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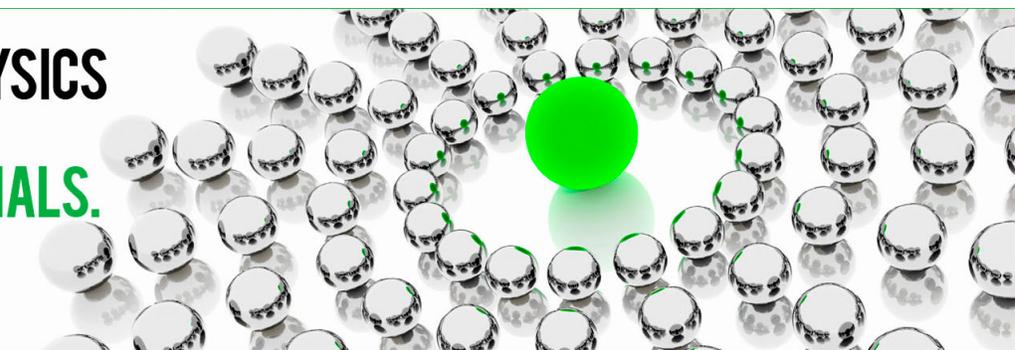
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Comment on: Deuterium nuclear fusion at room temperature: A pertinent inequality on barrier penetration

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In a recent letter, Rosen¹ claims to justify the large value apparently observed by Fleischmann and Pons² and Jones *et al.*³ for the fusion rate of deuterons embedded in palladium or titanium cathodes at room temperature. As we shall see, his reasoning contains some mistakes, and his conclusion is, in general, not valid.

Rosen estimates the fusion rate for D₂ molecules trapped in a metallic lattice by applying the WKB barrier penetration formula previously derived by Siclen and Jones⁴ for free D₂, to different vibrational states of the trapped molecule:

$$\Lambda(E) = (5.7 \times 10^8 \text{ s}^{-1}) \exp[-\lambda(E)] \quad (1)$$

with

$$\lambda(E) = \frac{2m_D^{1/2}}{\hbar} \int_a^b [V(r) - E]^{1/2} dr, \quad (2)$$

where m_D is the deuteron mass, r is the internuclear separation, $V(r)$ is the effective potential for linear molecular vibrations, b is the classical turning point for nuclear relative movement at the vibrational energy E , and a is the internuclear separation at which attractive nuclear forces begin to act.

In fact, the formula derived by Siclen and Jones⁴ was

$$\begin{aligned} \Lambda(E_0) &= \frac{A\alpha}{8\pi^{3/2}b_0} \exp[-\lambda(E_0)] \\ &= (5.7 \times 10^8 \text{ s}^{-1}) \exp[-\lambda(E_0)], \end{aligned} \quad (3)$$

where "0" subindices refer to the ground vibrational state, A is the nuclear reaction constant, $\alpha = (k_e m_D/2)^{1/2}/\hbar k_e$ being the harmonic force constant in the minimum of the nuclear motion potential function $V(r)$, $\lambda(E_0)$ is given by

$$\lambda(E_0) = \int_a^{b_0} \left\{ 2 \left(\frac{m_D}{\hbar^2} [V(r) - E_0] + \frac{1}{4r^2} \right)^{1/2} - \frac{1}{r} \right\} dr, \quad (4)$$

and the preexponential factor in the right-hand side of Eq. (3) is the one resulting for $a = 0$ (see Table 1 in Ref. 3).

The differences between formulas (1)–(2) and (3)–(4) deserve some comments.

(i) Siclen and Jones deduction applies only to the $v = 0$ molecular state, since the harmonic oscillator fundamental eigenfunction is used for determining the normalization constant in the WKB connection formula (page 215 in Ref. 4) [Siclen and Jones calculation of the normalization constant (β factor on page 215 of Ref. 4) contains a slight error, since $(Q_0(r_0))^{-1/2}$ instead of $(Q(r_0))^{-1/2}$ is used in its derivation]. For a vibrationally excited state a different eigenfunction should be used and a smaller normalization constant would be obtained, since penetration in the classically for-

bidden region decreases with vibrational excitation, so that a lower value would be obtained for the proportionally constant in (1). Therefore, Rosen's application of formula (1)–(2) to a vibrationally excited level should give a too high value for Λ .

