Calculations for developing a theoretical model for the cold fusion reaction

by

Taher Al-Jundi

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Researching in a new field like cold fusion is an enormously complex undertaking. But when you work under the supervision of a professor like Dr. Spinrad all troubles become easier. I would like to dedicate this work to my professor Dr. Bernard I. Spinrad, under whose supervision this research would not have been possible. Also thanks to him for stimulating my interest in this new field. I would like to extend my thanks to Dr. Monroe S. Wechsler for his valuable comments and corrections.

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CHAPTER 1. ABSTRACT

In this research we have developed a theoretical model for the cold fusion reaction by solving the Schrödinger wave equation for a deuteron pair inside a palladium cell until we get the asymptotic value of the wave function at the edge of the palladium cell. The wave function carries all the information about the system, and from the value of the wave function we can calculate the reaction rate constant as a function of the energy of the system. We have calibrated this model by attempting to reproduce the experimental d-d fusion reaction cross section. The results of our calculations indicate the possibility of achieving a controllable high reaction rate by varying the value of a negative potential applied to the cell, if a deuteron pair can be put in the vacant site of a palladium atom with a reasonable probability. This theoretical model might lead the experimental work toward the production of a predictable fusion reaction rate.

CHAPTER 2. INTRODUCTION

On March 23, 1989 two noted chemists called a press conference at the University of Utah in Salt Lake City. The scientists, Martin Fleischmann and B. Stanley Pons, announced that they had produced controlled nuclear fusion at room temperature in an electrochemical cell. "It was," one scientist asserted, "as important as the discovery of fire." "Simple experiment results in sustained nuclear fusion at room temperature for the first time. Break through process has potential to provide inexhaustible source of energy," read the headlines in the University of Utah's release [1]. For over 100 hours, Fleischmann and Pons had produced pure energy in a tiny glass jar, and the fuel they were using was as abundant as sea water.

A matter of days after the original announcement by Fleischmann and Pons, a second group announced that it had discovered room-temperature fusion. Moreover this announcement came from a university only forty miles away, in Provo, Utah. The announcement from Brigham Young University was more guarded in its claims. Although Brigham Young University's scientists had not seen the same large amounts of heat being produced as had the University of Utah team, neutrons were certainly detected. Group leader Steven E. Jones said "The discovery of cold fusion opens the possibility , at least, of a new path to fusion energy." [1]. Over the next few weeks, hopes were to rise and fall as evidence of new experiments from the United States, the

Soviet Union, Italy, India, Czechoslovakia, and the United Kingdom began to come in. At first some reports appeared to confirm the Fleischmann and Pons experiment; then others questioned the whole idea of cold fusion. By mid-April of the same year different laboratories were making almost daily conflicting claims.

It is agreed that there is no clear understanding of how a fusion reaction can take place at room temperature, and the controversies will continue unless an explanation of how solid-state fusion might be theoretically modeled is made.

Fusion of deuterium and tritium is the principal means of producing energy in the stars. In cold terrestrial conditions, however, the probability of two deuterium nuclei to fuse is of the order of $10^{-70}\ s^{-1}/(d-d)pair$[2]. This is due to the repulsive Coulomb barrier between nuclei. However, this probability may be increased dramatically by replacing the electron in a hydrogen molecular ion by a more massive negatively charged particle. Indeed the muon-catalyzed (a muon is a negatively charged massive particle) fusion reaction has been demonstrated to be an effective means of rapidly inducing fusion reactions in low-temperature hydrogen isotope mixture[2]. We are trying to see whether an equivalent effect can be produced by loading hydrogen isotope nuclei into a highly negatively charged metallic crystalline lattice.

In this research we have worked on two problems:

First, we have calculated the reaction cross section using two forms of the nuclear potential, and we have represented the wave function of a deuteron pair as a sum of a wave going into the palladium cell and one scattered out of it. The change in the outgoing wave has been calculated by simultaneously solving the wave function and its derivative at the edge of the cell. From this change the reaction cross section was calculated. Parameters of the potential model can be adjusted to make these results

agree with experiments.

The second problem was to calculate the reaction rate constant. This was done by considering the same model of the nuclear potential as was used in the cross-section calculation, and requiring that a deuteron pair be contained within a lattice cell. For this system a complex energy eigenvalue can be found; the imaginary part of the energy eigenvalue is related to the reaction rate constant.

Two models of the nuclear potential were considered in this study. The first and the easier to apply was the square well nuclear potential. The second model, more detailed and more realistic, was a Woods-Saxon nuclear potential. The two models (square well and Woods-Saxon) gave similar results for the reaction cross-section and for the reaction rate constant.

We assume in this thesis that a lattice cell as we have calculated contains two deuterons. A multiplicative factor on the reaction rate is the probability that a site will contain more then two deuterons. This probability is being investigated by Ms. Suneeta Singh. Thus, our work is considered an attempt to improve the theory of "cold fusion."

CHAPTER 3. LITERATURE REVIEW

Nuclear fusion of deuterium can take place through one of the following reactions:

$$^2D +^2 D \longrightarrow^3 T(1.01MeV) +^1 H(3.02MeV) \tag{3.1}$$

$$^2D +^2 D \longrightarrow^3 He(.82MeV) + n(2.45MeV) \tag{3.2}$$

$$^2D +^2 D \longrightarrow^4 He(.076MeV) + \gamma(23.772MeV) \tag{3.3}$$

The products of these reactions are the signatures of a (D-D) fusion reaction. Skepticism was growing over cold fusion because the original experiment reported by Pons and Fleischmann claimed the production of huge quantities of heat, but only very small amounts of fusion by-products were detected. Although many scientists contend that the heat must be of a chemical origin, this has never been proved. However, two scientists from the University of Utah, Cheves T. Walling and Jack Simons[3], propose that two deuterons can fuse to form an excited helium-4 nucleus which packs $24MeV$ of internal energy. Normally such a nucleus will fragment into helium-3 and a neutron, or a tritium and a proton. But when the excited helium-4 is formed inside the electron-rich palladium lattice, they claim it can return to the ground state by transferring its excess energy to the electrons. This process results in stable helium-4 and heat. Pons and his coworker, graduate student Marvin Hawkins, have used mass spectrometry to analyze the gas produced in the electrolytic cell. According to

Walling they got "a very appreciable helium-4 peak." The heat produced in the experiment seems to correspond to about $24MeV$ per helium-4 nucleus detected. That is what one would expect if internal conversion were the overriding pathway.

On April 12, 1989 at the 197th annual meeting of the American Chemical Society in Dallas, Pons reiterated how the Utah experiment involved passing an electrical current through heavy water and into a palladium electrode. Fusion in the rod produced four watts of energy for every watt used to run the cell. He even produced a picture of a test tube labeled "The Utah Tokamak."[1]. The major question in the cold-fusion claim was: could the energy release be explained in some other, chemical way ? Cold fusion depends critically upon the fusion of deuterium nuclei in the palladium electrode. The effect could not happen if light water were substituted for heavy water: calculations suggested that quantum tunneling would be unable to fuse light hydrogen nuclei, and no heat would be observed. But since light water is chemically identical to heavy water, if the heating effects are due to some chemical reaction and not nuclear, then nothing should change if light water were substituted in the cell. This was the critical experiment: repeat the steps as the original experiment but substitute light water for heavy water. If true cold fusion has been taking place, it will now stop; and no heat will be observed. But if the heat is the result of some unknown chemical effect, then the same heat production will be found with light as with heavy water. This key experiment (using the light water instead of heavy water) had already been carried out by Steven Jones at Brigham Young University and the results showed no heat or neutrons produced [1].

On April 17, 1989 Pons announced that in one cell the fusion reaction had been sustained for 800 hours and was producing eighty times more energy than it

consumed [1]. The power output was now up to sixty seven watts per cubic centimeter of electrode. Nineteen new fuel cells were being set up and the design for a small scale power reactor was under way. Scientists at Stanford University confirmed cold fusion but at a much lower heat production. In addition they performed a control experiment in which they repeated the whole procedure using ordinary light water in place of heavy water. The two cells were run for two weeks. As predicted by Fleischmann and Pons, since light water is chemically similar to heavy water but in nuclear terms quite different, the heating effect was not seen with light water. Two researchers at the University of Florida's Department of Nuclear Engineering Sciences, Glen J. Scoessow and John A. Wethington, claimed to have detected tritium during the cold fusion process (an important clue that fusion was actually taking place) but not when light water was used. [1].

On May 22-25, 1989, a workshop on Cold Fusion Phenomena was sponsored by the U.S. Department of Energy and hosted by the Los Alamos National Laboratory. This workshop was devoted to understand a complex, exciting, and potentially highly exploitable phenomenon of nuclear fusion at room temperature. The workshop brought key workers in the area of cold fusion from all around the world to a scientific forum, results were compared and debated on a scientific plane. The workshop began the process of bringing cold fusion research out of the bright glare of press conferences and back to in-depth probing and questioning. Some of the papers presented in the workshop were a search for experimental and theoretical insight into the phenomenon, others were reports of failed trials to reproduce the experiment, and one paper was an attempt to explain the results of Pons and Fleischmann's experiment on a metallurgical background. Here is a brief description of some of the papers that

were presented there:

A paper presented by K.L. Wolf and coworkers [4] from the Cyclone Institute and the Department of Chemistry of Texas A& M University. The paper reports some positive results for neutron emission and for tritium detection from the Fleischmann-Pons type of electrolytic cells. The experimental investigation was conducted on samples of palladium and titanium metals which have been loaded with deuterium through the electrolysis of D_2O and by absorption of D_2 gas. In approximately 200 experiments on 25 cells, statistically significant evidence for neutron emission was obtained in three separate experiments from one palladium cathode, the neutrons detected were at energies around $2.45MeV$ which corresponds to the reaction in equation 3.2. The results for tritium were more encouraging since nine Pd-Ni electrolytic cells have shown levels that are factors of $10^2 - 10^6$ above background.

Another study reported by Tsang-Lang Lin and Chi-Chang Liu from the Department of Nuclear Engineering, National Tsing-Hua University, Hsin-Chu, Taiwan[5] stated that they have repeated the cold fusion experiment by electrolyzing heavy water with $0.1M$ LiOD, with palladium rod as the cathode and platinum wire as the anode. They claimed that neutrons bursts were detected during a period of about 7 hours after electrolyzing for 11 days, the highest burst being 240 neutrons/5 min. while the background was 1. cpm.

A group of scientists from the Department of Chemistry in the University of Rome, Italy, in cooperation with four other research institutes in Italy[6] reported that they had tried to reproduce the experiment using a sintered palladium electrode instead of a cast metal electrode (which was used by Pons and Fleischmann [7]). After six days of electrolysis at $200mA/cm^2$ they detected a simultaneous emission of

neutrons, tritium excess in the electrolytic solution, and rapid temperature increase. During the event which lasted 4 minutes they counted $7.2 * 10^5$ neutrons; tritium was also detected in an excess quantity corresponds to $(2.14 \pm .04) * 10^{14}$ atoms related to the solution volume of $41ml$, while the palladium electrode temperature reached 150^0C. But the energy production in this experiment was higher than the amount of neutrons and tritium detected, which suggests that there may be helium-4 production. In the discussion after presenting this paper it was recommended to analyze the cathode and to look for helium-4.

