

QUANTUM MECHANICAL STUDY OF THE FLEISCHMANN-PONS EFFECT

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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; e.g., see Storms review.
 - 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 (LENR) where energy is released from a deuterium-deuterium (d-d) fusion.
- However, the probability of a d-d fusion under the conditions within a FPE cell, as we understand it, is vanishingly small.
- As stated by Pons et al., “it is necessary to reconsider the quantum mechanics of electrons and deuterons in such host lattices.”
 - We would add that other less exotic mechanisms of heat production within these lattices should also be investigated.

Study overview

- To predict changes in the probability of d-d fusion, caused by:
 - perturbations to the energy barriers;
 - or positive interference caused by the effects of adjacent atoms in a lattice.
 - Work is in its infancy, so here we report early results.
- First model: effect of adjacent lattice atoms on fusion examined in 1½ D model.
 - Quantum barrier model is formulated using the transfer matrix approach.
 - Then additional barriers are introduced in the form of adjacent atoms.
 - Initial results show **resonance** structure for the transmission of incoming deuterons through deuterium atom nuclei
 - This implies an **increase** in fusion probabilities at particular deuteron energies.
 - We will also discuss the possible effects of quantized deuteron energies.
- It is noted that the energy gains observed in FPE experiments often occur in highly dislocated metal lattices. The possible role of these dislocations in facilitating the d-d fusion process will also be examined.

One-Dimensional Transfer Matrices

The time-independent Schrödinger equation in 1-D has the solution

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

or in matrix notation,

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

Where k is the particle wave number, $k = \rho\sqrt{\varepsilon - v}$, $\rho = \sqrt{2mV_0}/\hbar$, m is the particle mass, V_0 is a potential energy used for non-dimensionalizing, and ε and v are the non-dimensionalized particle energy and potential felt by the particle.

The coordinate system can be translated to the left or right by a distance a , or **propagated** via straightforward multiplication, for example:

$$\begin{pmatrix} A \\ B \end{pmatrix}_{x=a} = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} \cdot \begin{pmatrix} A \\ B \end{pmatrix}_{x=0} \equiv \mathbf{p} \cdot \begin{pmatrix} A \\ B \end{pmatrix}_{x=0}$$

One-Dimensional Transfer Matrices, continued

In the same manner the potential, v , felt by a particle can be changed using a **discontinuity matrix** at $x = 0$, such as

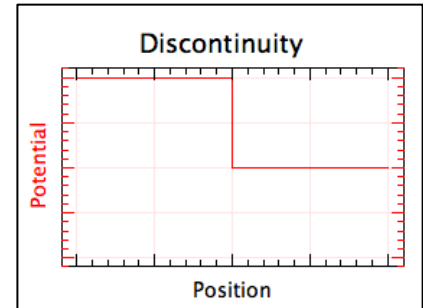
$$\begin{pmatrix} A \\ B \end{pmatrix}_{x^-} = \frac{1}{2} \begin{pmatrix} 1 + k^+/k^- & 1 - k^+/k^- \\ 1 - k^+/k^- & 1 + k^+/k^- \end{pmatrix} \cdot \begin{pmatrix} A \\ B \end{pmatrix}_{x^+} \equiv \mathbf{t} \cdot \begin{pmatrix} A \\ B \end{pmatrix}_{x^+}$$

or at $x = a$ by using a combination of propagation and discontinuity,

$$\begin{aligned} \begin{pmatrix} A \\ B \end{pmatrix}_{x^-} &= \begin{pmatrix} e^{-ika} & 0 \\ 0 & e^{ika} \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} 1 + k^+/k^- & 1 - k^+/k^- \\ 1 - k^+/k^- & 1 + k^+/k^- \end{pmatrix} \cdot \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} \cdot \begin{pmatrix} A \\ B \end{pmatrix}_{x^+} \\ &= \mathbf{p}_{-a} \cdot \mathbf{t} \cdot \mathbf{p}_{+a} \cdot \begin{pmatrix} A \\ B \end{pmatrix}_{x^+} \equiv \mathbf{t}_{total} \cdot \begin{pmatrix} A \\ B \end{pmatrix}_{x^+} \end{aligned}$$

