QUANTUM MECHANICAL STUDY OF THE FLEISCHMANN-PONS EFFECT

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The Fleischmann-Pons Effect [1] (FPE) was swiftly rejected when published in 1989, yet a significant number of researchers have since reported energy gains in similar experiments; for a review see ref. [2]. These gains have been associated with "cold fusion" or Low Energy Nuclear Reactions (LENR) where energy is released from a deuterium-deuterium (d-d) fusion. Clearly, this raises fundamental questions because the probability of a d-d fusion, under the conditions of the FPE cell, is extremely small. As stated in ref. [1], "it is necessary to reconsider the quantum mechanics of electrons and deuterons in such host lattices."

The goal of this paper is to predict possible 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. We report preliminary work on formulating quantum-mechanical models of the behavior of deuterium atoms trapped in a lattice.

In the first model we examine possible non-linear oscillation effects. A time *dependent* solution of the Schrödinger equation is presented for an oscillator problem in which (pseudo) 3-dimensional d-d particles are constrained to interact along a 1-dimensional axis. Non-linear excursions from stationary electronic configurations are investigated with the intent to understand possible enhancement of quantum barrier effects and enhanced probability of electron capture by protons.

In the second model the effect of adjacent lattice atoms on fusion is examined with a 1-½ dimensional model. First a quantum barrier model is formulated using the transfer matrix approach. Then additional barriers are introduced in the form of adjacent lattice atoms. Initial results show possible resonance structure for the transmission of incoming deuterons through deuterium atom nuclei, which implies an increase in fusion probabilities at particular 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 is examined. {LA-UR 09-03526.}

1. Fleischmann, M. and Pons, S., "Electrochemically induced nuclear fusion of deuterium," *Journal of Electroanalytical Chemistry*, 1989. **261**(2, Part 1): p. 301-308.
2. Storms, E., *The science of low energy nuclear reaction*. 2007, New Jersey: World-Scientific.

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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,

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

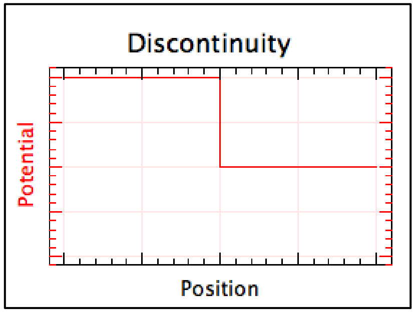
Where k is the particle wave number, $k = \rho\sqrt{\varepsilon - v}$, $\rho = \sqrt{2mV_0}/\hbar$, m is the particle mass, V_0 is a potential energy used for non-dimensionalizing, and ε and v are the non-dimensionalized particle energy and potential felt by the particle.

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,

$$\begin{pmatrix} A \\ B \end{pmatrix}_{x-} = \begin{pmatrix} e^{-ika} & 0 \\ 0 & e^{ika} \end{pmatrix}\cdot\frac{1}{2}\begin{pmatrix} 1+k^+/k^- & 1-k^+/k^- \\ 1-k^+/k^- & 1+k^+/k^- \end{pmatrix}\cdot\begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}\cdot\begin{pmatrix} A \\ B \end{pmatrix}_{x+}$$

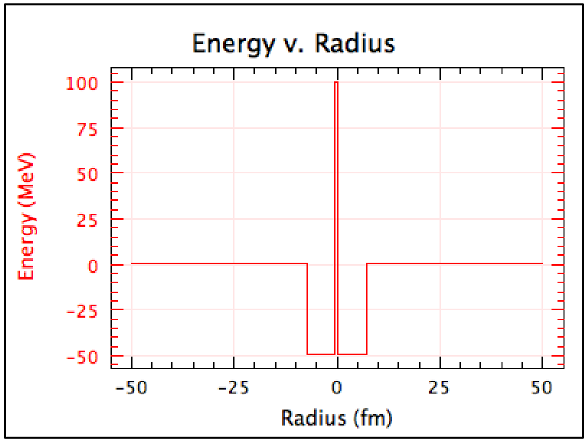
$$= \mathbf{p}_{-a}\cdot\mathbf{t}\cdot\mathbf{p}_{+a}\cdot\begin{pmatrix} A \\ B \end{pmatrix}_{x+} \equiv \mathbf{t}_{total}\cdot\begin{pmatrix} A \\ B \end{pmatrix}_{x+}$$

