets. In these definitions, the ratio $r_s = \frac{a}{a_B}$ denotes the ionic sphere radius *a* in terms of the ionic Bohr radius a_B. This situation asks, instead of classical MC simulations, computations including quantum characteristics. Path integral MC (PIMC) has been investigated by some authors [6, 7, 8] and shows different results with classical MC ones. And the MC values of the function *g*(*r*) depend not only on the coupling parameter Γ but this time on the quantum parameters η and ζ as well. For this reason, one should modify the formula obtained with classical OCP model.

Some authors have put forward expression for the enhancement factor h_0. One of the first works in literature must be the Jancovici's one [9]:

$$h_{0JAN}(\Gamma,\zeta) = \frac{1}{\Gamma}(1.0531\Gamma + 2.2931\Gamma^{\frac{1}{4}} - 0.5551\ln\Gamma - 2.35) - (\frac{5}{32})\zeta^2 \qquad (3)$$

with $1 \le \Gamma \le 155$ and $\zeta \le 1$.

In (3), the dependence of h_0 on the classical parameter Γ and the quantum one ζ is separated in two different parts. The plane representing h_0 with respect to Γ and ζ according to (3) is shown in Fig.1. One can compare (3) with PIMC data (black dots) [8] and observe that (3) is valid only for small value of Γ and ζ.

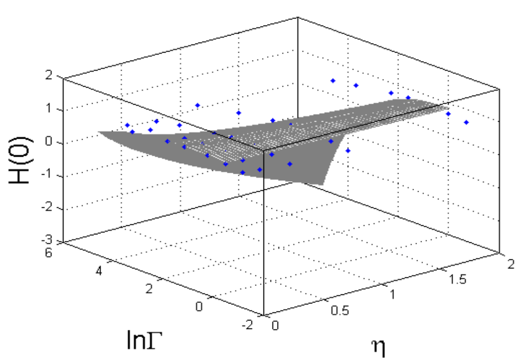

Fig 1. *The variation of h_0 with respect to Γ and ζ (3). Black spots are PIMC data.*

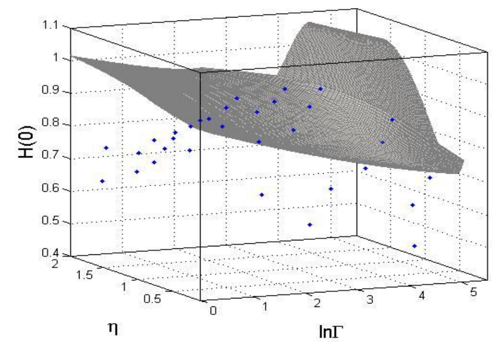

Fig 2. *The plane (4) does not match with PIMC data.*

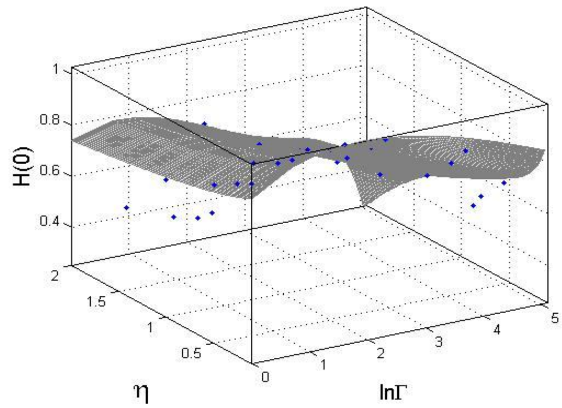

Fig 3. *The 3-D representation of (6) passes almost all the PIMC data with some error*

Another work concerning the coefficient h_0 comes from [6], where h_0 is

$$h_{0OGA}(\Gamma,\zeta) = h_{0OGA}(\Gamma) + h'_{0OGA}(\Gamma,\zeta)\,. \tag{4}$$

Where

$$h_{0OGA}(\Gamma) = 1.132 - 0.0094\ln\Gamma$$

is the purely classical part and

$$h'_{0OGA}(\Gamma,\zeta) = -(\frac{5}{32})\zeta^2(1-0.0348\zeta - 0.1388\zeta^2 + 0.0222\zeta^3) + 0.0015\zeta^3$$

is the part which combines classical and quantum effects.