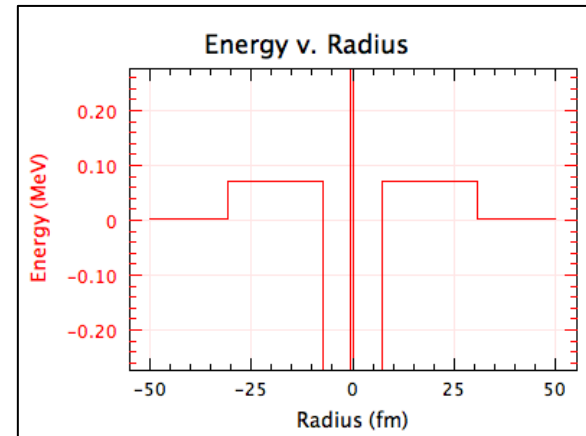
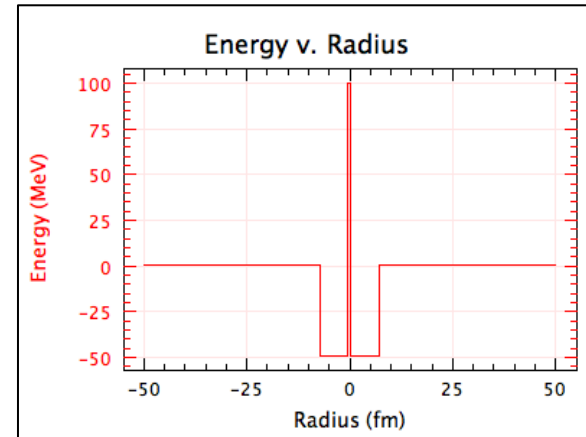
Finally, **transmission** through a system can be calculated using the formula