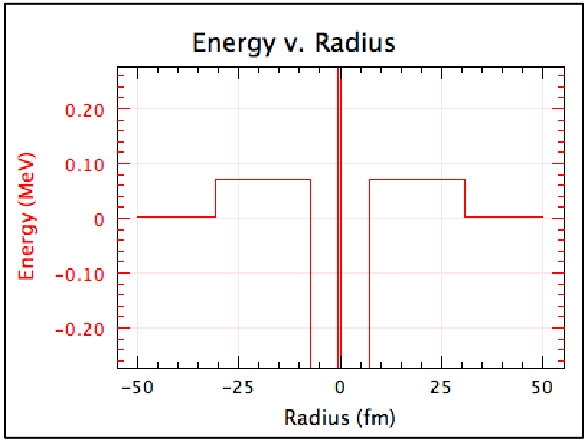
Finally, **transmission** through a system can be calculated using the formula

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

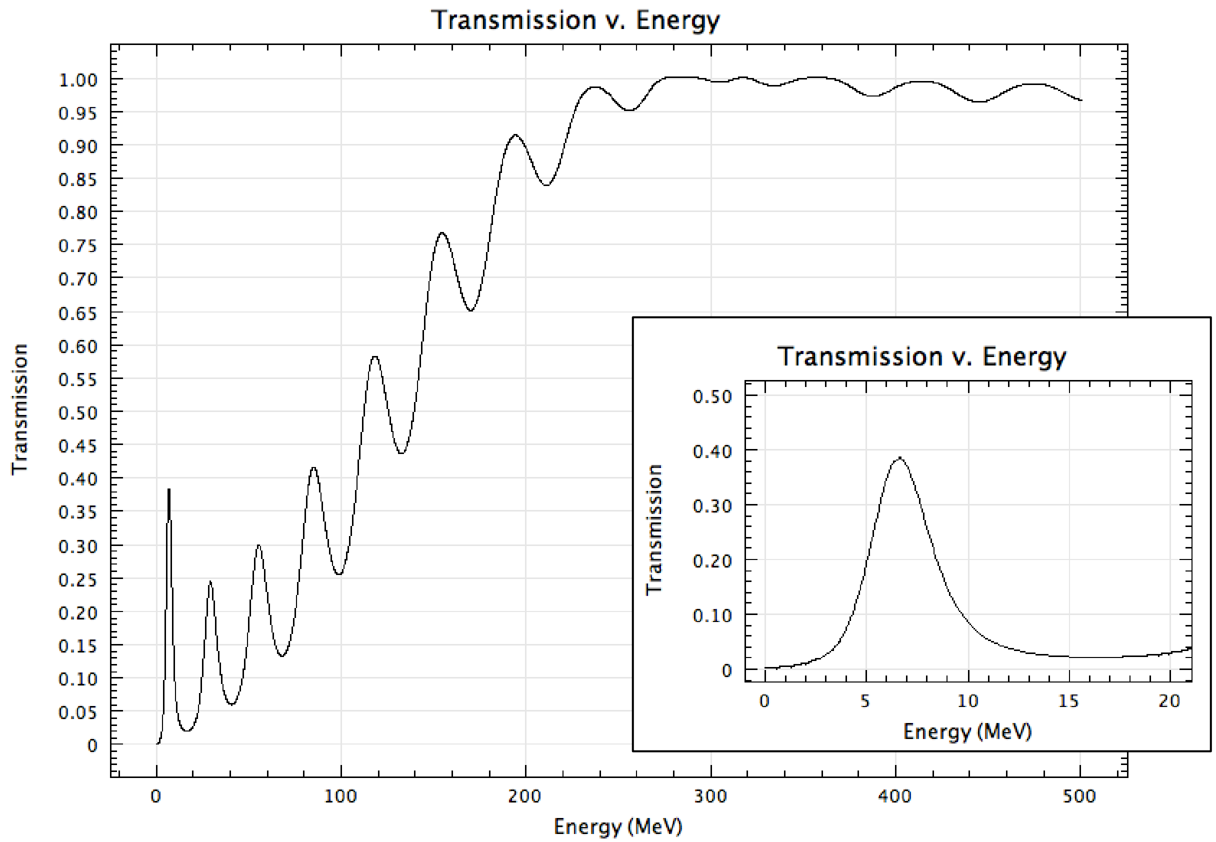
Simplistic Deuterium Atoms

- 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.