The above was a brief description of some of the papers which reported a success in detecting some of the by products of nuclear reactions. On the other hand, there was enormous number of papers which reported failure to find evidences of nuclear reactions. One of these papers reported a collaborative effort of a team which was formed at Los Alamos and supported by the U.S. Department of energy to investigate the claim that cold fusion may be occurring in electrochemical cells [8]. They have used palladium cathodes and platinum anodes in a LiOD solution electrolyte. Four electrochemical cells were constructed and operated for 3-5 weeks under various geometrical and electrical conditions. No conclusive evident was found for the production of neutrons above levels consistent with background. In subsequent precision calorimetric experiments performed in closed cells, there was no generation of "excess heat."

A paper presented by Ali AbuTaha [9], suggested that the palladium may have been the fuel in the electrochemical cell instead of the deuterium. The paper states that a considerable strain energy is stored in metals and alloys when processed from the ore. The energy balance is disturbed when cracks nucleate, grow, and propagate

within the bulk. Deuterium induces and propagates cracks in palladium and other metals and alloys. The sudden discharge of fracture energy during crack propagation generates a considerable amount of heat. The heat produced by the work-of-fracture can be substantial and can account for the excess enthalpy reported in cold fusion experiments. The paper claims that in all the cold fusion experiments, the release of heat was reported for a limited period of time (120 hours in the Pons and Fleischmann experiment) and this is due to the fact that the amount of fracture work that can be done on a metal is limited. The paper also explains the partially vaporized palladium sample in the Pons-Fleischmann experiments by a considerable power that can be generated if the fracture energy is released in shorter periods, this phenomena is known as the short-time release of fracture energy "The explosive crack propagation can be violent enough to produce traces of fusion by-products." The paper ends up with a conclusion that the fuel in the cold fusion experiment reported by Pons and Fleischmann was the palladium and not the deuterium.

Theoretical studies of the cold fusion phenomena were also conflicting, just as the experiments were. One of these studies was performed by a group of researchers from the Physics Department at Iowa State University [10]. They used the WKB approximation to calculate the Gamow transmission coefficient through a potential barrier for hydrogen-like ions confined in a potential well. Their calculations showed a fusion reaction rate of $10^{-64}/d - d/s$ (which is very low for all practical usages).

On the other hand, a paper written by Mario Robinowitz [11] suggested that "it appears that hitherto unconsidered physical mechanism must be present in the solid that are not present in the liquid." The paper claimed that there may be two means by which the fusion reaction rate in solids can be increased by several orders

of magnitude over that in liquids. These are:

- It is possible for the effective mass of the deuterium nuclei in a solid to be sufficiently less than the mass of deuterons in free space to increase the tunneling coefficient by many orders of magnitude.

- There may be preferential pathways in a solid that decrease the degree of freedom so that the fusing particle is confined essentially to one or two dimensional motion in the solid, that is the particle is able to move only in certain channels. Decreasing the dimensionality or the degrees of freedom, decreases the number of ways potentially colliding particles can miss each other.

Robinowitz goes on to claim that these two factors (the tunneling and the fusion probabilities) tend to be magnified by several orders of magnitudes in solids. The paper, however, assumed that the collision frequency is the same in solids as it is in the liquid state and in ordinary solid solutions. However, an article written by Bernard I. Spinrad from Iowa State University, Department of Nuclear Engineering [12], suggested that a high negative voltage applied on a metal into which deuterium is soaked should be just as effective as high-mass negative charges in permitting close approach of two deuterons to each other. "Another way of thinking about this is that the large negative potential effectively adds kinetic energy to the deuterons." This research was built on Dr. Spinrad's ideas of increasing the collision frequency by applying a high negative voltage to the cell, hence increasing the kinetic energy of the deuterons, and also of assuming that there is a preferential pathway for deuterium in solids.

In summary, three different scenarios for cold fusion have arisen. These are:

- Pons and Fleischmann have discovered controlled nuclear fusion, and practical applications are around the corner.

- The energy released within the Pons and Fleischmann experiment has nothing to do with any nuclear process, and is, for example, of chemical origin, or it is due to a destruction of the palladium metal.

- Nuclear fusion does indeed take place, but at the extremely low levels detected by Jones at Brigham Young University [2]. The phenomenon is of considerable scientific importance, but has no immediate relevance as a new energy source.

CHAPTER 4. THE MODEL

Introduction

At the beginning we need to define the word "cell". It has been established by neutron-diffraction studies, that hydrogen or deuterium atoms occupy the octahedral interstices of the face center cubic (FCC) palladium lattice, to give an H deficient NaCl structure in PdH [13]. The FCC structure of a palladium cell requires 14 atoms of Pd; 8 of them are shared by 8 neighboring cells each, and 6 of them are shared by 2 neighboring cells each, so the actual number of atoms per palladium cell equals $8(1/8) + 6(1/2) = 4$ atoms. As a result of electrical deuteration of a palladium cathode, we can reach the structure of PdD, this means that the combined number of Pd and D atoms in a PdD cell is 8. Knowing that the PdD has a cell parameter of $4.07\mathring{A}$ at room temperature [13], by simple calculations we find that the sphere which contains one atom in this structure has a radius of $1.26 * 10^5\ Fm$. In our calculations we have assumed a value of 125000 Fm, and the cell in this case is defined as the sphere which contains only one atom. This is effectively the volume within which a deuteron is normally to be found.

When a direct current is passed through a metallic conductor, macroscopic movement of lattice atoms may occur. This phenomenon is usually called electromigration. Electromigration is analogous to ionic transport in solid electrolytes in that the pres-

ence of an electric field provides the driving force for atomic transport. Although the migrating atom is acted upon by a constant external force, the atom is not uniformly accelerated because of interactions between the solute and the surrounding lattice, but the migrating atom still moves through the crystal with a macroscopically constant velocity proportional to the average electric field present [14]. The ratio of the velocity of migration to the applied potential is called the electric mobility. It should be noticed that it may be possible for an atom to be acted upon by a very large external force, yet have a very low migration velocity because of a high resistance to atomic transport in the lattice. However in this research we are assuming that the deuterium is free to move inside the palladium crystal.

Description of The Model

The model assumes that there exists a vacancy in a palladium deuteride lattice cell (the number of vacancies can be increased by several orders of magnitude by quenching the palladium) and the deuterons inside the palladium have preferential pathways toward these vacancies . As a result of the electrical deuteration process a deuteron exists in the palladium lattice. Another deuteron is introduced into the cell driven by a force due to the voltage applied to the electrochemical cell. It is further assumed that the center of mass of the two deuterons is fixed at the cell center. It is also assumed that the wave function of the deuteron pair is periodic. These assumptions, made to simplify calculations, are reasonable for deuterons confined in a single cell. The following approximations were made to calculate the wave function of the deuteron pair:

1. The nuclear potential is approximated by the optical model. This is a simple model used to account in a general way for elastic scattering in the presence of absorptive effects. In this model we represent the nuclear potential in terms of a complex potential $U(r)$:

$$U(r) = V(r) + iW(r) \tag{4.1}$$

where the real functions V and W are selected to give the potential its proper radial dependence. The real part $V(r)$ is mainly responsible for elastic scattering, and the imaginary part $iW(r)$ is responsible for absorption. Before applying the optical model we need to choose a form for the real part of the potential. Two forms were applied in this research: the first was a square well, and the second form was the Woods-Saxon, which is a more detailed form that was expected it gave better fit to the experimental D-D fusion reaction cross section [?] than the square well.

2. When calculating the D-D fusion reaction cross section, the cell radius was assumed to be 250000 Fm. This exaggerated value was used to assure that the wave function reaches its asymptotic value at the edge of the cell. The actual value of the radius ($R \simeq 125000\ Fm$) was used when calculating the reaction rate constant.

3. The delocalized deuteron pair has very low energy (mostly thermal). We have set this energy to zero and adopted as the eigenvalue of the system a negative potential acting on the site. How this site voltage relates to the potential applied on the palladium cathode requires further investigation.

Schrödinger Equation

The system in our model consists of two deuterons, and we are going to calculate the wave function of this system. To do so, we are going to convert the two-body problem into one particle problem by separating the coordinates of center of mass from the relative coordinates. The Hamiltonian in this case has the following general form:

$$H = \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + U(|r_1 - r_2|) \tag{4.2}$$

where P_1 and P_2 are the momenta of the first and second particles, and $|r_1 - r_2|$ is the distance between the two particles, and the Schrödinger equation has the form:

$$[\frac{-\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + U(|r_1 - r_2|)]\ \psi = E\ \psi \tag{4.3}$$

$$let \quad r = |r_1 - r_2| \qquad and \qquad R = \frac{m_1 r_1 + m_2 r_2}{m_1 + m_2} \tag{4.4}$$

Substituting equation 4.4 into equation 4.3 we get:

$$-\frac{\hbar^2}{2(m_1+m_2)}(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2})\psi - \frac{\hbar^2}{2\frac{m_1 m_2}{m_1+m_2}}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})\psi + U(r)\psi = E\psi \tag{4.5}$$

where $\psi = \psi(r, R)$ is a function of the relative coordinates $r(x, y, z)$ and the coordinates of the center of mass $R(X, Y, Z)$. The Hamiltonian is the sum:

$$H = H_R + H_r \tag{4.6}$$

and each of the sub Hamiltonians has a complete set of eigenfunctions. Hence all the eigenfunctions of equation 4.5 can be obtained by assuming that ψ is a product :

$$\psi(r, R) = \psi_r(r)\psi_{cm}(R) \tag{4.7}$$

and the energy is also a sum:

$$E = E_R + E_r \tag{4.8}$$

such that

$$-\frac{\hbar^2}{2(m_1+m_2)}\nabla^2\psi_{cm}(R) = E_R\psi_{cm}(R) \tag{4.9}$$

and

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi_r(r) + U(r)\psi_r(r) = E_r\psi_r(r) \tag{4.10}$$

where μ is the reduced mass $= \frac{m_1 m_2}{m_1+m_2}$. Since in our system we are assuming that the center of mass is fixed at the cell center , then $E_R = 0$, and we are only left with equation 4.10 to describe the system. At this point $E = E_r$ = applied voltage by the third approximation above. Equation 4.10 says that the relative motion of a system of two particles subject to central forces can be treated like a one-body problem if the reduced mass is used.