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

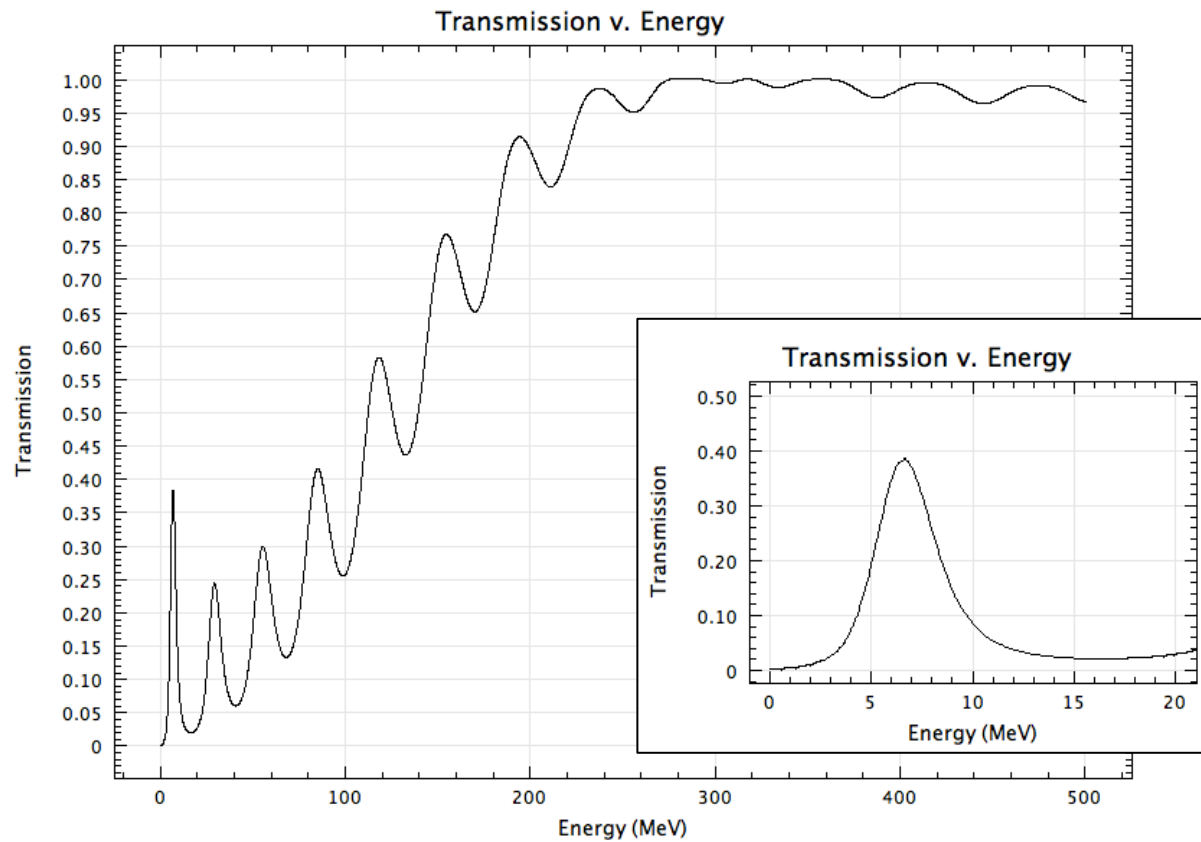


Simplistic Deuterium Atoms

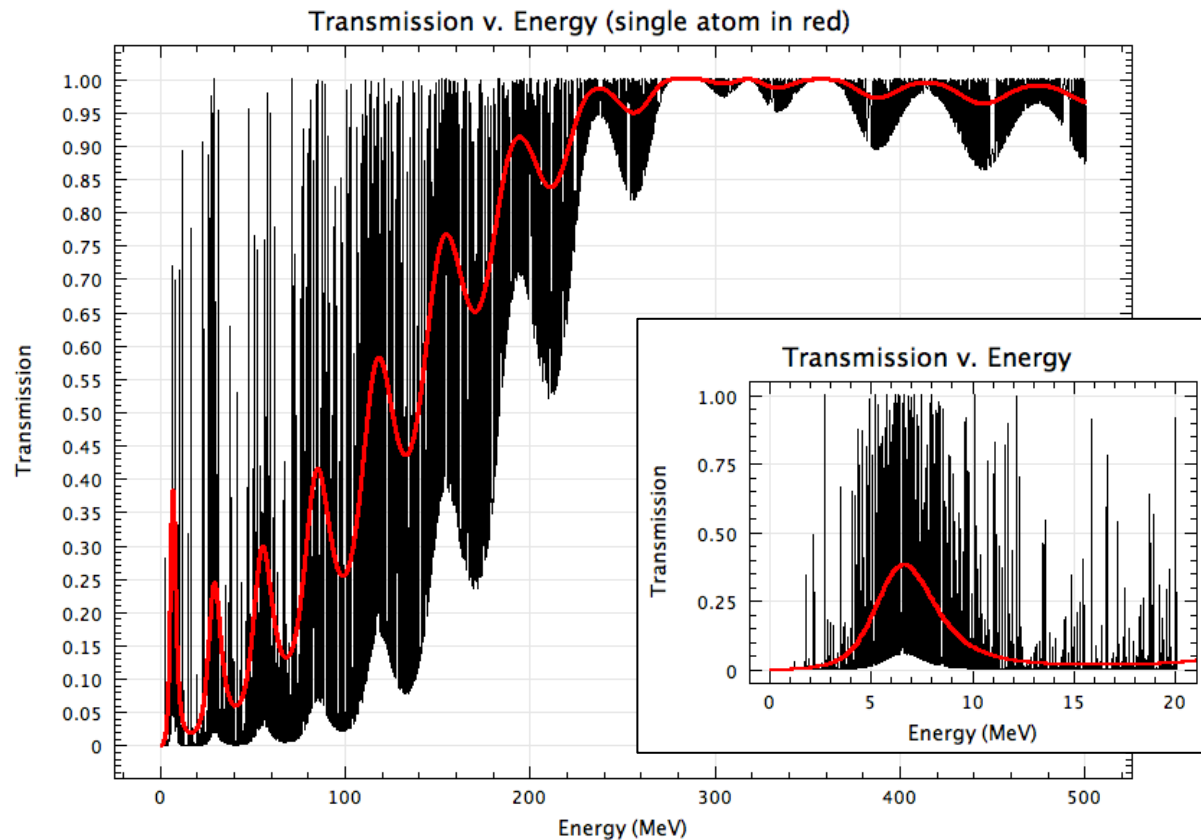
- Used the femtometer and the electron volt as characteristic scales.
 - Recognizable scales make results clear.
- Basic atom constructed from idealized deuterium with a 1s electron
 - 100 MeV repulsive hard core from the origin to a radius of 0.34 fm
 - -50 MeV symmetric (attractive) well from HC to radius of 7.24 fm
 - Optionally, a 70 keV coulomb repulsion from well to radius of 30.6 fm
 - A second coulomb repulsion section was sometimes added, but was found to be negligible.
 - This is a **rough** model, not an accurate model; hence the neglect of bonding effects or nearby Pd electron clouds.