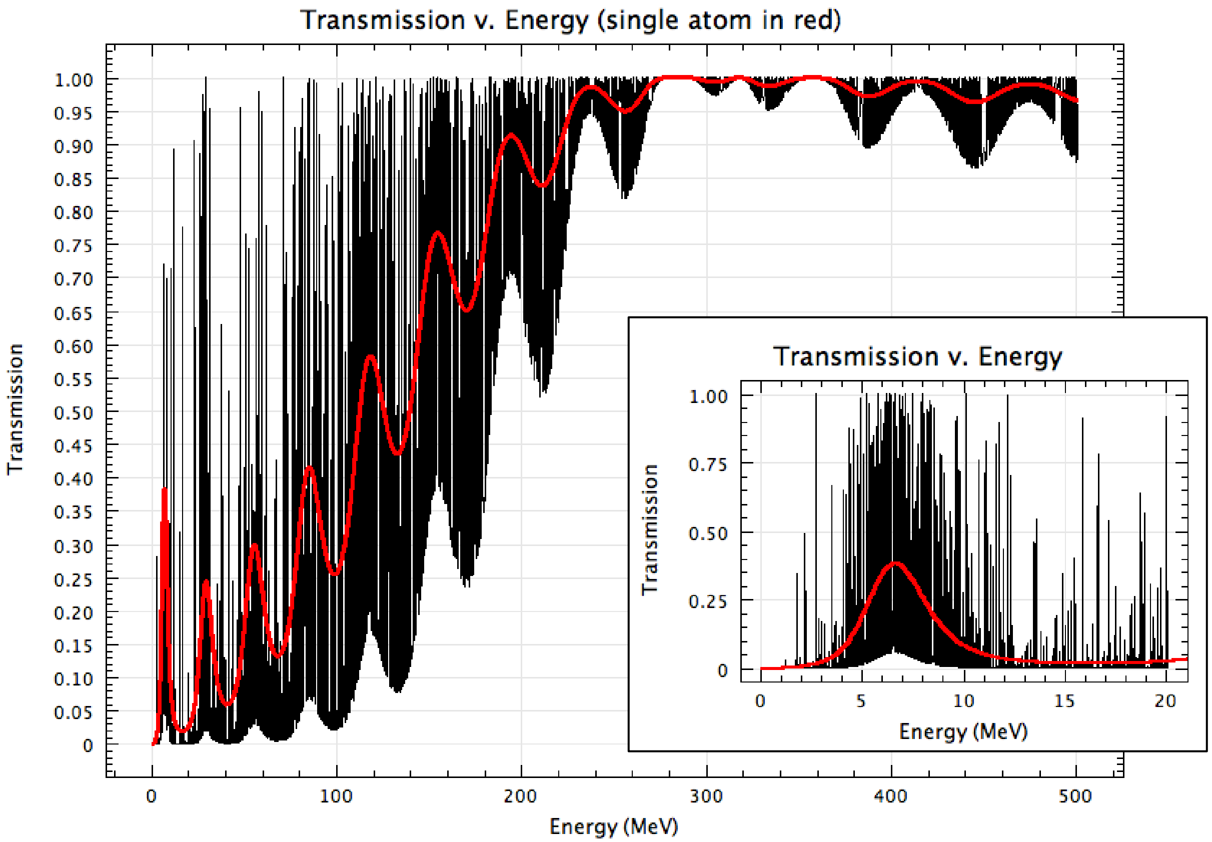




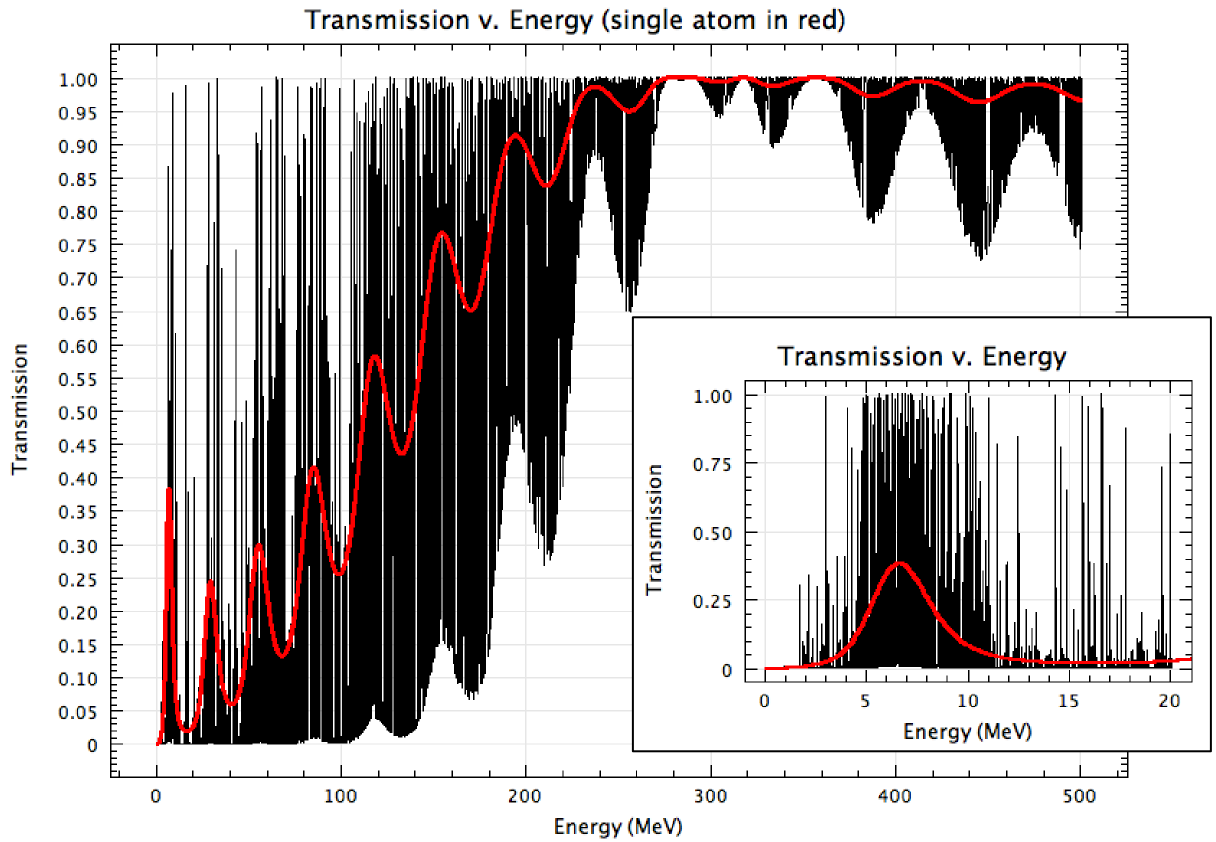