Eigenfunction

The eigenvalue of the cell problem is the value of E which solves equation 4.10 and satisfies the boundary conditions. We have assumed that the delocalized deuteron pair has very low energy, and we have adopted as the eigenvalue of the system the (negative) potential of the palladium cathode. With this eigenvalue equation 4.10 should satisfy the boundary condition $\psi_r'(R) = 0$. If it did not satisfy this condition , then the eigenvalue should be iterated till the above condition is satisfied within a pre-determined tolerance value, or till the number of iterations exceeds a certain number. The iteration formula is derived as the following:

The wave equation is converted into spherical coordinates, and the equation we

are solving is:

$$-\frac{\hbar^2}{2\mu}\phi_0'' + U(r)\phi_0 = E_0\phi_0 \tag{4.11}$$

where ϕ is the exact wave function $= r * \psi_r(r)$, ϕ_0 is the value we are calculating, and r is the separation distance between the two particles. The boundary conditions are $\phi(0) = \phi^*(0) = \phi(R) = \phi^*(R) = 0$. Multiplying equation 4.11 by the complex conjugate of the wave function and integrating all terms we get:

$$\int_0^R -\frac{\hbar^2}{2\mu}\phi_0''\phi^* dr + \int_0^R \phi_0 U\phi^* dr = \int_0^R E_0\phi_0\phi^* dr \tag{4.12}$$

Integrating the first term in the above equation by parts and applying the boundary conditions $\phi'(R) = \phi^{*'}(R) = 0$ where ϕ is the exact wave function; we get

$$\int_0^R -\frac{\hbar^2}{2\mu}\phi_0''\phi^* dr = \int_0^R -\phi_0\frac{\hbar^2}{2\mu}\phi^{*''} dr - \frac{\hbar^2}{2\mu}\phi^*(R)\phi_0'(R) \tag{4.13}$$

Then equation 4.12 becomes:

$$-\int_0^R \phi_0\frac{\hbar^2}{2\mu}\phi^{*''} dr - \frac{\hbar^2}{2\mu}\phi^*(R)\phi_0'(R) + \int_0^R \phi_0 U\phi^* dr = E_0\int_0^R \phi_0\phi^* dr \tag{4.14}$$

Now take the complex conjugate of the exact wave equation and multiply it by ϕ_0 and integrate to get:

$$\int_0^R -\phi_0\frac{\hbar^2}{2\mu}\phi^{*''} dr + \int_0^R \phi_0 U^*\phi^* dr = \int_0^R \phi_0 E^*\phi^* dr \tag{4.15}$$

Subtracting equation 4.15 from equation 4.14, we find

$$-\frac{\hbar^2}{2\mu}\phi^*(R)\phi_0'(R) + \int_0^R \phi_0(U - U^*)\phi^* dr = (E_0 - E^*)\int_0^R \phi_0\phi^* dr. \tag{4.16}$$

$$\implies \quad E_0 - E^* = \frac{\int_0^R \phi_0(U - U^*)\phi^* dr - \frac{\hbar^2}{2\mu}\phi^*(R)\phi_0'(R)}{\int_0^R \phi_0\phi^* dr} \tag{4.17}$$

Since ϕ^* appears as a "weighting function" in numerator and denominator , we expect that using ϕ_0^* for ϕ^* will be a good approximation. Thus the new value of E can be obtained from the relation:

$$E^* = E_0 + \frac{\frac{\hbar^2}{2\mu}\phi_0^*(R)\phi_0'(R) - \int_0^R \phi_0(U-U^*)\phi_0^* dr}{\int_0^R \phi_0\phi_0^* dr} \tag{4.18}$$

Reaction Rate Constant

Once we have got a reasonable approximation of the eigenvalue, the eigenfunction of the system is given by introducing a time dependence. If E is now the total energy of the particle asymptotically, we would have:

$$\begin{aligned} \phi(r,t) &= f(t) * \phi(r) \\ E\phi(r,t) &= -i\hbar\frac{d\phi(r,t)}{dt} \\ \phi(r,t) &= e^{iEt/\hbar}\ \phi(r) \end{aligned} \tag{4.19}$$

if $E = E_{real} + iE_{imaginary}$

$$\Longrightarrow \quad \phi(r,t) = e^{iE_R t/\hbar}\ e^{-E_{Im}t/\hbar}\ \phi(r) \tag{4.20}$$

multiply the above equation by the complex conjugate of the wave function:

$$\phi^*(r,t)\phi(r,t) = e^{-2E_{Im}t/\hbar}\ \phi(r)\phi^*(r) \tag{4.21}$$

but $\phi\phi^*$ = density of matter = ρ

so $\rho = \rho_0 e^{-2E_{Im}t/\hbar} \equiv \rho_0 e{-}\lambda t$

and the reaction rate constant is:

$$\lambda = \frac{2E_{Im}}{\hbar} \qquad s^{-1}/(D-D)pair \tag{4.22}$$

CHAPTER 5. REACTION CROSS SECTION AND REACTION RATE CONSTANT

The model was first calibrated by attempting to reproduce the experimental D-D reaction cross section. The nuclear potential was first assumed to be a square well; then,the calculations were repeated using a Woods- Saxon potential.

Square Well

This is an oversimplification of the problem, but it is sufficient for at least some qualitative conclusions. The range of the strong attractive nuclear forces is taken to be the radius of a helium atom $(1.25 \pm .05)A^{1/3}\ Fm$ rounded upward, an actual value of 2.1 Fm was used. Beyond this distance the only force in the system is the Coulomb repulsive force. The depth of the nuclear potential is a fitting parameter, i.e there is no exact way for calculating its value, though the following method was used to get a first estimate of the real part of the strength of this potential; then by trial and error the exact real and imaginary parts which give the best fit to the experimental cross section were obtained. The nuclear potential is represented by a three dimensional square well, as shown in figure 5.1.

$$\begin{aligned} V(r) &= -V_0 \qquad for \quad r < R_n \\ &= 0 \qquad for \quad r > R_n \end{aligned} \tag{5.1}$$

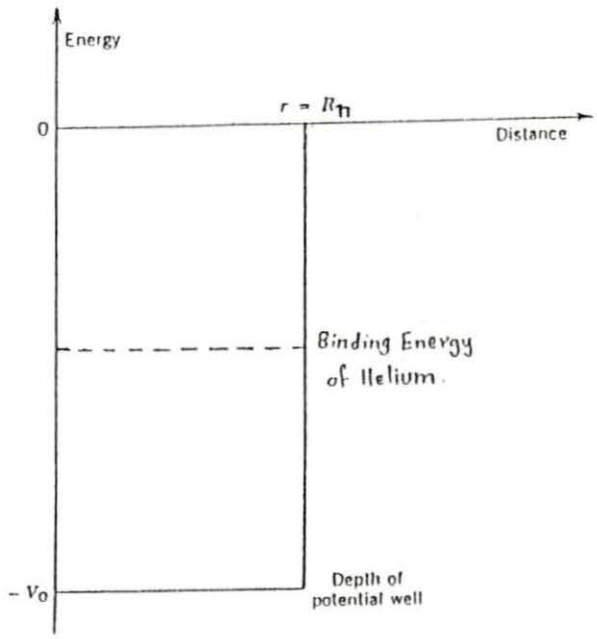

Figure 5.1: The square-well potential is an approximation to the nuclear potential, the depth of the well is $-V_0$

Note that we are ignoring the electrical repulsion of the two deuterons here, because this repulsion is very small compared to the attractive force due to the nuclear potential.

The assumption that only s-wave interactions exist in the system requires that the angular momentum of a deuteron should be zero. The wave function of the system $\psi(r)$ consists of a superposition of radial and angular wave functions, but for s-waves the angular function is 1. If we define the radial part of $\psi(r)$ as $\phi(r)/r$, then we can write the Schrödinger wave equation as

$$\frac{-\hbar^2}{2m}\frac{d^2\phi}{dr^2} + V(r)\phi(r) = E\phi(r). \tag{5.2}$$

The solution for this differential equation is given by

$$\phi(r) = A\sin k_1 r + B\cos k_1 r \qquad for \quad r < R_n \tag{5.3}$$

where $k_1 = \sqrt{\frac{2\mu(E+V_0)}{\hbar^2}}$

$$\phi(r) = Ce^{-k_2 r} + De^{k_2 r} \qquad for \quad r > R_n \tag{5.4}$$

where $k_2 = \sqrt{\frac{-2\mu E}{\hbar^2}}$. The boundary conditions are

1. $\phi(r)$ is finite as $r \to \infty$

2. $\phi(r) \to 0$ as $r \to 0$

From the first boundary condition we must have $D = 0$, and from the second condition we must have $B = 0$. Applying the continuity condition on $\phi(r)$ and $d\phi(r)/dr$ at $r = R_n$ we obtain

$$k_1 \cot k_1 R_n = -k_2. \tag{5.5}$$

Substituting for k_1 and k_2 we get

$$\tan \sqrt{\frac{-2\mu E}{\hbar^2}} * R_n \sqrt{\frac{-(E+V_0)}{E}} = -\sqrt{-\frac{(E+V_0)}{E}} \tag{5.6}$$

let $\sqrt{\frac{-2\mu E}{\hbar^2}}\, R_n = b$ = constant, and

$$\sqrt{-\frac{(E+V_0)}{E}} = x \tag{5.7}$$

$\Longrightarrow$ $-\tan bx = x$ substituting the following numerical values:

1. The binding energy E is obtained from the mass defect of helium= $-25.$ MeV.

2. $\hbar$ is Planck's constant= $6.58217 * 10^{-16}$ eV.s.

3. μ is the reduced mass of the deuteron pair= 938.0700206 MeV/c^2

we get the following transcendental equation

$$-\tan(2.19504197)x = x \tag{5.8}$$

The only unknown in the above equation is V_0. Solving equation 5.8 numerically, the result is 50.92 MeV. This value is only a first estimate of the real part of the nuclear potential. The actual value of the real and imaginary parts of the potential are found by looking for a value with a real part around the above calculated value and an imaginary part with a value around 10% of the real part such that the potential will give best estimate of the D-D experimental cross section. This value was found to be $(51.37 * 10^6 + i4.367 * 10^6)$ eV. This result was obtained by numerical integration of the wave equation. Starting with a zero initial value for the radial part of the wave function, and 1. for the first derivative, the second through the seventh derivatives were calculated using the Schrödinger wave equation as follows:

$$\begin{aligned}
\phi_0(0) &= 0 \\
\phi_0'(0) &= 1 \\
\phi_0''(0) &= \frac{2\mu}{\hbar^2}(-E - V_0)\phi_0 \\
&\vdots \\
\phi_0^{vii}(0) &= \frac{2\mu}{\hbar^2}(-E - V_0)\phi_0^{vi}
\end{aligned} \tag{5.9}$$

where V_0 is the depth of the square well nuclear potential $= (51.37 * 10^6 + i4.367 * 10^6)$eV. Starting from a zero separation distance between the two deuterons, and using Taylor series we have calculated the wave function to a high precision at a point further out. The process was repeated all through the cell until the separation distance was equal to the diameter of the cell 500000 Fm. The actual equation used

was:

$$\phi_0(r+H) = \phi_0(x) + H\phi_0'(x) + H^2\phi_0''(x)/2! + \cdots + H^6\phi_0^{vi}(x)/6! \tag{5.10}$$

A similar relation was used to calculate the first derivative. The step H is given by

$$H = \left|10^{-6} * 720(\phi_0' + .2\phi_0'')/\phi_0^{vii}\right|^{1/6} \tag{5.11}$$

At a separation distance of 2.1 Fm and beyond, the only force in the system is the Coulomb repulsive force, and V_0 in equations 5.9 is given by

$$V(r) = \frac{1.44 * 10^6}{r} \tag{5.12}$$

where V is in MeV, and r is the separation distance in between two deuterons. Thus and when calculating the derivatives of the wave function, the potential should be differentiated also.