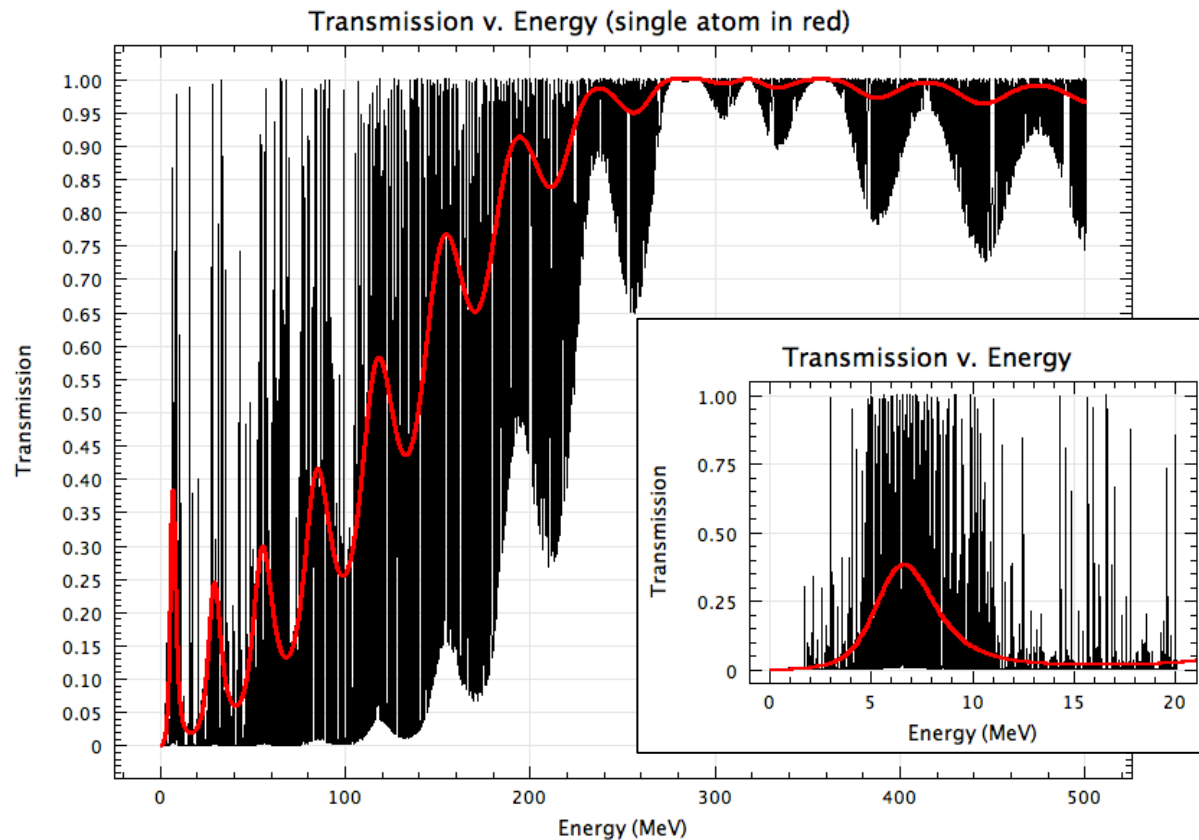
Single Atom Transmission



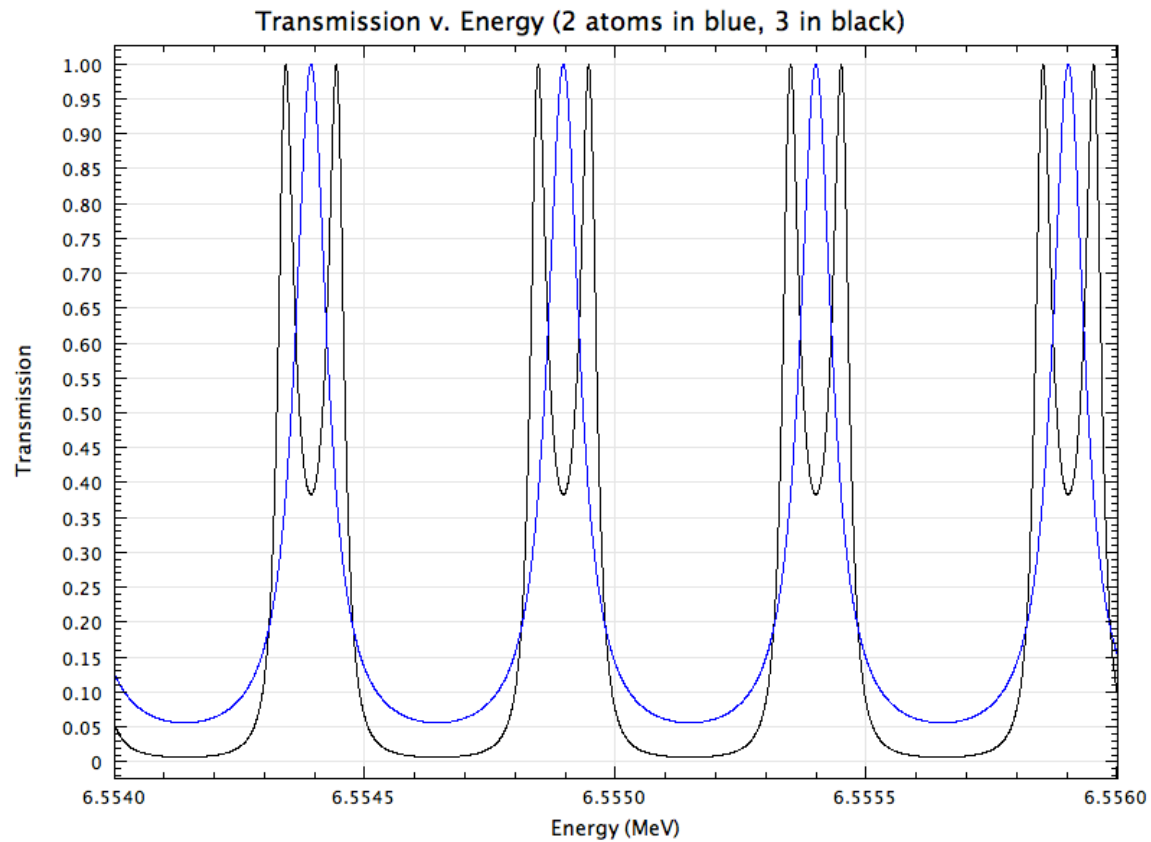