Single Atom Transmission



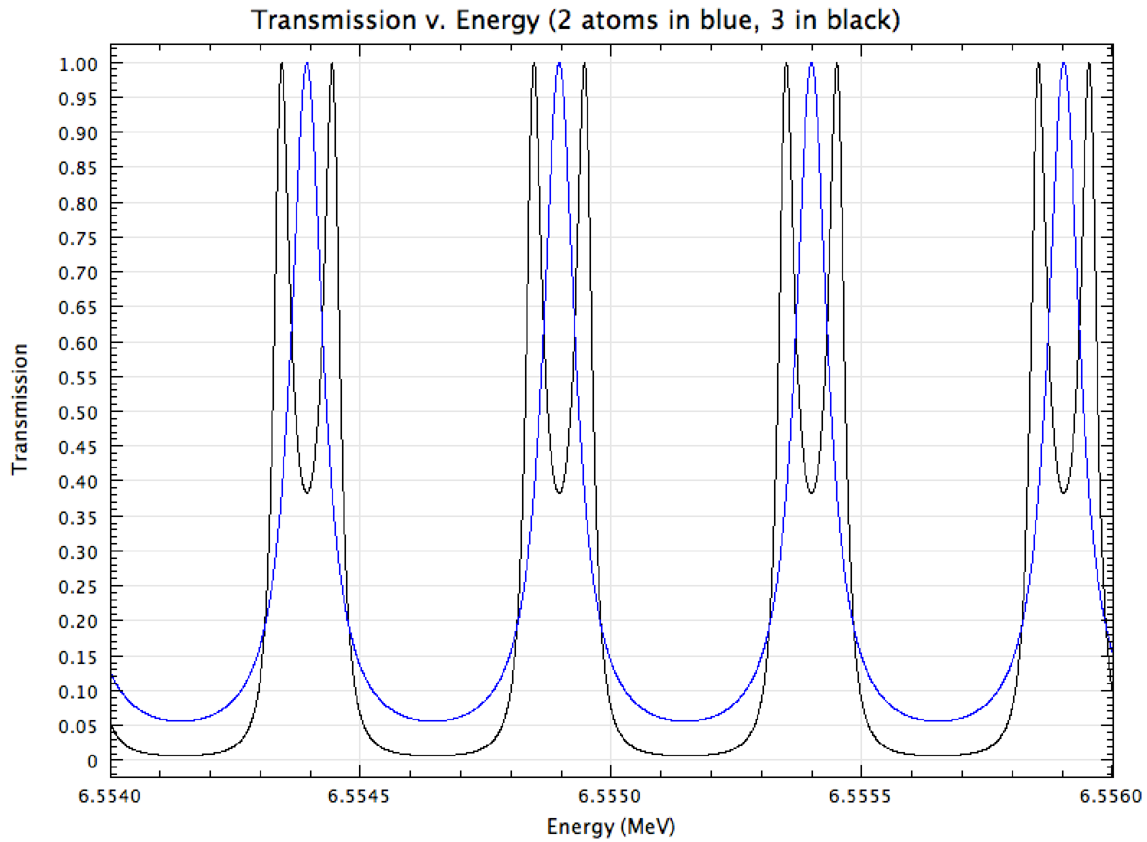
Two Atom Transmission (1-Å separation)



Three Atom Transmission (1-Å separation)



Peak Splitting (1-Å separation)



