Quantum Mechanical Study of the Fleischmann-Pons Effect

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Abstract. Resonances in deuterium-deuterium fusion were examined by calculating the transmission behavior of a single deuteron through a deuterium atom, or through a system comprising two or three deuterium atoms, using transfer matrix methodology. Many unit-transmission resonance peaks were observed in the results of the calculations, even at incoming deuteron energies of a few electron volts, but resonance peak widths were found to be very narrow at low energies, so that the probabilities of fusion would be small.

1. Introduction

The Fleischmann-Pons Effect (FPE) was swiftly rejected when first published in 1989, yet many researchers have since reported energy gains in similar experiments [1]. The body of evidence suggests that the energy gains are real, even though the heat production powers are small and often difficult to replicate. Fleischmann and Pons suggested that these gains are the result of "cold fusion", or low energy nuclear reactions, where energy is released from a deuterium-deuterium (D-D) fusion. However, the probability of D-D fusion under the conditions of an FPE cell is vanishingly small as currently understood. As stated by Pons, et al., "It is necessary to reconsider the quantum mechanics of electrons and deuterons in such host lattices" [2].

The current work undertook a simple study of resonance bands that may exist for quantum-mechanical deuterium particles to penetrate through the nucleus of a deuterium atom. Solutions to Schrödinger's equation were developed first for a single-atom system, and then for multi-atom systems using the transfer matrix methodology. The effect of energy perturbations on the atom potentials was also examined.

1.1 Time-Independent Schrödinger's Equation in One Dimension

Phenomena of interest were examined using the simplified, one-dimensional and time-independent Schrödinger's equation for quantum mechanics. This equation can be written

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = (E - V(x))\cdot\psi(x) \tag{1}$$

where m is the particle mass, E the particle energy, x the spatial variable, and $V(x)$ is the background potential energy of the system encountered by the particle. The general solution of this equation is the wave equation,

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{2}$$

where A and B are wave magnitudes and $k = \frac{\sqrt{2m}}{\hbar}\sqrt{E-V}$ is the wave number of the particle at position x.

1.2 One-Dimensional Transfer Matrices

The above wave solution can be drafted in matrix notation as

$$\psi(x) = \begin{pmatrix} e^{ikx} & e^{-ikx} \end{pmatrix}\cdot\begin{pmatrix} A \\ B \end{pmatrix} \tag{3}$$

From this it can be observed that the wave can be "propagated" to the left or right by a distance a via the straightforward matrix operation

$$\begin{pmatrix} A \\ B \end{pmatrix}_{x=a} = \begin{pmatrix} e^{ikx} & 0 \\ 0 & e^{-ikx} \end{pmatrix} \cdot \begin{pmatrix} A \\ B \end{pmatrix}_{x=0} \equiv \mathbf{P}(V,a) \cdot \begin{pmatrix} A \\ B \end{pmatrix}_{x=0} \tag{4}$$

Likewise, the background potential can be changed discontinuously from V_1 to V_2 via the "discontinuity matrix" at the origin

$$\mathbf{D}(V_1, V_2)_{x=0} = \begin{pmatrix} 1+\dfrac{k_1}{k_2} & 1-\dfrac{k_1}{k_2} \\ 1-\dfrac{k_1}{k_2} & 1+\dfrac{k_1}{k_2} \end{pmatrix} \tag{5}$$

where the subscripts indicate wave numbers at the respective potentials. A similar discontinuity can be applied at $x = a$ using a combination of the above discontinuity matrix and suitable backward and forward propagation matrices,

$$\mathbf{D}(V_1, V_2)_{x=a} = \mathbf{P}(v_2, -a) \cdot \mathbf{D}(v_1, v_2) \cdot \mathbf{P}(v_1, a) \equiv \mathbf{t}_{total} \tag{6}$$

Finally, the transmission through a system comprising multiple discontinuities, all contained within a system transfer matrix $\mathbf{t}_{total}$, can be calculated using the formula

$$T = 1 - \frac{|\mathbf{t}_{total,21}|^2}{|\mathbf{t}_{total,11}|^2} \tag{7}$$

where the subscripts indicate particular matrix elements by row and column. [3]

2. Methodology

2.1 Basic Atom

A single deuterium atom was represented by stepped discontinuities in potential energy.