Two Atom Transmission (1-Å separation)



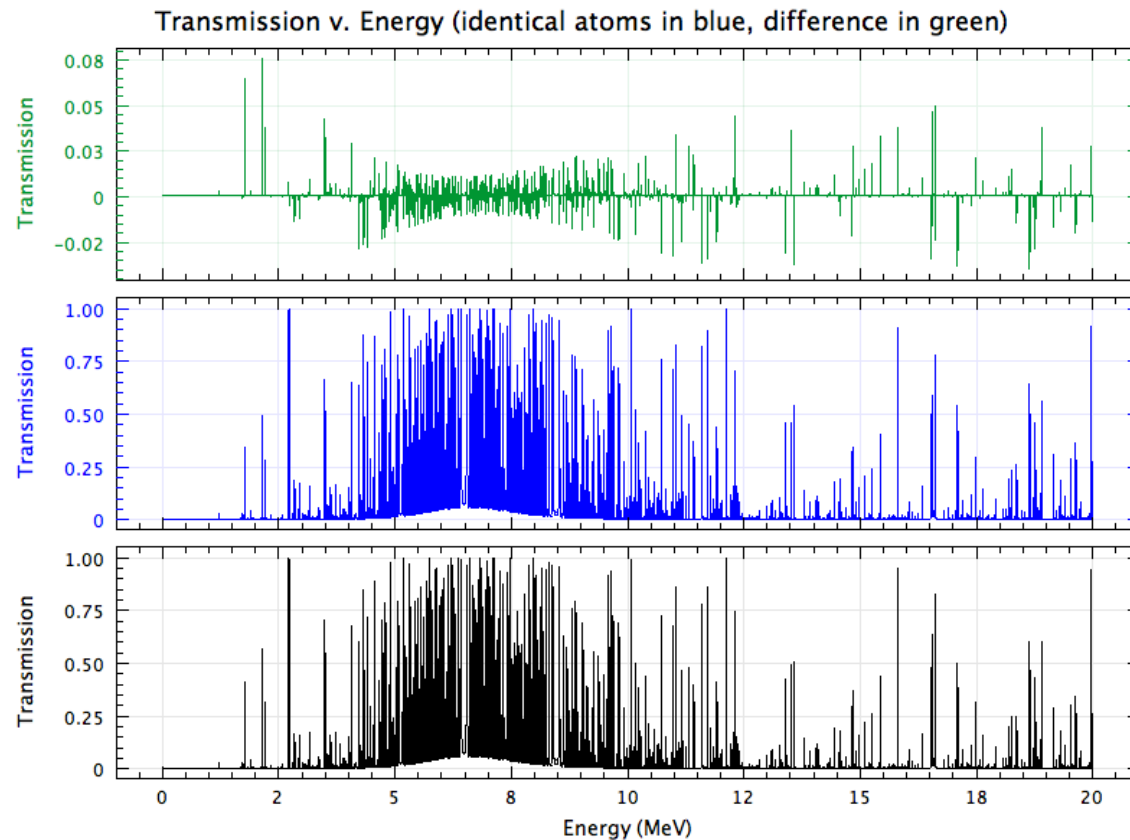
Three Atom Transmission (1-Å separation)