(ii) Siclen and Jones use Langer's modification⁵ of the WKB method which, for a potential approaching the origin as $1/r$, gives a better approximation to the wave function in the neighborhood of $r = 0$ than the standard WKB method.⁶ In fact, the real $V(r)$ decreases when attractive nuclear interactions begin to act ($r < a$), but this behavior does not affect the present calculations since, for a given vibrational energy, the barrier penetration rate only depends on the potential shape for $a < r < b_0$, as follows from Eqs. (4) or (2). Given the small value of "a" ($\approx 10^{-4}$ a.u.), it is advisable to use Langer's modification of the WKB method. Rosen's formulas (1)–(2) differ, even when applied to the E_0 level, from both, the one obtained using the standard WKB method and that resulting in Langer's modification: in the latter case, the $1/4r^2$ and $-1/r$ terms do not cancel in the integral in (4) and, in the former case, the relationship between $\lambda(E_0)$ and $\Lambda(E_0)$ is no longer that of (1) or (3), but

$$\Lambda(E_0) = \frac{A\alpha\hbar}{16\pi^{3/2}m_D^{1/2}a^2(V(a) - E_0)^{1/2}} \exp[-\lambda(E_0)], \quad (5)$$

where we have assumed $v = J = 0$, and $\lambda(E_0)$ coincides with Eq. (2) for $E = E_0$. In particular, if we take $a = 0$, the preexponential factor in (5), as well as $\Lambda(E_0)$ diverge, making indispensable to use Langer's method. The values adopted by Rosen for $\lambda(E_0)$ and $\Lambda(E_0)$ are those calculated by Siclen and Jones for $a = 0$ (Table 1 in Ref. 4) and therefore, are inconsistent with Rosen's formula (1)–(2).

In order to appreciate how the basic WKB method detaches from Langer's modification as $a \rightarrow 0$, we present in Table I the values of $\lambda(E_0)$, $\Lambda(E_0)$ and the preexponential factor $\Lambda(E_0)/\exp[-\lambda(E_0)]$ calculated by us using formulas (5)–(2) and (3)–(4).

Those data have been obtained with the $V(r)$ values calculated by Kolos and Wolniewicz⁷ for free D₂. Instead of doing a direct analytical fit to $V(r)$ (using, for instance, a Morse function), we have made a polynomial fitting of the electronic energies ($V(r) - 1/r$), which have a much smoother behavior and a well defined $r \rightarrow 0$ limit (for $r = 0$, the Helium atomic energy is used). Adding the nuclear repulsion to this polynomial, an analytical function is obtained that fits $V(r)$ in the whole $(0, r_e)$ interval much better than the Morse or similar curves. This procedure corrects an error introduced in the evaluation of integral (4) by Siclen and Jones,⁴ who use a Morse curve for $r > 0.5$ a.u. and $V = 1/r$

TABLE I. Calculated values of $\lambda(E_0)$, $\Lambda(E_0)/\exp[-\lambda(E_0)]$ and $\Lambda(E_0)$ using formulas (3)–(4) (WKB–Langer) and (5)–(2) (basic WKB) with $A = 2 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1} = 1.35 \times 10^9 \text{ bohr}^3 \text{ s}^{-1}$ and the Kolos and Wolniewicz⁷ values for $V(r)$.

$a/a.u.$	Method	$\lambda(E_0)$	$\frac{\Lambda(E_0)}{\exp[-\lambda(E_0)]}/\text{s}^{-1}$	$\Lambda(E_0)/\text{s}^{-1}$
0	Basic WKB	177	∞	∞
0	WKB–Langer	166	6.04×10^8	4.35×10^{-64}
10^{-12}	Basic WKB	177	6.12×10^{24}	1.34×10^{-52}
10^{-12}	WKB–Langer	166	6.04×10^8	4.35×10^{-64}
10^{-6}	Basic WKB	176	6.12×10^{15}	1.71×10^{-61}
10^{-6}	WKB–Langer	166	6.04×10^8	4.38×10^{-64}
10^{-4}	Basic WKB	174	6.12×10^{12}	1.51×10^{-63}
10^{-4}	WKB–Langer	165	6.04×10^8	8.25×10^{-64}

for $r < 0.5$ a.u., thus omitting the electronic energy in the latter zone (see also Koonin and Nauenberg⁸). For the numerical calculations, the NAG package⁹ has been used.