The most basic atom comprised only a hard core potential at 100 MeV and a potential well at -50 MeV. These values were chosen as representative of the energies in a real atom, but were not meant to be precise duplicates of real potentials. As was discovered in developing the results documented below, a choice of different values of these potentials did affect the locations of the resonance bands found, but did not change the overall resonance structure of the systems in question. Plots of the potential energies for this atom are shown in Fig. 1. The radius chosen for the hard core potential was 0.34 femtometers [4], and a radius of 7.24 femtometers was chosen for the Yukawa well; this is the radius at which a simple Yukawa attractive potential would adopt a value of -50 MeV [adapted from equations in reference 5].

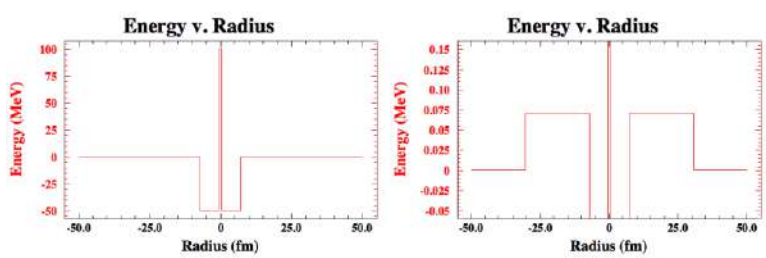

Fig. 1 – Basic atom potentials, including first coulomb potential.

More complicated atoms included additional potentials, which were used to represent the coulomb attraction experienced by a deuteron near a deuterium atom. These included a 70-keV potential from the edge of the Yukawa well to a radius of 30.6 femtometers, to represent the peak energy of a $1s^-$ electron orbital and the radius at which that orbital's energy drops to one-half its peak value. However, differences in the results of those calculations were found to be negligible; for brevity the results have not been included in this paper.

2.2 Systems Studied
Transmission of a deuteron through a single deuterium was studied first, followed by an examination of the additional resonances generated in transmission through two atoms. Finally, results of the two-atom case were compared with those of a system with three atoms.

3. Results

3.1 Single Atom Transmission
Single-atom transmission is perhaps the least interesting case studied, with several resonances below the hard-core energy of 100 MeV, but no unit resonance until well above the hard-core energy. A plot of the result can be seen in Fig. 2.