To reduce the numerical error accumulation in the process of calculating the wave function, the reasoning of the WKB method was employed to separate the wave function into two real functions with complex coefficients, as follows:

At a separation distance of 2.1 Fm the square well nuclear potential is zero and the radial part of the wave function can be approximated by a superposition of Bessel functions with complex coefficients:

$$\begin{aligned} \phi_0(r) &= AxI_1(x) + BxK_1(x) \\ \phi_0'(r) &= [AxI_0(x) - BxK_0(x)]\frac{dx}{dr} \end{aligned} \tag{5.13}$$

where I_0, I_1, K_0,and K_1 are the modified Bessel functions of the first and second kinds. The argument x is given by

$$x = \frac{\lambda^2}{k}\arcsin(\frac{k\sqrt{r}}{\lambda}) + \sqrt{\lambda^2 r - k^2 r^2}$$

$$\begin{aligned} \lambda^2 &= \frac{2\mu e^2}{\hbar^2} \\ k &= wave\ number = \sqrt{\frac{2\mu E}{\hbar^2}} \\ \frac{dx}{dr} &= \sqrt{\frac{\lambda^2}{r} - k^2}. \end{aligned} \tag{5.14}$$

and r is the separation distance between the two deuterons. A and B are the complex coefficients, found by solving equations 5.13 simultaneously at r= 2.1 Fm. The numerical integration was carried out for the two separate real functions and the complex coefficients were saved till the separation distance was equal to the diameter of the cell. At this point the eigenfunction of the wave equation is given by a superposition of the following functions:

$$\phi_I = AF_I \qquad \phi_k = BF_K \tag{5.15}$$

and the derivative of the eigenfunction is also given by the superposition of the following functions

$$\phi'_I = AF'_I \qquad \phi'_K = BF'_K \tag{5.16}$$

where F_I, F_K, F'_I, F'_K are real functions. At this point the wave function represents a superposition of an incident and scattered wave. The change in the outgoing (scattered) partial wave is accounted for by introducing the complex coefficient μ_0, (The interaction is assumed to be only with s-waves). Thus, the wave function is:

$$\phi_0 = \frac{c}{2k} i(e^{-ikr} - \mu_0 e^{ikr}) \tag{5.17}$$

and its derivative is

$$\phi'_0 = \frac{c}{2k} i(-ike^{-ikr} - ik\mu_0 e^{ikr}) \tag{5.18}$$

Solving 5.17 and 5.18 simultaneously, we get the following expression for $|\mu_0|^2$

$$|\mu_0|^2 = \left| \frac{1 + \frac{\phi_0'}{ik\phi}}{1 - \frac{\phi_0'}{ik\phi}} \right|^2 \tag{5.19}$$

Substituting 5.15 and 5.16 into equation 5.19

$$|\mu_0|^2 = \left| \frac{ik + \frac{F_I' + \frac{B}{A}F_K'}{F_I + \frac{B}{A}F_K}}{ik - \frac{F_I' + \frac{B}{A}F_K'}{F_I + \frac{B}{A}F_K}} \right|^2 \tag{5.20}$$

where B and A are complex constants. Let $B/A = Re + iJ$, substitute this into equation 5.20 and simplify the expression to get

$$1 - |\mu_0|^2 = \frac{4.kJ(F_K F_I' - F_K' F_I)}{(F_I' + ReF_K' + kF_I)^2 + (kF_I + kReF_K - JF_K')^2} \tag{5.21}$$

The constant μ_0 was introduced to account for the change in the outgoing partial s-wave. A reduction in the amplitude of the wave suggests that there are fewer particles coming out than there were going in. The rate at which particles are disappearing is the difference between the incoming current and the outgoing current, and the reaction cross section is given by [15]

$$\sigma_r = \pi\bar{\lambda}^2(1 - |\mu_0|^2) \tag{5.22}$$

where $\bar{\lambda} = \lambda/2\pi$ is called the reduced deBroglie wavelength. $\bar{\lambda} = k^{-1}$, and the last term in the above equation is given by equation 5.21.

Woods-Saxon Form of the Potential

The square well is not realistic, simply because the nuclear potential does not have a sharp edge. Actually the nuclear charge and matter distribution falls smoothly

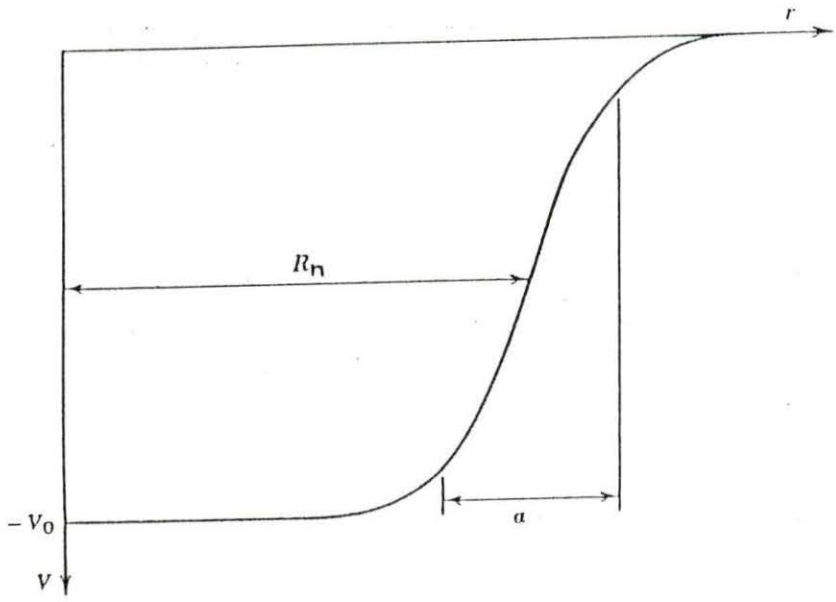

Figure 5.2: A realistic form for the potential is the Woods-Saxon potential, the distance "a" is called the "skin thickness."

to zero beyond the main radius. A more realistic form of the potential is the Woods-Saxon potential:

$$V = \frac{-V_0}{1 + e^{\frac{r-R_n}{a}}} \tag{5.23}$$

which is shown in figure 5. The parameters R_n and a give, respectively, the mean radius and the skin thickness. The skin thickness is defined as the distance over which the potential changes from $.9V_0$ to $.1V_0$. Again R_n, a, and V_0 are fitting parameters, their values are adjusted to give the best fit to the experimental D-D reaction cross section [15]. The following values where obtained for these parameters:

$V_0 = (51.37 * 10^6 + i7.848 * 10^6)$ eV

$a = .631\ Fm$ $\qquad$ and $\qquad$ $R_n = 1.575\ Fm.$

The forces in the system are:

1. Attractive force due to the Woods-Saxon nuclear potential.

2. Repulsive force due to the Coulomb potential.

These two forces act against each other until the separation distance equals 10 Fm. After the separation distance exceeds 10 Fm, the nuclear force is very small, so that practically the only force that exists in the system is a pure Coulomb repulsion. As we have done in the square well form of the potential, at a certain distance, when the nuclear attractive force is weak compared to the Coulomb repulsive force, the WKB method was used, and the radial part of the eigenfunction for the Schrödinger equation can be written in the form of equations 5.9. A correction factor on the Coulomb potential was used to account for the shielding of the two positive charges of the deuteron pair due to the presence of 4 electrons inside the cell, three valence electrons of the palladium atom and 1 electron from the deuterium atom. The four electrons are uniformly distributed in the cell (This is a conservative assumption, because if one of the electrons is closer to the deuterium atom, its shielding effect will be larger and this will reduce the repulsive force between the two positive charges by a great amount.) such that their density is $4*3/4\pi*R^3$, and at radius r the electrons inside r act like a central charge of $4r^3/R^3$. This charge acts separately on each of the two deuterons, yielding an additional (attractive) potential of $-8r^2e^2/R^3$ for the two deuteron system.

The reaction cross section was calculated using this form of the nuclear potential. Table 5.1 shows the values of the D-D cross section obtained by using the square well form and then the Woods-Saxon form compared to the standard values obtained experimentally.

As it was expected the Woods-Saxon form is more realistic, and it gives a better fit for the true values of reaction cross section. Figure 5.3 shows the reaction cross

Table 5.1: Fusion reaction cross sections as functions of the system energy

Energy	*Experimental value*[15]	*Square Well*[a]	*Woods − Saxon*[b]
KeV	mb	mb	mb
11	.758	.7838	.771
15	2.22	2.220	2.220
20	4.99	4.911	4.96
30	12.75	11.749	12.13
40	22.1	18.81	19.87
50	30.6	25.22	27.21
60	34.9	30.76	33.88

a. Radius of the cell= 250000 Fm.
$V = (51.37 * 10^6 + i4.367 * 10^6)eV$.
b. Radius of the cell = 250000 Fm.
$V = (51.37 * 10^6 + i7.848 * 10^6)eV$.
Skin thickness = .631 Fm.
$R_n = 1.575\ Fm$.

sections for both models compared to the reaction cross sections obtained experimentally.

Reaction Rate Constant

The reaction rate constant, which is given by equation 4.22, was calculated for both forms of the nuclear potential. The results showed a slight increase of the reaction rate constant when the Woods-Saxon potential was used, but the square well potential still showed to be a good approximation.

Before calculating the reaction rate constant we need to find an eigenvalue for the cell. As was explained in the previous chapter this is done by iterating equation 4.18.The integrals in this equation were calculated numerically all through the cell, from a zero separation distance to the edge of the cell (The actual cell radius was used =125000 Fm). A new value for the energy is obtained from equation 4.18.

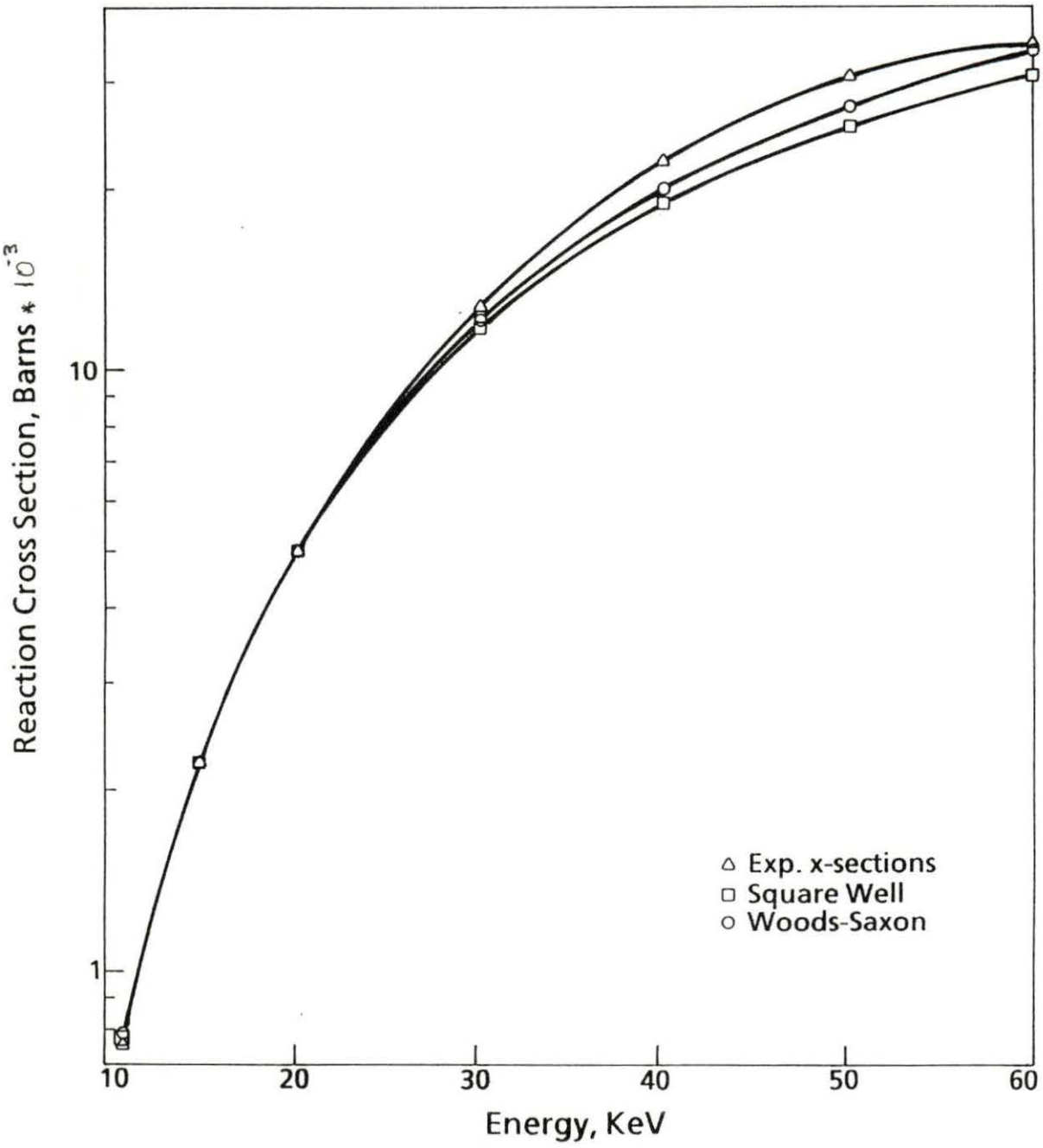

Figure 1. Comparison of the experimental reaction cross sections for the fusion reaction with those obtained theoretically by using the square well and Wood-Saxon nuclear potentials.