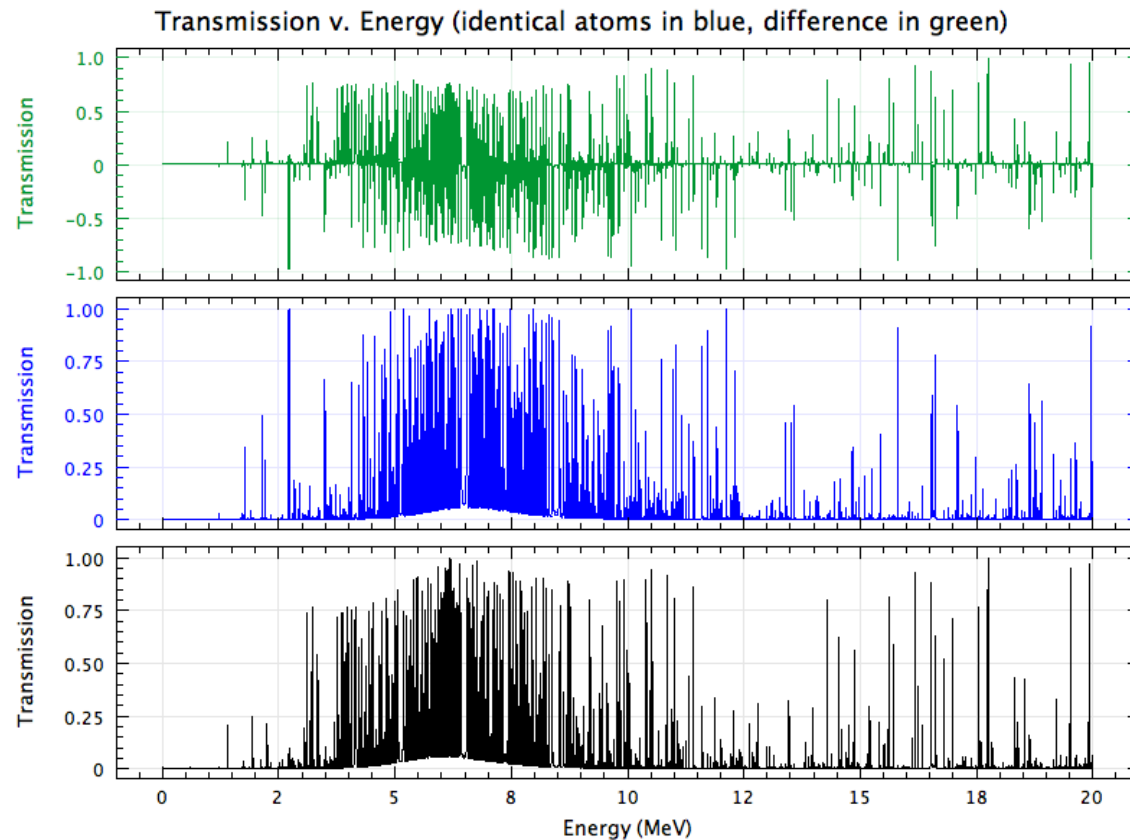
Peak Splitting (1-Å separation)