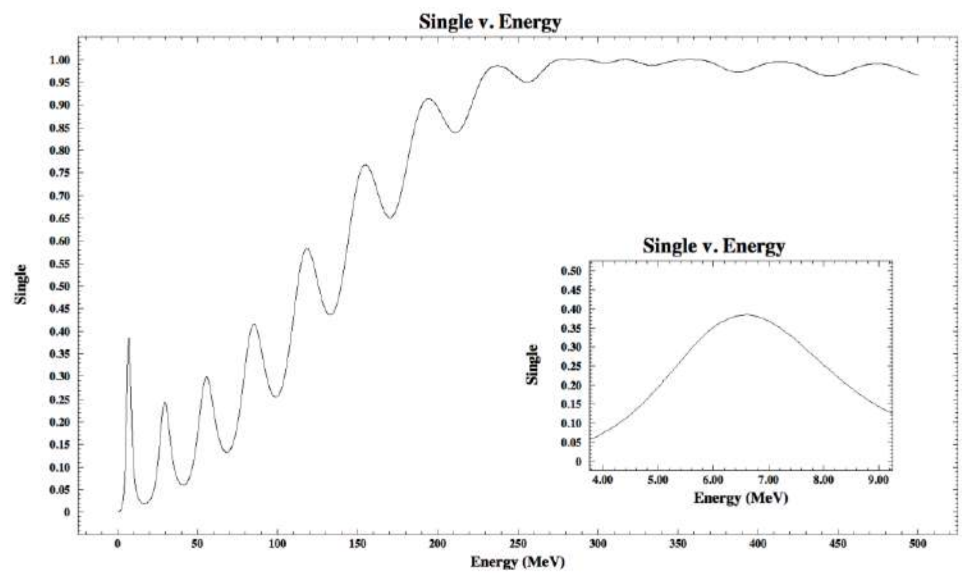

Fig. 2 – Transmission through a single basic atom; the inset shows magnification of the first peak.

3.2 Two- and Three-Atom Transmission
Fig. 3 and Fig. 4 show the transmission through two atoms and three atoms, respectively. Atoms in the system calculated were duplicates of the basic atom above, separated from one another by a distance of one angstrom.

Perturbation of the energy levels in any of the atoms in the multi-atom system had very little effect on the structure of the results, except for changing the particular energies at which resonance bands occur. For brevity, plots have not been included here.

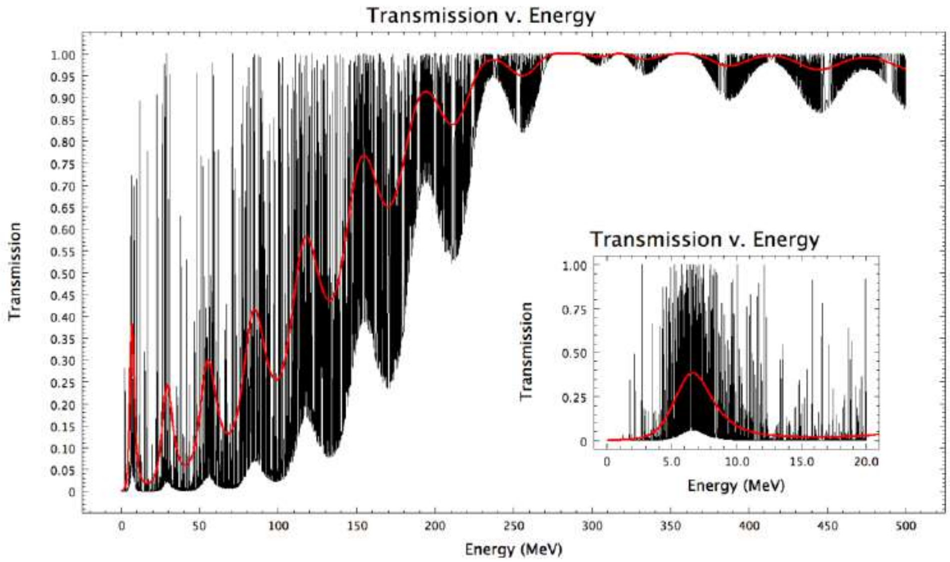

Fig. 3 – Transmission through two atoms separated by 1 angstrom (black curve); the single atom transmission curve from Fig. 2 is shown in red. The inset shows magnification of the first peak in the single-atom spectrum.