Leaving aside the above-mentioned inconsistencies implicit in the formula (1)–(2), Rosen uses it together with the inequality

$$V(\hat{r}) - V(r) \leq (E - E_0) \quad \text{for } a \leq r \leq b_0 \quad \text{and } E > E_0, \quad (6)$$

where

$$\hat{r} \equiv \beta(r - a) + a \quad \text{and} \quad \beta \equiv \frac{b - a}{b_0 - a}, \quad (7)$$

to deduce the relationship

$$\lambda(E) < \frac{b - a}{b_0 - a} \lambda(E_0), \quad (8)$$

which, for $E = 9$ eV and taking a free deuterium Morse function for $V(r)$, leads to $\Lambda \geq 2.8 \times 10^{-20} \text{ s}^{-1}$ [Eq. (7) of Ref. 1].

We shall now show that inequalities (6) and (8) do not, in general, hold. The relationship (6) can be put in the form

$$W(r) \leq W(b_0) \quad (9)$$

with $W(r) \equiv V(\hat{r}) - V(r)$. If, for simplicity, we take $a = 0$ in (7), it can easily be seen that Eq. (9) is not fulfilled by any potential of the form $C + 1/r^n$ in any point of the interval (a, b_0) . Effectively, inequality (9) now reads

$$\frac{1}{(\beta r)^n} - \frac{1}{r^n} \leq \frac{1}{(\beta b_0)^n} - \frac{1}{b_0^n}, \quad (10)$$

which requires $r^n > b_0^n$. Other kinds of potential functions, like e^{-ar} , can lead to $(dW/dr) \geq 0$ for $r < b_0$, this being a sufficient condition for (9) to be satisfied. In effect, for that function

$$dW/dr = -ae^{-ar}\beta + ae^{-ar}, \quad (11)$$

TABLE II. Calculated values of $\lambda(E)$ and $\beta\lambda(E_0)$ using formulas (3)–(4) (WKB–Langer) and (5)–(2) (basic WKB) with $A = 2 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1} = 1.35 \times 10^9 \text{ bohr}^3 \text{ s}^{-1}$, $E = 9$ eV = 0.331 hartree, $E_0 = -4.54$ eV = -0.154 hartree and the Kolos and Wolniewicz (Ref. 7) values for $V(r)$.

$a/a.u.$	Method	$\lambda(E)$	$\beta\lambda(E_0)$
0	Basic WKB	137	79.6
0	WKB–Langer	127	74.9
10^{-4}	Basic WKB	134	78.5
10^{-4}	WKB–Langer	127	74.6

which is ≥ 0 for r less than a critical value

$$r_c = \frac{\ln \beta}{\alpha(\beta - 1)} = b_0 \frac{\ln b - \ln b_0}{\alpha(b - b_0)}. \quad (12)$$

Choosing a sufficiently small value for α , we can always obtain an $r_c > b_0$.

However, it is well known that exponential functions (e.g. the Morse curve), although qualitatively reproducing the global behavior of $V(r)$, they cannot give a good representation of that potential for r values close to and above “ a ,” where it should approximately behave as $C + 1/r$ (the changes in electronic energy and in the repulsions with other nuclei when varying r will be much less than that of the intramolecular nuclear repulsion). Therefore, it is to be expected that inequality (8) does not, in general, hold and that the high value obtained by Rosen for Λ not be significant to cold fusion experiments. To corroborate this, we have used the basic WKB and WKB–Langer formulas to calculate $\lambda(E)$ for the two energy values considered by Rosen (using the procedure described for Table I and forgetting about the incorrectness of applying it for $E \neq E_0$). The results are collected in Table II, which evidences that Rosen’s inequality is not satisfied, and that use of one or the other method is not essential at this point.

In conclusion, Rosen’s values for $\Lambda(E)$ are incorrect.

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