229(4): Transmission Coefficient for Lennard-Jones and Woods-Saxon Potentials.

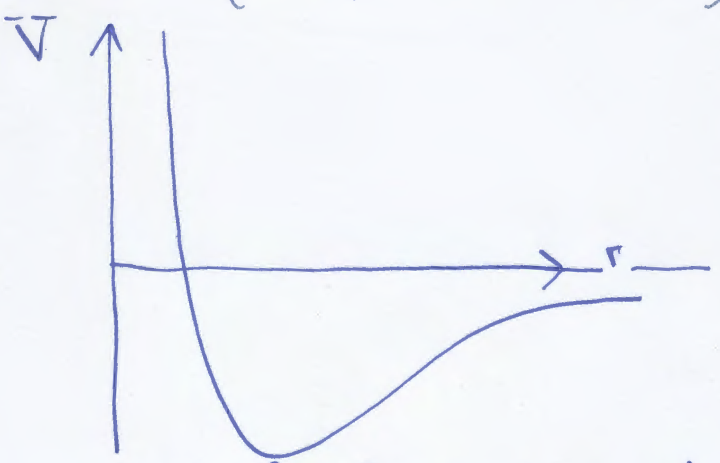
When two neutral atoms or molecules interact, they do so through the Lennard-Jones potential:

$$V_{LJ} = \frac{A}{r^{12}} - \frac{B}{r^6} \quad -(1)$$

which is an approximation of:

$$V = \gamma \left(\exp\left(-\frac{r}{r_0} - \left(\frac{r_0}{r} \right)^6 \right) \right) \quad -(2)$$

Fig (1)



The r^{-12} term describes the Pauli repulsion due to overlapping electron orbitals and the r^{-6} term the long range van der Waals dispersion force.

This potential is often used in molecular dynamics computer simulation.

The transmission coefficient is:

$$T = \frac{4}{\left(2\theta + \frac{1}{2\theta} \right)^2} \quad -(3)$$

2) where:

$$\theta = \exp\left(\frac{(2m)^{1/2}}{\hbar} \int_a^b \left(V(x) - E \right)^{1/2} dx \right) \quad -(4)$$

where

$$V(x) = \frac{A}{x^{12}} - \frac{B}{x^{6}} \quad -(5)$$

The atom or molecule is neutral when there is no free electron. Otherwise it is an ion. In low energy nuclear reaction two neutral atoms collide, or approach each other. In order for nuclear fusion to occur, the short range repulsion must be overcome, and the transmission coefficient must be substantially greater than zero.

Computer algebra can be used to calculate T for the Lennard-Jones potential, in the WKB approximation.

The Woods Saxon potential is a mean field potential for nucleons inside a nucleus. If it is assumed that the nuclei of two atoms have fused, then the combined nucleus is described by:

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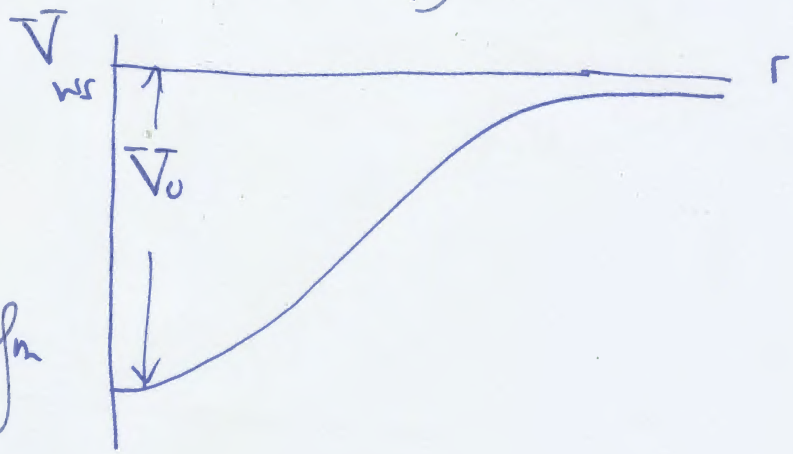
$$V_{WS} = - \frac{V_0}{1 + \exp\left(\frac{r - R}{a_1}\right)} \quad -(6)$$

Fig (2)



V_0 = potential well depth,
a_1 = surface thickness,
$R = r_0 A^{1/3}$, $r_0 = 1.25$ fm
A = mass number.

In one dimension the combined potential may be modelled as:

$$V = \frac{A}{x^{12}} - \frac{B}{x^{6}} - \frac{V_0}{1 + \exp\left(\frac{x - r_0 A^{1/3}}{a_1}\right)} \quad -(7)$$

and can be used to work out the transmission coefficient from eqs. (3) and (4).

For the Coulomb potential of note 229(1), computer algebra shows that T is maximized for low E and large n.