is used to calculate the wave function and its derivatives along with their complex conjugates. The integrals in equation ?? are calculated again, and another value of the energy was obtained. The process was repeated until the number of iterations exceeds a certain value, or the change in the energy is less than a pre-set value. The energy obtained in the above process is a complex number, and it is taken as the eigenvalue of the cell. As was shown in the previous chapter, the imaginary part of this eigenvalue is responsible for the absorption of particles in the system. The reaction rate constant is calculated using equation ?? which is rewritten here:

$$\lambda = \frac{2E_{Im}}{\hbar} \quad S^{-1}/(D-D)pair \tag{5.24}$$

Table ?? shows the energy eigenvalue and the corresponding reaction rate constants obtained for the two forms of nuclear potential:

Figure ?? shows the reaction rate constant as a function of the energy of the deuteron pair (The voltage applied to the lattice). The reaction rate constant has a suitable value for practical usages at an applied voltage of 400 V. However, the reaction rate can be increased by several orders of magnitude if the site voltage is increased. Practically, it is not difficult to apply a voltage of several thousands of volts to an electrochemical cell. However, it remains to be investigated how this applied voltage translates into a site voltage.

Table 5.2: Fusion reaction rate constant as a function of the system energy eigenvalues

$Square\ Well^a$		$Woods - Saxon^b$	
Energy (eV)	Reac. Rate Cons. (per second)	Energy(eV)	Reac. Rate Cons. (per second)
10.0043411	$.129492284 * 10^{-122}$	9.92969984	$.386935602 * 10^{-93}$
14.8647220	$.450693798 * 10^{-98}$	15.1140380	$.54532347 * 10^{-83}$
25.0361217	$.271039311 * 10^{-72}$	24.7653660	$.530966854 * 10^{-68}$
49.9133860	$.560661574 * 10^{-47}$	50.0870709	$.925649399 * 10^{-46}$
99.8594709	$.637014272 * 10^{-29}$	99.8944151	$.299839016 * 10^{-28}$
200.468394	$.464405994 * 10^{-16}$	201.160690	$.176241614 * 10^{-15}$
300.197438	$.213262776 * 10^{-10}$	300.102797	$.824439830 * 10^{-10}$
399.029355	$.496035291 * 10^{-7}$	400.753020	$.208443334 * 10^{-6}$
500.178676	$.112797925 * 10^{-4}$	500.732673	$.442359127 * 10^{-4}$
999.573148	7.0679	1000.63905	27.0254
2001.76995	100721.979	2001.89475	377871.0
3002.85741	7244569.24	2997.74189	26871214.2
3997.2455	93389927.4	4002.715	354826427.0
4997.02063	547562253.0	4998.73	$.206862373 * 10^{10}$
11000.2783	$.7827599 * 10^{11}$	11001.1810	$.29886 * 10^{12}$
19995.7615	$.1196336 * 10^{13}$	19997.4238	$.468805384 * 10^{13}$
29999.8055	$.5226378 * 10^{13}$	30006.6919	$.211245092 * 10^{14}$
39990.8643	$.128 * 10^{14}$	40005.7981	$.533275094 * 10^{14}$
50000.1305	$.238836101 * 10^{14}$	49994.7464	$.101922547 * 10^{15}$
60000.7705	$.38097 * 10^{14}$	59997.6600	$.166156978 * 10^{15}$

a. $V = (51.37 * 10^6 + i4.367 * 10^6)eV$

b. $V = 51.37 * 10^6 + i7.848 * 10^6)eV$

$R_n = 1.575\ Fm$ $\qquad$ $Skin\ thickness = .631\ Fm$

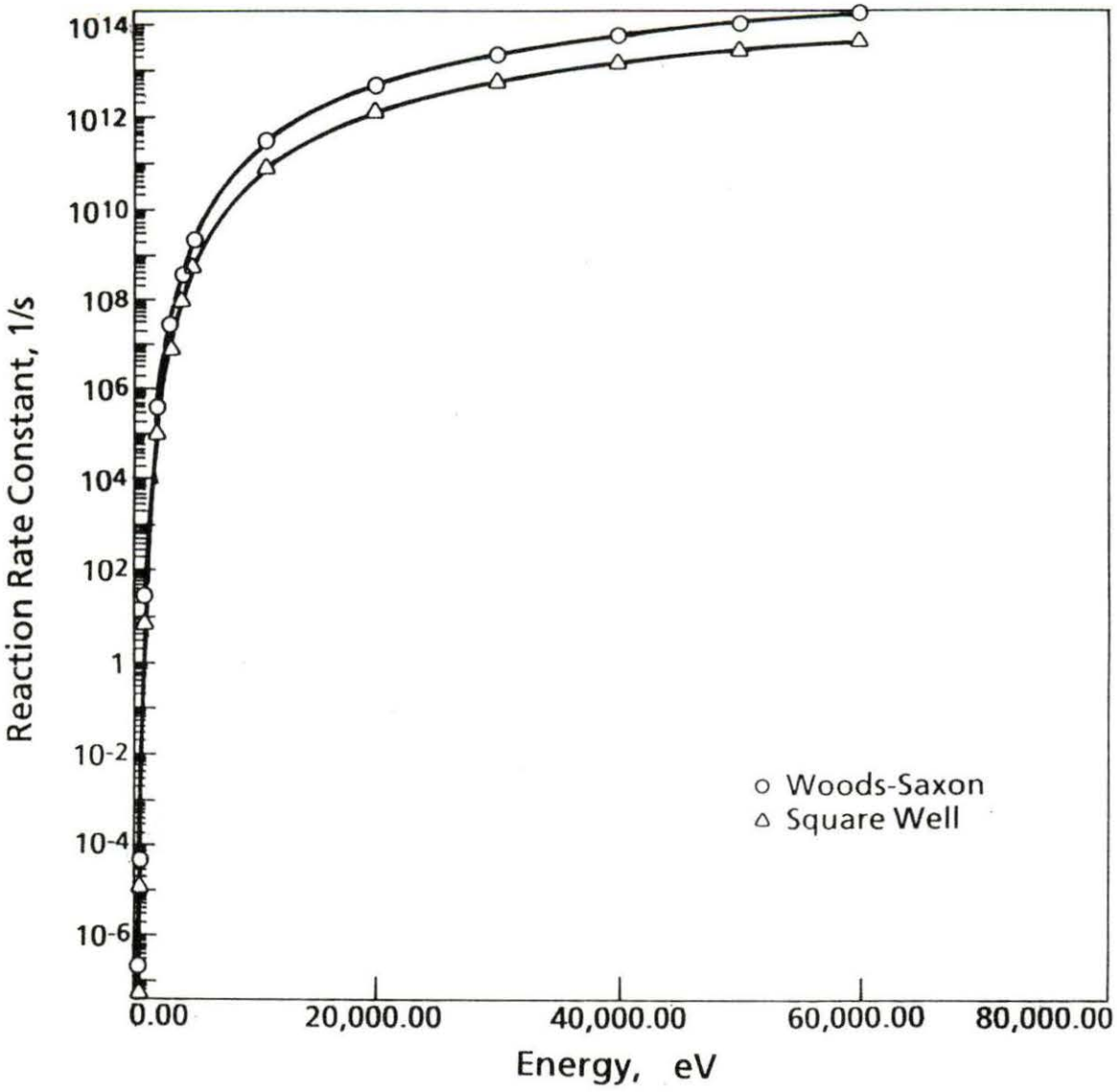

Figure 2. **The reaction rate constant as a function of the energy of the deuton pair for both models of the nuclear potential.**

CHAPTER 6. CONCLUSION

The striking conclusion of this research is that the cold fusion reaction can be made to happen at various reaction rates. A high energy deuteron confined in the palladium can increase the reaction rate by several orders of magnitude. If such energy, of the order of of 1 KeV, can be acheived by electrical means, this could control the power production level in the electrochemical cell. The reaction rates obtained above can be translated into energy production if we know how many deuterons are in the palladium cathode (The extent to which we can pump deuterons into the cathode before it starts bubbling off as gas at the surface of the metal). Simply, not all the lattice cells in the palladium cathode are occupied by deuteron pairs. The amount of deuterons that can be soaked into the palladium depends on the way in which the metal was formed, and the finishing of the surface.

Cold fusion is a new field of science, and it opens the door for a wide range of new knowledge. A lot of research is still needed to reach a complete understanding of the new phenomenon. Scientists need to research in the mechanisms of a new and unknown phenomenon that is capable of generating large excursions of heat from a palladium electrode that has been saturated with deuterium. A variety of physics and chemistry pathways and theories will have to be explored. The understanding of this phenomenon will also require a detailed study of the process of electrolysis

along with an understanding of the physical, metallurgical, and chemical changes that are taking place in the electrode. Moreover, studies are needed in the field of material science, especially metal structure and the electrodiffusion of hydrogen and deuterium in metals.

Finally, this work is a step on the long way to a complete understanding of the new and promising phenomenon of cold fusion.

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APPENDIX A. THE UTAH CELL

The Utah fusion cell[1] contains 99.5% heavy water with 0.5% light water.(Also, 0.1 M of LiOD was added to the cell.)

Electrical current for a given area of electrode surface: Highest used was $512 mA/cm^2$.

Neutron flux: 4000./sec for the $.4cm$ diameter electrode.

Heat output: Up to 1224.% of break even value (that is , up to $21 W/cm^3$ of the electrode.

Configurations:

- Negative electrode: a palladium sheet. Positive electrode: platinum sheet.
- Negative electrode: 10 cm palladium rods with diameters of 1.,2., and 4.mm. Positive electrode: platinum wire wound on a cage of glass rods.
- Negative electrode: a palladium cube ($1cm * 1cm * 1cm$). In this case the electrode heated to its melting point (1554 degrees Celsius) vaporized and destroyed part of the cupboard housing experiment.