As one can see in Fig. 2, the compatibility between (4) and PIMC data is not good enough though the authors have the idea of splitting the classical contribution apart in (4).

More recently, Chugunov *et al* recommended more sophisticated formula to compute h_0 [7]:

$$h_{0CHU}(\Gamma,\zeta) = h_{0CHU}(\Gamma) + h'_{0CHU}(\Gamma,\zeta) = h_{0CHU}(\Gamma',\zeta) \tag{5}$$

where

$$h_{0CHU}(\Gamma) = \Gamma^{3/2}\left(\frac{A_1}{\sqrt{A_2+\Gamma}} + \frac{A_3}{1+\Gamma}\right) + \frac{B_1\Gamma}{B_2+\Gamma} + \frac{B_3\Gamma}{B_4+\Gamma^2}$$

with

$A_1 = 2.7822$, $A_2 = 98.34$, $A_3 = \sqrt{3} - A_1/\sqrt{A_2} = 1.4515$, $B_1 = -1.7476$,

$B_2 = 66.07$, $B_3 = 1.12$, and $B_4 = 65$,

and $h'_{0CHU}(\Gamma,\zeta)$ is the quantum contribution, with $1 \le \Gamma \le 155$ and $0 \le \zeta \le 2$.

Note that in (5), the supplementary variable *Γ'* is computed from classical and quantum parameters *Γ* and *ζ*

$$\Gamma' = \frac{\Gamma}{(1+0.022\zeta+(0.41-0.6/\Gamma)\zeta^2+(0.06+2.2/\Gamma)\zeta^3)^{1/3}}.$$

One of the features of (5) is that one can deduce the asymptotic value of h_0 for fluid plasmas $h_{0CHU}=\sqrt{3}\Gamma^{1/2}$ ($\Gamma \ll 1$) in Debye-Hückel theory. Still, there exists some error with respect to the PIMC data in the region as one can recognize in Fig.3.

In this paper, taking into account (2a, b, and c), we suggest a new expression for $h_0$depending at the same time the classical and quantum parameters:

$$h_0 = h_{0\Gamma}(\Gamma) + h_{0\Gamma\zeta}(\Gamma,\zeta) + h_{0\zeta}(\zeta) \tag{6a}$$

where $h_{0\Gamma}(\Gamma)$ is computed from (2), which expresses the dependence of h_0 on Γ only,

$$h_{0\Gamma\zeta}(\Gamma,\zeta) = 0.03914\zeta^{1/2}\ln\Gamma \tag{6b}$$

is the part which reflects the influence of the « hybrid » classical and quantum parameters on the nuclear fusion, and the last part,

$$h_{0\zeta}(\zeta) = -0.06797\zeta - 0.23498\zeta^2 + 0.08694\zeta^3 - 0.00947\zeta^4, \tag{6c}$$

reveals the pure effect of quantum variable *ζ* on the enhancement factor.

In Table 2, we list some numerical values given by PIMC simulations [8] and those coming from the formulae (3), (4), (5), and (6a, b, and c). Their variation and the errors committed between those expressions and PIMC data are shown in Table 3 and Fig. 4, 5. We mention a very small discordance of about 9% between (6) and PIMC data provided by [8].