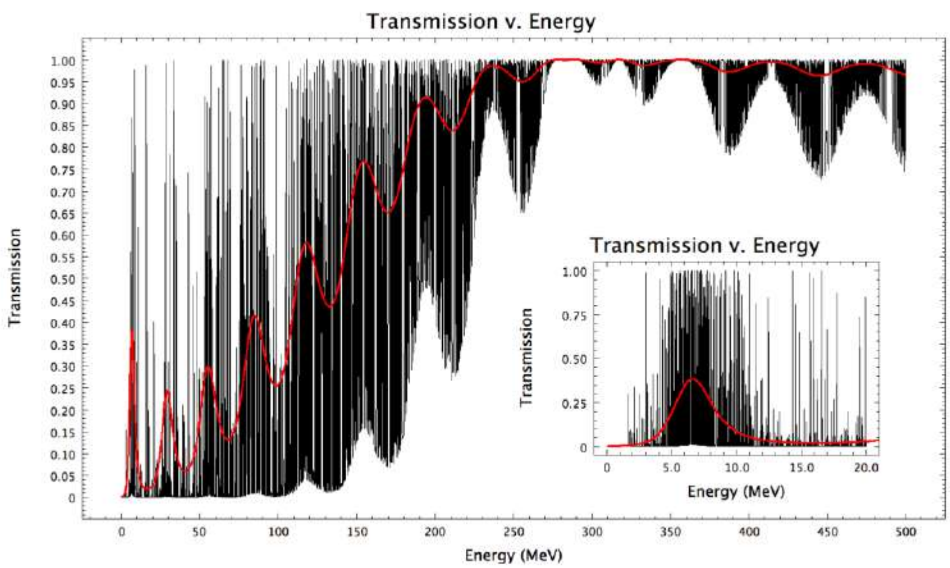

Fig. 4 – Transmission through three atoms separated by 1 angstrom (black curve); the single atom transmission curve from Fig. 2 is shown in red. The inset shows magnification of the first peak in the single-atom spectrum.

Zooming in on various energy regions to examine the resonance bands in greater detail revealed two interesting phenomena. First, the difference between the two-atom case and the three-atom case was noticed to resemble the peak splitting observed in optical spectroscopy or magnetic resonance imaging. A plot of this splitting is shown in Fig. 5.

Second, even at very low energies, the resonance bands that look like spike noise in the coarse plots of Fig. 3 and Fig. 4 were revealed to be *unit* transmission peaks. A plot at low energy with greatly increased resolution can be seen in Fig. 6. The plot illustrates the unit-transmission character of only one peak, but others were examined and found to also be peaks of unit transmission. This character was not obvious in the above figures because the resonance peaks have such narrow energies: a high degree of granularity was required in the transmission calculation to produce transmission values of one.

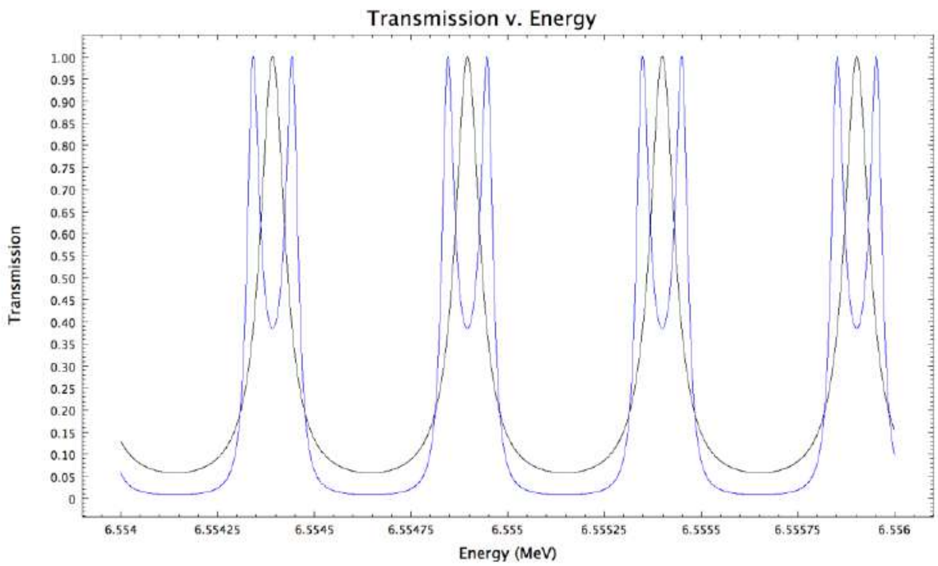

Fig. 5 – Peak splitting observed between two-atom transmission (black curve) and three-atom transmission (blue curve)