APPENDIX B. COMPUTER PROGRAMS

```
C                       TS.FOR
C
C      THIS PROGRAM IS USED TO GENERATE THE WAVE FUNCTION AND ITS
C      DERIVATIVE  WHICH ARE USED TO CALCULATE THE REACTION
C      CROSS-SECTION.
C      THIS PROGRAM USES THE SQUARE WELL AS THE NUCLEAR POTENTIAL.
C      THE PROGRAM USES THE WKB APPROXIMATION TO CALCULATE THE
C      WAVE FUNCTION BEYOND R=2.1 Fm.

       REAL*8 X,X1,E,FI,FID,FK,FKD
       COMPLEX*16 F1,F2,F3,F4,F5,F6,F7,F8,V1,V2,V3,Z,H
       COMPLEX*16 V4,V5,V6,F11,F22,A,B,COEF

        X=(0.D0,0.0D0)
       F1=(0.D0,0.D0)
       F2=(1.D0,0.D0)

       E=(60000.D0,0.0D0)
       Z=(4.8182D-8,0.0D0)
       OPEN (UNIT=11,status='UNKNOWN',FILE='SS.DAT')
         J=0
         IFLAG=1
 1       DO 50 I=1,100000000

         IF (X.LT.2.1) THEN
         V1=(51.37D6,4.373D6)
         F3=(-E-V1)*F1*Z
         F4=(-E-V1)*F2*Z
         F5=(-E-V1)*F3*Z
```

```
      F6=(-E-V1)*F4*Z
      F7=(-E-V1)*F5*Z
      F8=(-E-V1)*F6*Z

      ELSE
      IF (IFLAG.EQ.1)          CALL BES(X,X1,F1,F2,F11,F22,Z,E,A,B)
      IFLAG=0
      V1=(1.44D6)/(X)
      V2=(-1.44D6)/(X**2)
      V3=(2.D0*1.44D6)/(X**3)
      V4=(-6.D0*1.44D6)/(X**4)
      V5=(24.D0*1.44D0)/(X**5)
      V6=(-120.D0*1.44D6)/(X**6)

      F3=(-E+V1)*F1*Z
      F4=((-E+V1)*F2+V2*F1)*Z
      F5=((-E+V1)*F3+2.D0*V2*F2+V3*F1)*Z
      F6=((-E+V1)*F4+3.D0*V2*F3+3.D0*
     +  V3*F2+V4*F1)*Z
      F7=((-E+V1)*F5+4.D0*V2*F4+6.D0*
     +  V3*F3+4.D0*V4*F2+V5*F1)*Z
      F8=((-E+V1)*F6+5.D0*V2*F5+10.D0*
     +  V3*F4+10.D0*V4*F3+5.D0*V5*F2
     +  +V6*F1)*Z

      ENDIF

      H=(ABS(1.D-6*720.D0*(F2+.2D0*F3)/F8))**
     +  (1.D0/6.D0)
      X=X+H

      IF (X.GT.500000.) GOTO 250

            F1=F1+H*F2+(H**2)*F3/2.D0+
     +      (H**3)*F4/6.D0+(H**4)*F5/24.D0+(H**
     +      5)*F6/120.D0

            F2=F2+H*F3+(H**2)*F4/2.D0+
     +      (H**3)*F5/6.D0+(H**4)*F6/24.D0+(H**
     +      5)*F7/120.D0
```

```
50    CONTINUE

250   X=X-H
      WRITE(11,41) X,F1,F2
41    FORMAT(F15.4,G16.9,G16.9,G16.9,G16.9)
      H=500000.-X

            F1=F1+H*F2+(H**2)*F3/2.D0+
     +      (H**3)*F4/6.D0+(H**4)*F5/24.D0+(H**5)*F6/120.D0

            F2=F2+H*F3+(H**2)*F4/2.D0+
     +      (H**3)*F5/6.D0+(H**4)*F6/24.D0+(H**5)*F7/120.D0
      X=X+H
      OPEN (UNIT=50,STATUS='UNKNOWN',FILE='S.DAT')
        COEF=B/A
        IF (J.EQ.0) THEN
           FI=DBLE(F1)
           FID=DBLE(F2)
           WRITE(50,55) X,FI,FID
        ELSE
           FK=DBLE(F1)
           FKD=DBLE(F2)
           WRITE(50,56) X,FK,FKD,COEF,E
        ENDIF
55    FORMAT(F10.2,G16.9,G16.9,G16.9,G16.9)
56    FORMAT(F10.2,G16.9,G16.9,G16.9,G16.9,/,G16.9,G16.9,G16.9)
        F1=F11
        F2=F22
        X=X1
        J=J+1
        IF(J.EQ.1) GOTO 1
344   STOP
        END

        SUBROUTINE BES (X,X1,F1,F2,F11,F22,Z,E,A,B)
        REAL*8 X,X1,T,R,E
        COMPLEX*16  I0,I1,K0,K1,SPIN
        COMPLEX*16  LAM,LAMSQ,K,KSQ,DXDR
        COMPLEX*16 Z,A,B,F1,F2,F11,F22
        CALL UNDER0(IFLAG)
```

```
      LAMSQ=Z*1.44002E6
      KSQ=Z*E
      LAM=SQRT(LAMSQ)
      K=SQRT(KSQ)
      x=2.1
9     R=(LAMSQ/K)*DASIN(K*SQRT(X)/LAM)+SQRT(LAMSQ*X-KSQ*X**2)
      DXDR=SQRT(LAMSQ/X-KSQ)
      T=R/3.75
      IF (R.LT.3.75) THEN
      I0=1.+3.5156229*T**2+3.0899424*T**4+1.2067492*t**6
     +    +.2659732*t**8+.0360768*t**10+.0045813*t**12
      I1=(.5+.87890594*t**2+.51498869*t**4+.15084934*t**6
     +     +.02658733*T**8+.00301532*T**10+.00032411*T**12)/R
      ELSE
      I0=(.39894228+.01328592*t**(-1)+.00225319*t**(-2)-.0015
     +7565*t**(-3)+.00916281*t**(-4)-.02057706*T**(-5)+.02635537*
     +T**(-6)-.01647633*T**(-7)+.00392377*T**(-8))/(DSQRT(R)*EXP(-R))
      I1=(.39894228-.03988024*t**(-1)-.00362018*t**(-2)+.00163801
     +    *t**(-3)-.01031555*t**(-4)+.02282967*t**(-5)-.02895312*t
     +    **(-6)+.01787654*t**(-7)-.00420059*t**(-8))/(DSQRT(R)*EX
     +    P(-R))
      ENDIF
      K0=(1.25331414-.07832358*2./R+.02189568*(2./R)**2
     +    -.01062446*(2./R)**3+.00587872*(2./R)**4-.002
     +    51540*(2./R)**5+.00053208*(2./R)**6)/(DSQRT(R)*EXP(R))
      K1=(1.25331414+.23498619*(2./R)-.03655620*(2./R)**2
     +    +.01504268*(2./R)**3-.00780353*(2./R)**4
     +    +.00325614*(2./R)**5-.00068245*(2./R)**6)/(DSQRT(R)
     +     *EXP(R))
      IF (X.GT.2.3) goto 4
      B=(I0*F1-F2*I1/DXDR)
      A=(F1*K0+F2*K1/DXDR)
      F1=R*I1
      F2=R*I0*DXDR
      F11=R*K1
      F22=-1.*R*K0*DXDR
      X1=X
      RETURN
      END
```

```
C                       TW.FOR
C
C      THIS PROGRAM IS USED TO GENERATE THE WAVE FUNCTION AND ITS
C      DERIVATIVE  WHICH ARE USED TO CALCULATE THE REACTION CROSS-SECTION.
C      THIS PROGRAM USES THE WOODS-SAXON POTENTIAL AS THE
C      NUCLEAR POTENTIAL. AND THE WKB APPROXIMATION FOR
C      CALCULATING THE WAVE FUNCTION BEYOND R=10. Fm.

       REAL*8 X,X11,Y11,Y,X1,E,R,A,R0,FI,FID,FK,FKD
       COMPLEX*16 F1,F2,F3,F4,F5,F6,F7,F8,V1,V2,V3,Z,H,COEF
       COMPLEX*16 V4,V5,V6,F11,F22,V0,B,C
       X=0.00000000002
       F1=(0.D0,0.D0)
       F2=(1.D0,0.D0)
         R=250000.

       v0=(51.37d6,7.848d6)
       a=0.631
       r0=1.575
        x1=Dexp(2)*Dexp(-r0/a)
       E=(15000.D0,0.0D0)
       Z=(4.8182D-8,0.0D0)
       OPEN (UNIT=11,status='UNKNOWN',FILE='SS.DAT')
         J=0
         IFLAG=1
 1       DO 50 I=1,100000000

          IF (X.LT.10.0) THEN

c        v1 this is the nuclear potential which is a Wood's-Saxon potential.
c        f3-f8 are the second through seventh derivatives of the wave function.
          y=exp((x-r0)/a)
          y11=x+x*y
         V1=(x*(-v0)-x1*(exp(x/a)-1))/(y11)
         v2=(-v0-(x1/a)*exp(x/a)-v1*(1+y+x/a*y))/y11
         v3=(-(x1*exp(x/a))/a**2)-(v1*x/(a**2))*y-2*v1*y/a-v2*x*y/a
     +      -2*v2*(y+1)/y11
         v4=(((-x1*exp(x/a))/a**3)-3*v1*y/a**2-v1*x*y/a**3-5*v2*y/a
     +      -3*v3*(y+1)-2*v3*x*y/a-2*v2*x*y/a**2)/y11
```

```
      v5=(-x1*exp(x/a)/a**4-10*v2*y/a**2-4*v1*y/a**3-3*v2*x*y/a**3
     +    -v1*x*y/a**4-10*v3*y/a-4*v3*(y+1)-3*v4*x*y/a-4*v3*x*y/
     +    a**2)/y11
      v6=((-x1*exp(x/a)/a**5)-24*v3*y/a**2-17*v2*y/a**3-5*v1*y/a**4
     +    -7*v3*x*y/a**3-4*v2*x*y/a**4-v1*x*y/a**5-17*v4*y/a-5*v5*(1+y)
     +    -4*v5*x*y/a-7*v4*x*y/a**2)/y11

      F3=-(E+V1)*F1*Z
      F4=-((E+V1)*F2+V2*F1)*Z
      F5=-((E+V1)*F3+2.D0*V2*F2+V3*F1)*Z
      F6=-((E+V1)*F4+3.D0*V2*F3+3.D0*V3*F2+V4*F1)*Z
      F7=-((E+V1)*F5+4.D0*V2*F4+6.D0*V3*F3+4.D0*V4*F2+V5*F1)*Z
      F8=-((E+V1)*F6+5.D0*V2*F5+10.D0*V3*F4+10.D0*V4*F3+5.D0*V5*F2
     +    +V6*F1)*Z

      ELSE

      IF (IFLAG.EQ.1)         CALL BES(X,X11,F1,F2,F11,F22,Z,E,B,C)
      IFLAG=0

      V1=(1.44D6)/(X)-(2.*1.44D6*X**2)/R**3
      V2=(-1.44D6)/(X**2)-4.*1.44D6*X/R**3
      V3=(2.D0*1.44D6)/(X**3)-4.*1.44D6/R**3
      V4=(-6.D0*1.44D6)/(X**4)
      V5=(24.D0*1.44D0)/(X**5)
      V6=(-120.D0*1.44D6)/(X**6)
      ENDIF

      F3=(-E+V1)*F1*Z
      F4=((-E+V1)*F2+V2*F1)*Z
      F5=((-E+V1)*F3+2.D0*V2*F2+V3*F1)*Z
      F6=((-E+V1)*F4+3.D0*V2*F3+3.D0*V3*F2+V4*F1)*Z
      F7=((-E+V1)*F5+4.D0*V2*F4+6.D0*V3*F3+4.D0*V4*F2+V5*F1)*Z
      F8=((-E+V1)*F6+5.D0*V2*F5+10.D0*V3*F4+10.D0*V4*F3+5.D0*V5*F2
     +    +V6*F1)*Z

      H=(ABS(1.D-6*720.D0*(F2+.2D0*F3)/F8))**(1.D0/6.D0)
      X=X+H