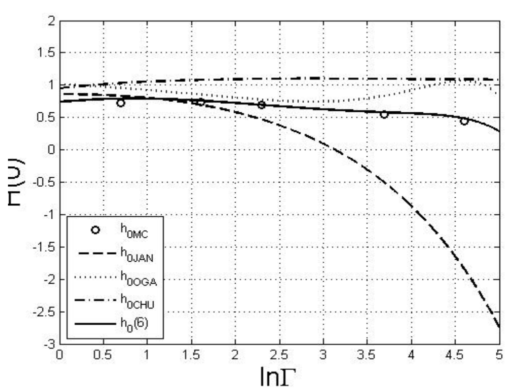

***Fig. 4.** The dependence of h_0 on Γ with η = 2*

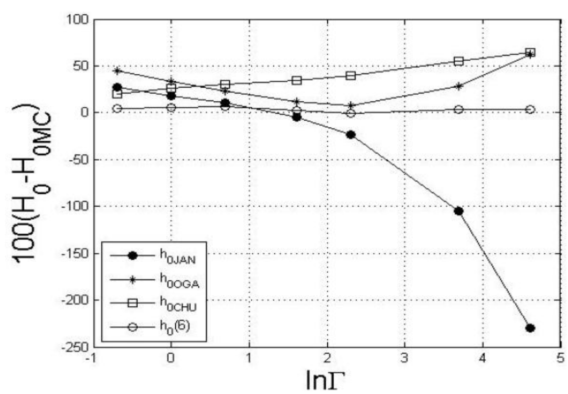

***Fig. 5.** Error of (3), (4), (5), and (6) with respect to the PIMC data with η = 2*

Table 2. *Some numerical values of PIMC data [8]*
and of formulae proposed by various authors (3), (4), (5,) and (6)

η	Γ	h_0[7]	h_{0JAN} (3)	h_{0OGA}(4)	h_{0CHU} (5)	h_0(6)
0.1	0.5	0.87(4)	0.9675	1.1272	0.8750	0.7813
0.1	1	0.95(3)	0.9778	1.1141	0.9926	0.8973
0.1	2	1.01(3)	1.0199	1.0975	1.0559	0.9934
0.1	5	1.03(2)	1.0363	1.0667	1.0906	1.0368
0.1	10	1.02(3)	1.0125	1.0333	1.1006	1.0303
0.1	40	0.91(4)	0.8717	0.9265	1.0897	0.9632
0.25	0.5	0.82(2)	0.9578	1.1179	0.8693	0.7602
0.25	1	0.92(3)	0.9622	1.0997	0.9878	0.8706
0.25	2	0.97(3)	0.9953	1.0753	1.0531	0.9586
0.25	5	0.98(2)	0.9909	1.0287	1.0890	0.9860
0.25	10	0.957(3)	0.9404	0.9783	1.1003	0.9628
0.25	40	0.83(4)	0.6901	0.8327	1.0909	0.8557
0.25	100	0.71(4)	0.3449	0.7383	1.0828	0.7691
0.5	0.5	0.773(14)	0.9452	1.1062	0.8596	0.7369
0.5	1	0.869(19)	0.9423	1.0818	0.9804	0.8405
0.5	2	0.92(2)	0.9636	1.0485	1.0490	0.9190
0.5	5	0.93(2)	0.9326	0.9848	1.0869	0.9293
0.5	10	0.869(14)	0.8478	0.9186	1.0997	0.8904
0.5	40	0.734(16)	0.4568	0.7627	1.0921	0.7583
0.5	100	0.61(2)	-0.0848	0.7436	1.0843	0.6823
1	0.5	0.708(9)	0.9252	1.0884	0.8420	0.7045
1	1	0.787(11)	0.9106	1.0550	0.9673	0.7984
1	2	0.844(14)	0.9134	1.0092	1.0421	0.8641
1	5	0.85(2)	0.8400	0.9251	1.0837	0.8535
1	10	0.797(19)	0.7009	0.8457	1.0984	0.7987
1	40	0.637(15)	0.0865	0.7386	1.0936	0.6613
1	200	0.442(14)	-1.8567	1.0598	1.0801	0.5331
2	0.5	0.6184(18)	0.8936	1.0615	0.8138	0.6598
2	1	0.682(5)	0.8604	1.0157	0.9466	0.7407
2	2	0.725(7)	0.8336	0.9546	1.0309	0.7905

2	5	0.737(13)	0.6930	0.8522	1.0791	0.7580
2	10	0.698(16)	0.4676	0.7758	1.0960	0.6929
2	40	0.546(12)	-0.5014	0.8322	1.0953	0.5795
2	100	0.443(8)	-1.8499	1.0663	1.0878	0.4828

Table 3. *Errors in percentages committed between PIMC data and formulae (3), (4), (5), and (6) for some values of η and Γ*