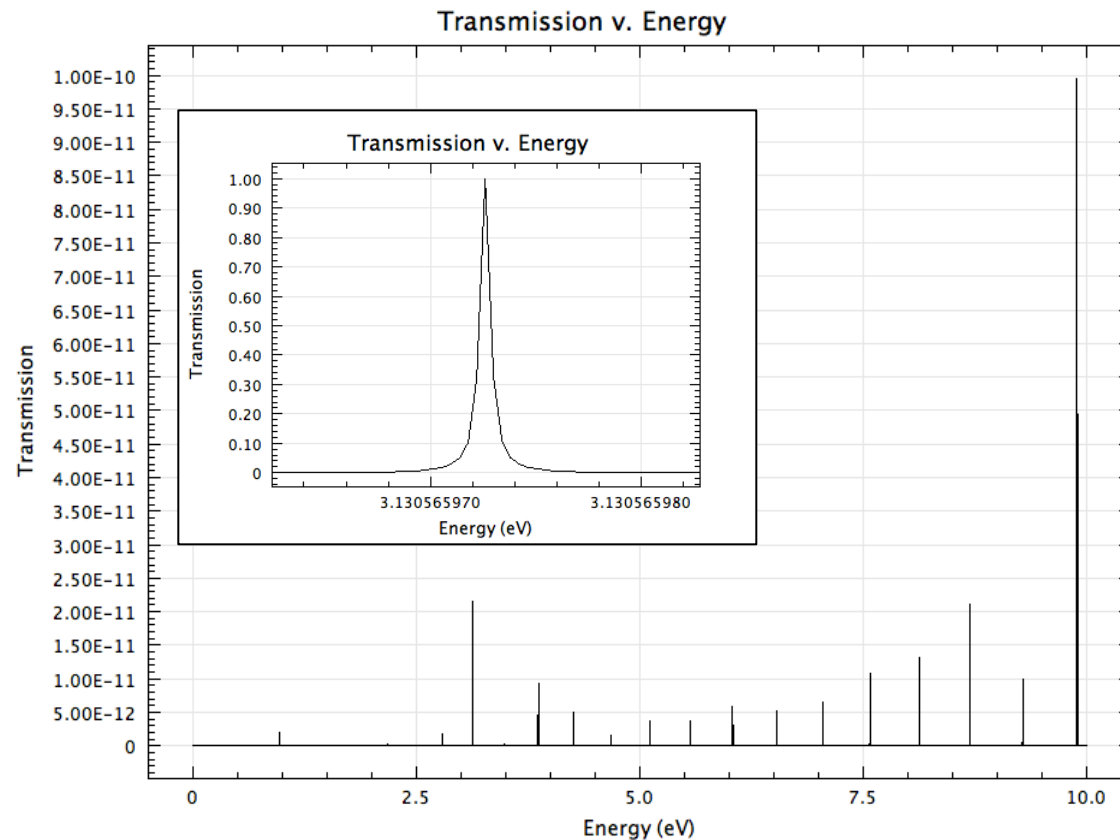
Large Energy Perturbation of +10 keV (2 atoms)



Extreme Energy Perturbation of +1 MeV (2 atoms)



Some Unit Transmission Even at a Few eV (2 atoms)



Conclusions

- Transmission has been estimated for a deuteron through one or more deuterium atoms.
 - Estimate is rough, but representative
 - Transmission through entire atoms is closely related to fusion with one of the atoms.
- Complicated resonance structure exists for even 2 atom transmission
 - Resonance peaks are regularly spaced
 - Resonance peaks are extremely narrow (but with unit transmission)
- Large (10 keV) perturbations in deuterium-deuteron attractive or repulsive potential have very little effect on transmission resonances.

Discussion of Probabilities

- Narrow resonance peaks would imply that transmission is extremely improbable when waves encounter 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.
- **Overlaps** between quantized energy levels and narrow resonance peaks may drastically **increase the transmission probability**.
 - Requires further study: energy levels of deuterium within a particular lattice should be fully understood before drawing any further conclusions.

Future work

- Perform calculations to understand the effect that quantized deuterium energies may have on transmission probabilities – as just discussed
- Another planned approach is to examine possible non-linear oscillation effects.
- Examine the role of a highly dislocated lattice on the d-d fusion process.
- To our knowledge, all previous Q-M studies of the FPE have been based on the time independent solution to the Schrödinger equation
- We propose formulating a time dependent solution for an oscillator problem
 - (Quasi) 3-D d-d particles are constrained to interact along a 1-D axis.
 - Non-linear excursions from stationary electronic configurations are investigated.
 - We will seek possible enhancement of quantum barrier effects and enhanced probability of electron capture by protons.

Acknowledgements

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