      IF (X.GT.500000.) GOTO 250
```

```
              F1=F1+H*F2+(H**2)*F3/2.D0+
     +        (H**3)*F4/6.D0+(H**4)*F5/24.D0+(H**
     +        5)*F6/120.D0

              F2=F2+H*F3+(H**2)*F4/2.D0+
     +        (H**3)*F5/6.D0+(H**4)*F6/24.D0+(H**
     +        5)*F7/120.D0
50     CONTINUE

250    X=X-H
       WRITE(11,41) X,F1,F2
41     FORMAT(F15.4,G16.9,G16.9,G16.9,G16.9)
       H=500000.-X

              F1=F1+H*F2+(H**2)*F3/2.D0+
     +        (H**3)*F4/6.D0+(H**4)*F5/24.D0+(H**
     +        5)*F6/120.D0

              F2=F2+H*F3+(H**2)*F4/2.D0+
     +        (H**3)*F5/6.D0+(H**4)*F6/24.D0+(H**
     +        5)*F7/120.D0
      X=X+H
      OPEN (UNIT=50,STATUS='UNKNOWN',FILE='S.DAT')
        COEF=B/C
        IF (J.EQ.0) THEN
          FI=DBLE(F1)
          FID=DBLE(F2)
          WRITE(50,55) X,FI,FID
        ELSE
          FK=DBLE(F1)
          FKD=DBLE(F2)
          WRITE(50,56) X,FK,FKD,COEF,E
        ENDIF
55     FORMAT(F10.2,G16.9,G16.9,G16.9,G16.9)
56     FORMAT(F10.2,3G16.9,/,3G16.9)
        F1=F11
        F2=F22
        X=X11
        J=J+1
```

```
      IF(J.EQ.1) GOTO 1
344   STOP
      END

      SUBROUTINE BES (X,X11,F1,F2,F11,F22,Z,E,B,C)
      REAL*8 X,X11,T,R,E
      COMPLEX*16  I0,I1,K0,K1
      COMPLEX*16  LAM,LAMSQ,K,KSQ,DXDR
      COMPLEX*16 Z,C,B,F1,F2,F11,F22
      CALL UNDER0(IFLAG)
      LAMSQ=Z*1.44002E6
      KSQ=Z*E
      LAM=SQRT(LAMSQ)
      K=SQRT(KSQ)
      x=10.
 9    R=(LAMSQ/K)*DASIN(K*SQRT(X)/LAM)+SQRT(LAMSQ*X-KSQ*X**2)
      DXDR=SQRT(LAMSQ/X-KSQ)
      T=R/3.75
      IF (R.LT.3.75) THEN
      I0=1.+3.5156229*T**2+3.0899424*T**4+1.2067492*t**6.
     +     +.2659732*t**8.+.0360768*t**10.+.0045813*t**12.
      I1=(.5+.87890594*t**2.+.51498869*t**4.+.15084934*t**6.
     +      +.02658733*T**8.+.00301532*T**10.+.00032411*T**12.)/R
      ELSE
      I0=(.39894228+.01328592*t**(-1.)+.00225319*t**(-2.)-.0015
     +  7565*t**(-3.)+.00916281*t**(-4.)-.02057706*T**(-5.)+.02635537*
     +  T**(-6.)-.01647633*T**(-7.)+.00392377*T**(-8.))/(DSQRT(R)*
     +  EXP(-R))
      I1=(.39894228-.03988024*t**(-1)-.00362018*t**(-2)+.00163801
     +     *t**(-3)-.01031555*t**(-4)+.02282967*t**(-5)-.02895312*t
     +     **(-6)+.01787654*t**(-7)-.00420059*t**(-8))/(DSQRT(R)*EX
     +     P(-R))
      ENDIF
      K0=(1.25331414-.07832358*2./R+.02189568*(2./R)**2
     +     -.01062446*(2./R)**3+.00587872*(2./R)**4-.002
     +     51540*(2./R)**5+.00053208*(2./R)**6)/(DSQRT(R)*EXP(R))
      K1=(1.25331414+.23498619*(2./R)-.03655620*(2./R)**2
     +     +.01504268*(2./R)**3-.00780353*(2./R)**4
     +     +.00325614*(2./R)**5-.00068245*(2./R)**6)/(DSQRT(R)
     +      *EXP(R))
```

```
IF (X.GT.10.1) goto 4
B=(I0*F1-F2*I1/DXDR)
C=(F1*K0+F2*K1/DXDR)
F1=R*I1
F2=R*I0*DXDR
F11=R*K1
F22=-1.*R*K0*DXDR
X11=X
RETURN
END
```

```
c                          FINA.FOR
c
c     THIS PROGRAM IS USED TO CALCULATE THE REACTION RATE CONSTANT.
c     IT USES A SQURE WELL AS THE NUCLEAR POTENTIAL.
c

      REAL*8 X,R,Y1,Y2
      COMPLEX*16 F1,F2,F3,F4,F5,F6,F7,F8,V1,V2,V3,Z,H,E
      COMPLEX*16 V4,V5,V6,CF1,CF2,CF3,CF4,CF5,CF6,DER,DEI,INT
      COMPLEX*16 PR,FPR,FINT,CV1,CFD10,CC,Y3,Y4

c       THE ENERGY OF THE SYSTEM.
        E=(11000.D0,0.D0)
        J=0
        R=500000.
      OPEN (UNIT=50,STATUS='UNKNOWN',FILE='INT.DAT')
      OPEN (UNIT=51,STATUS='UNKNOWN',FILE='sum.DAT')

 6      X=(0.D0,0.0D0)

C     THE WAVE FUNCTION AND ITS FIRST DERIVATIVE.
      F1=(0.D0,0.D0)
      F2=(1.D0,0.D0)
        J=J+1
        WRITE(50,*)
        WRITE(50,*)
        WRITE(50,7)J
 7      FORMAT(I8)
      INT=0.0
      FINT=0.0

      Z=(4.8182D-8,0.0D0)

      DO 3 I=1,100000000
        IF (X.LT.2.1) THEN

c       v1 this is the nuclear potential which is a square well
c       f3-f8 are the second through seventh derivatives
c       of the wave function
```

```
      V1=(51.37D6,4.367D6)
      F3=(-E-V1)*F1*Z
      F4=(-E-V1)*F2*Z
      F5=(-E-V1)*F3*Z
      F6=(-E-V1)*F4*Z
      F7=(-E-V1)*F5*Z
      F8=(-E-V1)*F6*Z

      ELSE
c     this is the colomb barrier and its derivatives, plus the
c     screening effect.
c     the f's are the wave function derivatives

      V1=(1.44D6)/(X)-(8*X**2)/R**3
      V2=(-1.44D6)/(X**2)-16*X/R**3
      V3=(2.D0*1.44D6)/(X**3)-16/R**3
      V4=(-6.D0*1.44D6)/(X**4)
      V5=(24.D0*1.44D0)/(X**5)
      V6=(-120.D0*1.44D6)/(X**6)

      F3=(-E+V1)*F1*Z
      F4=((-E+V1)*F2+V2*F1)*Z
      F5=((-E+V1)*F3+2.D0*V2*F2+V3*F1)*Z
      F6=((-E+V1)*F4+3.D0*V2*F3+3.D0*
     +  V3*F2+V4*F1)*Z
      F7=((-E+V1)*F5+4.D0*V2*F4+6.D0*
     +  V3*F3+4.D0*V4*F2+V5*F1)*Z
      F8=((-E+V1)*F6+5.D0*V2*F5+10.D0*
     +  V3*F4+10.D0*V4*F3+5.D0*V5*F2
     +  +V6*F1)*Z
      ENDIF
c     this is the steps we are moving from the center of the cell
c     towared the edge,in order to calculate the wave function.

      H=(ABS(1.D-6*720.D0*(F2+.2D0*F3)/F8))**
     +  (1.D0/6.D0)

      X=X+H
      IF (X.GT.R) GOTO 250
```

```
c       these are the complex conjugates of the wave
c         function and its derivatives and the complex conjugate
c         of the nuclear potential.

        CV1=DCONJG(V1)
        CF1=DCONJG(F1)
        CF2=DCONJG(F2)
        CF3=DCONJG(F3)
        CF4=DCONJG(F4)
        CF5=DCONJG(F5)
        CF6=DCONJG(F6)

c       FPR is the value of the last part in the iteration formula.

        FPR=(H*(F1*CF1)+(H**2)/2.*(F1*CF2+F2*CF1)+(H**3)/3.*((F1*CF3/2.D0
     +  )+F2*CF2+(F3*CF1/2.D0))+(H**4)/4.*((F1*CF4/6.D0)+(F2*CF3/
     +  2.D0)+(F3*CF2/2.D0)+(F4*CF1/6.D0))+(H**5)/5.*((F1*CF5/24
     + .D0)+(F2*CF4/6.D0)+(F3*CF3/4.D0)+(F4*CF2/6.D0)+(F5*CF1
     + /24.D0))+(H**6)/6.*((F1*CF6/120.D0)+(F2*CF5/24.D0)+(F3*CF
     + 4/12.D0)+(F4*CF3/12.D0)+(F5*CF2/24.D0)+(F6*CF1/120.D0)
     + )+(H**7)/7.*((F2*CF6/120.D0)+(F3*CF5/48.D0)+(F4*CF4/36.D0
     + )+(F5*CF3/48.D0)+(F6*CF2/120.D0))+(H**8)/8.*((F3*CF6/240.
     + D0)+(F4*CF5/144.D0)+(F5*CF4/144.D0)+(F6*CF3/240.D0))+(
     + H**9)/9.*((F4*CF6/720.D0)+(F5*CF5/576.D0)+(F6*CF4/720.D0))
     + +(H**10)/10.*((F6*CF5/2800.D0)+(F5*CF6/2800.D0))+(H**11)/11.*(F6
     + *CF6/14400.D0))

c       PR is the value of the first part in the iteration formula.
        PR=FPR*(V1-CV1)

c       FINT is the last integral in the iteration formula.
c       INT is the first integral in the iteration formula.

        FINT=FINT+FPR
        INT=INT+PR

              F1=F1+H*F2+(H**2)*F3/2.D0+
     +           (H**3)*F4/6.D0+(H**4)*F5/24.D0+(H**
     +           5)*F6/120.D0
              F2=F2+H*F3+(H**2)*F4/2.D0+(H**3)*F5/6.D0+(H**4)*
```

```
     +           F6/24.D0+(H**5)*F7/120.D0
 3       CONTINUE
c             This part of the program is to calculate the wave
c             function and the integral of page X7 exactly at the
c             edge of the cell.
 250          X=X-H
              H=R-X

         OPEN(4,'SS.DAT')
         WRITE(4,32)X,F1,F2

               F1=F1+H*F2+(H**2)*F3/2.D0+
     +            (H**3)*F4/6.D0+(H**4)*F5/24.D0+(H**
     +            5)*F6/120.D0
               F2=F2+H*F3+(H**2)*F4/2.D0+(H**3)*F5/6.D0+(H**4)*
     +            F6/24.D0+(H**5)*F7/120.D0
         X=X+H
         OPEN(1,'S.DAT')
         WRITE(1,32)X,F1,F2
 32      FORMAT(F15.4,3X,G16.9,G16.9,4X,G16.9,G16.9)