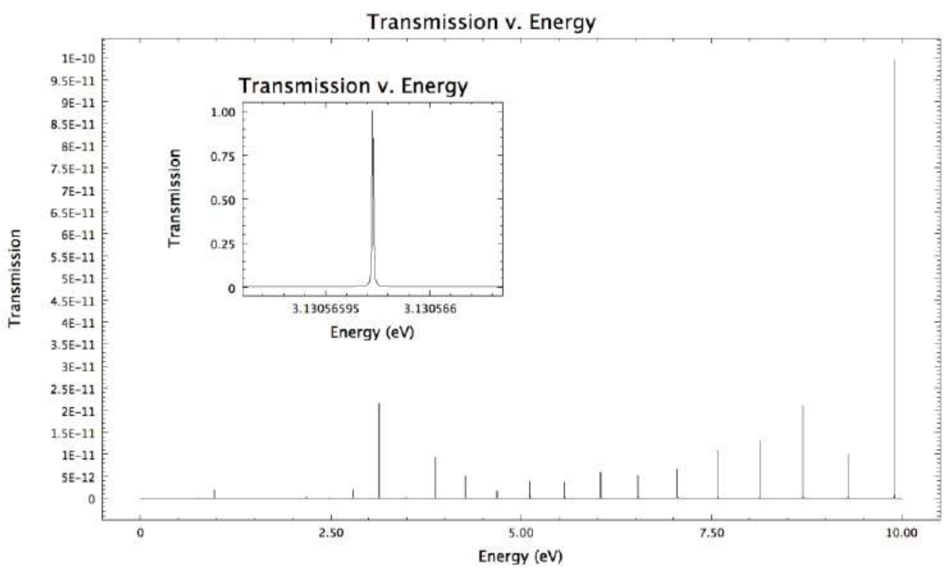

Fig. 6 – Resonance peaks from 0 to 10 eV (outer plot) and the particular peak near 3.1306 eV (inset plot); the ordinate scale on the outer plot is narrow only because the energies in the curve were too coarsely spaced to include larger transmission values – high granularity at each resonance was required in order to observe unit transmission.

4. Conclusions

Transmission has been estimated for a deuteron through one or more deuterium atoms. The estimate was approximate, but the resonance structure observed should represent that of real systems.

A complicated structure of unit-transmission resonance was found for multi-atom systems, even for transmission through a two-atom system.

Large (1%) perturbations in the deuterium-deuterium attractive or repulsive potential energies had very little effect on transmission resonances.

Resonance peaks observed in transmission through two- and three-atom systems are regularly spaced, and a comparison of the two systems illustrated peak splitting reminiscent of optical spectroscopy or magnetic resonance imaging in the chemistry lab.

Resonance peaks at low deuteron energies were extremely narrow.

5. Discussion and Future Work

The narrowness of resonance peaks would imply that transmission is highly improbable when deuteron waves encounter deuterium particles in free space; this is due to the broad, continuous energy distribution of particles in free space. However, deuterium atoms trapped in a lattice structure would behave as "particles in a box", and hence have quantized energy levels. Therefore it is possible that overlaps between the quantized energy levels of trapped deuterium atoms in a palladium lattice, and the narrow resonance peaks for transmission, could lead to an increased probability of transmission, and therefore an increased probability of D-D fusion in the lattice-bound system.

First and foremost, the next segment of this research should relate transmission spectra – such as those included in this paper – with fusion interaction probabilities. For instance, the area under the curve for the 3.1306-eV resonant peak shown in Fig. 6 is only 8.9×10^{-10} eV. However, it is not immediately obvious how this relates to a reaction cross-section.

Future work in this field should include a study of the energy levels deuterium atoms may occupy within a palladium lattice, and some examination of whether those energy levels may overlap with resonance peaks for transmission through real bound-deuterium systems, thereby increasing the fusion probability.

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