η	Γ	Δh_{0JAN} (3)	Δh_{0OGA}(4)	Δh_{0CHU} (5)	Δh_0 (6)
0.1	0.5	-9.35	25.32	0.10	9.27
0.1	1	-2.48	16.11	3.96	-5.57
0.1	2	-0.69	8.45	4.29	-1.96
0.1	5	-0.43	3.47	5.86	0.48
0.1	10	1.05	1.03	7.76	0.73
0.1	40	4.23	1.25	17.57	4.92
0.25	0.5	-13.58	29.59	4.73	-6.18
0.25	1	-3.92	17.67	6.48	-5.24
0.25	2	-2.23	10.23	8.01	-1.44
0.25	5	-0.89	4.67	10.79	0.40
0.25	10	1.69	2.10	14.30	0.55
0.25	40	14.39	-0.13	25.69	2.17
0.25	100	36.91	2.43	36.88	5.51
0.5	0.5	-17.21	33.31	8.65	-3.63
0.5	1	-7.31	21.26	11.12	-2.87
0.5	2	-4.16	12.65	12.70	-0.30
0.5	5	-0.06	5.28	15.49	-0.27
0.5	10	2.13	4.94	23.06	2.12
0.5	40	27.73	2.86	35.79	2.41
0.5	100	69.68	13.16	47.23	7.03
1	0.5	-21.63	37.94	13.31	-0.44
1	1	-12.35	26.79	18.02	1.13
1	2	-6.92	16.51	19.80	2.00
1	5	1.20	7.31	23.17	0.15
1	10	9.63	4.85	30.12	0.15

1	40	55.07	10.144	45.64	2.41
1	200	229.9	61.77	63.80	9.09
2	0.5	-27.52	44.31	19.54	4.14
2	1	-17.79	33.32	26.41	5.82
2	2	-10.79	22.89	30.52	6.45
2	5	4.41	11.51	34.19	2.09
2	10	23.06	7.76	39.78	-0.52
2	40	104.75	28.61	54.92	3.33
2	100	229.38	62.25	64.50	3.90

4. Conclusion

Pycnonuclear fusion reactions are produced in ultradense matters, for example, in white dwarfs, neutron stars and in some laboratories such as in Lawrence Livermore National Laboratory (LIFE project to produce artificial stars using a large number of high power lasers).

An analytic expression for the enhancement factor of this kind of reaction is then very important for codes of numerical computations. The result for classical OCP has been obtained with high accuracy but the dependence of this factor on quantum parameters is revealed to be clear so that in this work, we put in advance a formula which combines the classical and quantum effects in the fusion process of two nuclei in ultradense plasmas. The agreement between this and PIMC data is shown to be satisfactory.

Anyway, further investigations should be followed, especially ones concerning the mixture of heterogeneous nuclei plasmas or the influence of free-electron inhomogeneity on the process fusion.

REFERENCES

1. Gasques L. R., Afanasjev A. V., Aguilera E. F., Beard M., Chamon L. C., Ring P., Wiescher M., and Yakovlev D. G. (2005), "Nuclear fusion in dense matter: Reaction rate and carbon burning", *Phys. Rev.*,72(2), pp.025806-1-025806-14.
2. Cameron, A. G. W. (1959), "Pycnonuclear Reactions and Nova Explosions", *Astrophysical Journal*, **130**, pp.916-940.
3. DeWitt H., Slattery W., and Chabrier G. (1996), "Numerical simulation of strongly coupled binary ionic plasmas", *Physica B*, 228(1-2), pp. 21-26.
4. Do Xuan Hoi, Phan Cong Thanh (2012), "Screening potential at the crystallization point of ultradense OCP plasmas", *Journal of Science* –Natural Science and Technology, *Ho Chi Minh City University of Education*, 36(70), 05-2012**,** pp. 63-73.

5. Lê Thị Thúy Ngân (2015), “Hiệu ứng lượng tử trong quá trình tổng hợp hạt nhân trong plasmas cực đậm đặc”, *Master's Thesis in Physics*, HCMC University of Pedagogy (in preparation).
6. Ogata S., Iyetomi H., and Ichimaru S., (1991), “*Nuclear reaction rates in dense carbon-oxygen mixtures*”, *Astrophys. J.*, 372, 259.
7. Chugunov A. I., DeWitt H. E., Yakovlev D. G. (2007), “Coulomb tunneling for fusion reactions in dense matter: Path integral Monte Carlo versus mean field”, *Phys. Rev. D*, 76(2), pp.025028-1-025028-13.
8. Militzer B., Pollock E. L. (2004), “Equilibrium contact probabilities in dense plasma”, *Phys. Rev. B*, 71, 134303.
9. Jancovici B. (1977), “Pair correlation function in a dense plasma and pycnonuclear reactions in stars”, *J. Stat. Phys.*, 17(5), pp.357-370.

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