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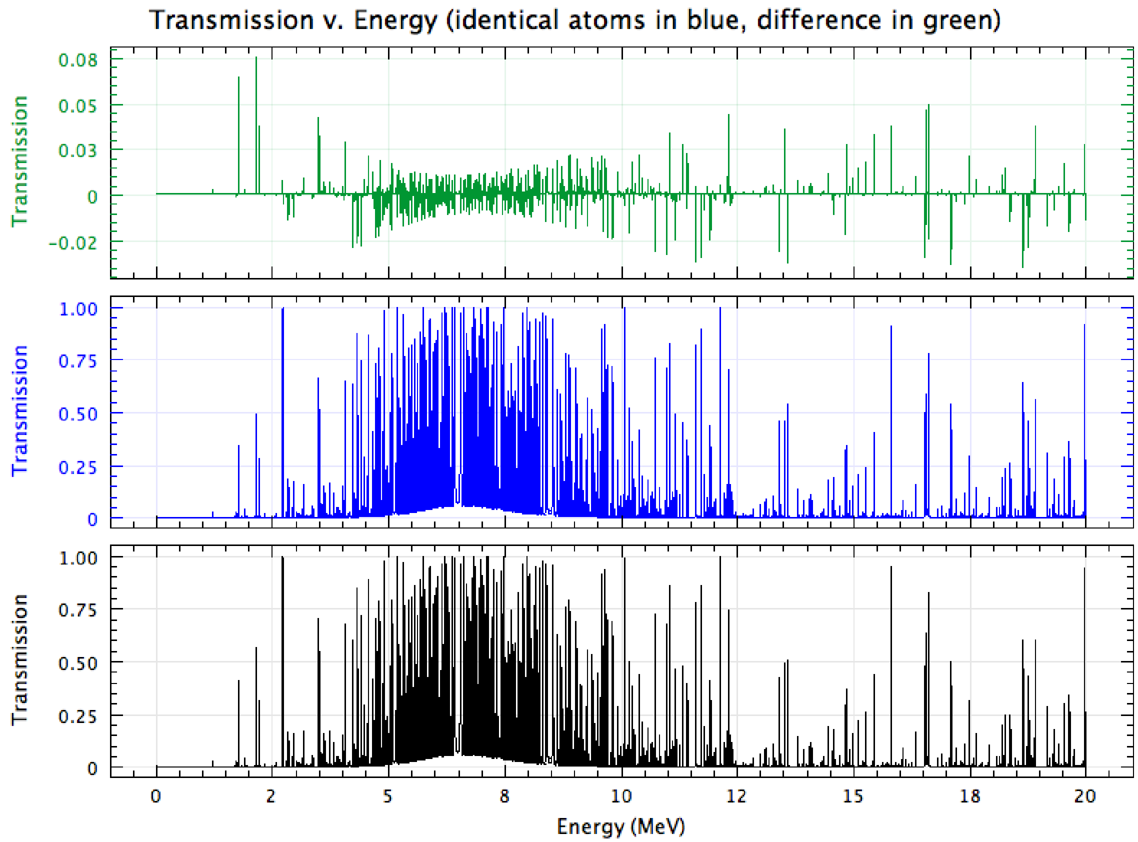
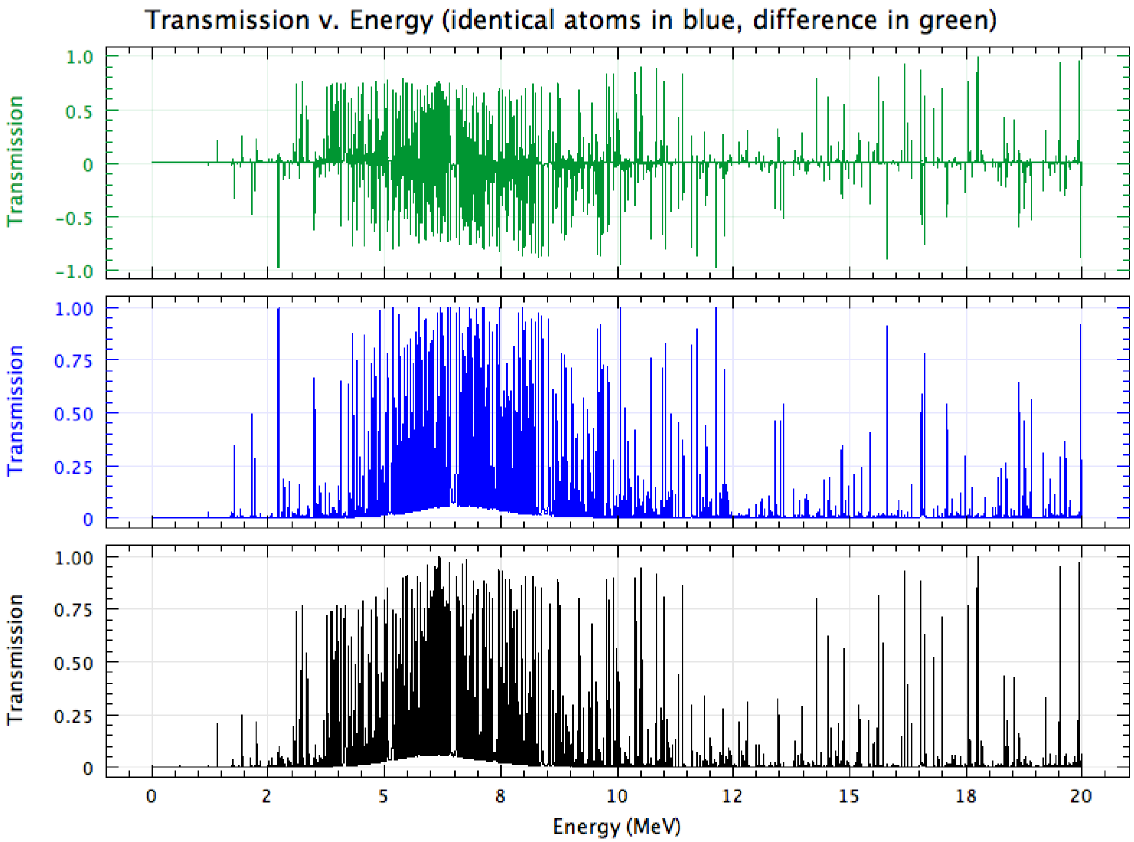
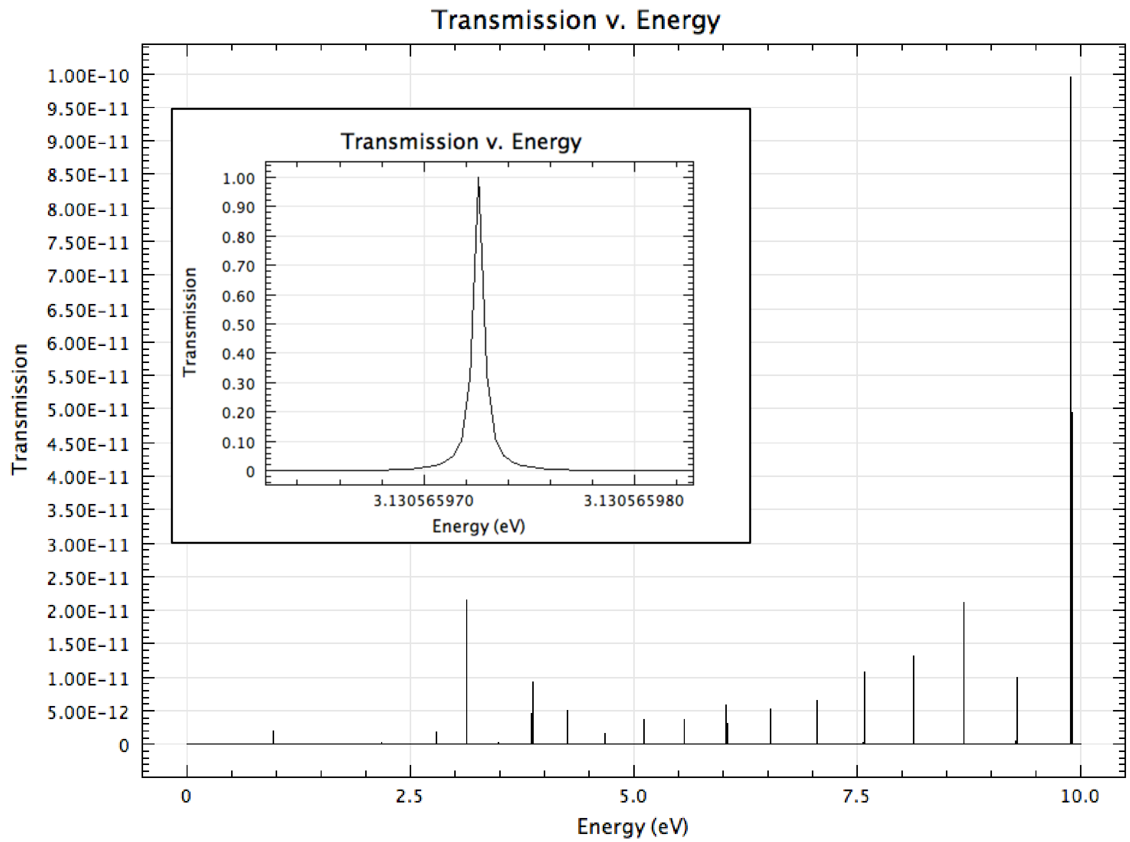
Large Energy Perturbation of +10 keV (2 atoms)



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.

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