         V1=(1.44D6)/(X)-(8*X**2)/R**3
         V2=(-1.44D6)/(X**2)-16*X/R**3
         V3=(2.D0*1.44D6)/(X**3)-16/R**3
         V4=(-6.D0*1.44D6)/(X**4)
         V5=(24.D0*1.44D0)/(X**5)
         V6=(-120.D0*1.44D6)/(X**6)
         F3=(-E+V1)*F1*Z
         F4=((-E+V1)*F2+V2*F1)*Z
         F5=((-E+V1)*F3+2.D0*V2*F2+V3*F1)*Z
         F6=((-E+V1)*F4+3.D0*V2*F3+3.D0*
     +   V3*F2+V4*F1)*Z
         F7=((-E+V1)*F5+4.D0*V2*F4+6.D0*
     +   V3*F3+4.D0*V4*F2+V5*F1)*Z
         F8=((-E+V1)*F6+5.D0*V2*F5+10.D0*
     +   V3*F4+10.D0*V4*F3+5.D0*V5*F2
     +   +V6*F1)*Z

         CV1=DCONJG(V1)
         CF1=DCONJG(F1)
```

```
      CF2=DCONJG(F2)
      CF3=DCONJG(F3)
      CF4=DCONJG(F4)
      CF5=DCONJG(F5)
      CF6=DCONJG(F6)

c     FPR  this is the value of thelast part in the iteration formula for
c     the energy (page x7 from the notes).

      FPR=(H*(F1*CF1)+(H**2)/2.*(F1*CF2+F2*CF1)+(H**3)/3.*((F1*CF3/2.D0
     +  )+F2*CF2+(F3*CF1/2.D0))+(H**4)/4.*((F1*CF4/6.D0)+(F2*CF3/
     +  2.D0)+(F3*CF2/2.D0)+(F4*CF1/6.D0))+(H**5)/5.*((F1*CF5/24
     + .D0)+(F2*CF4/6.D0)+(F3*CF3/4.D0)+(F4*CF2/6.D0)+(F5*CF1
     + /24.D0))+(H**6)/6.*((F1*CF6/120.D0)+(F2*CF5/24.D0)+(F3*CF
     + 4/12.D0)+(F4*CF3/12.D0)+(F5*CF2/24.D0)+(F6*CF1/120.D0)
     + )+(H**7)/7.*((F2*CF6/120.D0)+(F3*CF5/48.D0)+(F4*CF4/36.D0
     + )+(F5*CF3/48.D0)+(F6*CF2/120.D0))+(H**8)/8.*((F3*CF6/240.
     + D0)+(F4*CF5/144.D0)+(F5*CF4/144.D0)+(F6*CF3/240.D0))+(
     + H**9)/9.*((F4*CF6/720.D0)+(F5*CF5/576.D0)+(F6*CF4/720.D0))
     + +(H**10)/10.*((F6*CF5/2800.D0)+(F5*CF6/2800.D0))+(H**11)/11.*(F6
     + *CF6/14400.D0))

c     PR   this is the value of the first part in the iteration formula for
c     the energy (page X7 from the notes)

      PR=FPR*(V1-CV1)
       INT=INT+PR
       FINT=FINT+FPR

       CFD10=DCONJG(F2)
       CC=(2./9.6364E-8)*F1*(CFD10)
       Y1=DBLE(CC)
       Y2=DBLE(FINT)
       Y3=DBLE(INT)
       Y4=INT-Y3

       WRITE(50,19)I
       WRITE(50,20)Y4
       WRITE(50,21)Y2
       WRITE(50,22)Y1
```

```
      DER=(Y3+Y1)/Y2
      DEI=Y4/Y2
      E=E+DER
      E=E+(0.D0,1.D0)*DEI

      WRITE(50,*)
      WRITE(50,8) E
      WRITE(50,9)DER
      WRITE(50,10)DEI

      IF(CDABS(DER).LT.1.D-15) GOTO 66
      IF(J.GT.3) GO TO 66
      GO TO 6
66

19    FORMAT(2X,'NO. OF ITERATIONS=',I8)
20    FORMAT(2X,'INT.=',G16.9,2X,G16.9)
21    FORMAT(2X,'FINT.='G16.9,2X,G16.9)
22    FORMAT(2X,'CC   ='G16.9,2X,G16.9)
9     FORMAT(4X,'DE REAL   =',G16.9,3X,G16.9)
8     FORMAT(4X,'THE ENERGY=',G16.9,3X,G16.9)
10    FORMAT(4X,'DEIMAG.   =',G16.9,3X,G16.9)
      STOP
      END
```

```
C                    FINAL11.FOR

C     THIS PROGRAM USES A WOOD'S-SAXON NUCLEAR POTENTIAL AND
C     FOR THE COULOMB BARRIER, AND THE SCREENING POTENTIAL DUE
C     TO THE ELECTRON DISTRIBUTION WITHIN THE CELL.
C     THE RADIUS OF THE CELL IS 125000. Fm.

      REAL*8 X,R,Y1,Y2
      COMPLEX*16 F1,F2,F3,F4,F5,F6,F7,F8,V1,V2,V3,Z,H,E
      COMPLEX*16 V4,V5,V6,CF1,CF2,CF3,CF4,CF5,CF6,DER,DEI,INT
      COMPLEX*16 PR,FPR,FINT,CV1,CFD10,CC,Y3,Y4,y,y11,v0,LAMDA
        IK=1
c       The energy of the cell.
        E=(100.D0,0.D0)
        J=0
c       the radius of the cell in Femto-meters.
        R=125000.
      OPEN (UNIT=50,STATUS='UNKNOWN',FILE='INT8.DAT')
      OPEN (UNIT=51,STATUS='UNKNOWN',FILE='sum.DAT')
 6      X=.00000000002
c       the wave function and its first derivative.
      F1=(0.D0,0.D0)
      F2=(1.D0,0.D0)
        J=J+1
        WRITE(50,*)
        WRITE(50,*)
        WRITE(50,7)J
 7      FORMAT(I8)
      INT=0.0
      FINT=0.0

      Z=(4.8182D-8,0.0D0)
      v0=(51.37d6,7.848d6)
      a=0.631
      r0=1.575
       x1=exp(2)*exp(-r0/a)

      DO 3 I=1,100000000
         IF (X.LT.10.0) THEN
c       v1 this is the nuclear potential which is a Wood's-Saxon potential.
```

```
c       f3-f8 are the second through seventh derivatives of the wave function.
         y=exp((x-r0)/a)
         y11=x+x*y
        V1=(x*(v0)-x1*(exp(x/a)-1))/(y11)
        v2=(v0-(x1/a)*exp(x/a)-v1*(1+y+x/a*y))/y11
        v3=(-(x1*exp(x/a))/a**2)-(v1*x/(a**2))*y-2*v1*y/a-v2*x*y/a
     +  -2*v2*(y+1)/y11
       v4=(((-x1*exp(x/a))/a**3)-3*v1*y/a**2-v1*x*y/a**3-5*v2*y/a
     + -3*v3*(y+1)-2*v3*x*y/a-2*v2*x*y/a**2)/y11
       v5=(-x1*exp(x/a)/a**4-10*v2*y/a**2-4*v1*y/a**3-3*v2*x*y/a**3
     +  -v1*x*y/a**4-10*v3*y/a-4*v3*(y+1)-3*v4*x*y/a-4*v3*x*y/a**2)/y11
        v6=((-x1*exp(x/a)/a**5)-24*v3*y/a**2-17*v2*y/a**3-5*v1*y/a**4
     + -7*v3*x*y/a**3-4*v2*x*y/a**4-v1*x*y/a**5-17*v4*y/a-5*v5*(1+y)
     +  -4*v5*x*y/a-7*v4*x*y/a**2)/y11

        F3=-(E+V1)*F1*Z
        F4=-((E+V1)*F2+V2*F1)*Z
        F5=-((E+V1)*F3+2.D0*V2*F2+V3*F1)*Z
        F6=-((E+V1)*F4+3.D0*V2*F3+3.D0* V3*F2+V4*F1)*Z
        F7=-((E+V1)*F5+4.D0*V2*F4+6.D0*V3*F3+4.D0*V4*F2+V5*F1)*Z
        F8=-((E+V1)*F6+5.D0*V2*F5+10.D0*V3*F4+10.D0*V4*F3+5.D0*V5*F2
     +  +V6*F1)*Z

        ELSE

c       this is the colomb potential and its derivatives, and the screening
c       potential due to the electron distribution within the cell.
c       the f's are the wave function derivatives.

        V1=(1.44D6)/(X)-(2.*1.44d6*X**2)/R**3
        V2=(-1.44D6)/(X**2)-4.*1.44d6*X/R**3
        V3=(2.D0*1.44D6)/(X**3)-4.*1.44d6/R**3
        V4=(-6.D0*1.44D6)/(X**4)
        V5=(24.D0*1.44D0)/(X**5)
        V6=(-120.D0*1.44D6)/(X**6)

        ENDIF

        F3=(-E+V1)*F1*Z
        F4=((-E+V1)*F2+V2*F1)*Z
```

```
      F5=((-E+V1)*F3+2.D0*V2*F2+V3*F1)*Z
      F6=((-E+V1)*F4+3.D0*V2*F3+3.D0*V3*F2+V4*F1)*Z
      F7=((-E+V1)*F5+4.D0*V2*F4+6.D0*V3*F3+4.D0*V4*F2+V5*F1)*Z
      F8=((-E+V1)*F6+5.D0*V2*F5+10.D0*V3*F4+10.D0*V4*F3+5.D0*V5*F2
     +  +V6*F1)*Z

c     this is the steps we are moving from the center of the cell
c     towared the edge in order to calculate the wave function.

      H=(ABS(1.D-6*720.D0*(F2+.2D0*F3)/F8))**(1.D0/6.D0)

      X=X+H
      IF (X.GT.250000.) GOTO 250

c     these are the complex conjugates of the wave
c       function and its derivatives and the complex conjugate
c       of the nuclear potential.

      CV1=DCONJG(V1)
      CF1=DCONJG(F1)
      CF2=DCONJG(F2)
      CF3=DCONJG(F3)
      CF4=DCONJG(F4)
      CF5=DCONJG(F5)
      CF6=DCONJG(F6)

c     FPR  this is the value of thelast part in the iteration formula.

      FPR=(H*(F1*CF1)+(H**2)/2.*(F1*CF2+F2*CF1)+(H**3)/3.*((F1*CF3/2.D0
     +  )+F2*CF2+(F3*CF1/2.D0))+(H**4)/4.*((F1*CF4/6.D0)+(F2*CF3/
     +  2.D0)+(F3*CF2/2.D0)+(F4*CF1/6.D0))+(H**5)/5.*((F1*CF5/24
     + .D0)+(F2*CF4/6.D0)+(F3*CF3/4.D0)+(F4*CF2/6.D0)+(F5*CF1
     + /24.D0))+(H**6)/6.*((F1*CF6/120.D0)+(F2*CF5/24.D0)+(F3*CF
     + 4/12.D0)+(F4*CF3/12.D0)+(F5*CF2/24.D0)+(F6*CF1/120.D0)
     + )+(H**7)/7.*((F2*CF6/120.D0)+(F3*CF5/48.D0)+(F4*CF4/36.D0
     + )+(F5*CF3/48.D0)+(F6*CF2/120.D0))+(H**8)/8.*((F3*CF6/240.
     + D0)+(F4*CF5/144.D0)+(F5*CF4/144.D0)+(F6*CF3/240.D0))+(
     + H**9)/9.*((F4*CF6/720.D0)+(F5*CF5/576.D0)+(F6*CF4/720.D0))
     + +(H**10)/10.*((F6*CF5/2800.D0)+(F5*CF6/2800.D0))+(H**11)/11.*(F6
     + *CF6/14400.D0))
```

```
c      PR   this is the value of the first part in the iteration formula.

      PR=FPR*(V1-CV1)
c       FINT  this is the last integral in the iteration formula.
c       INT   this is the first integral in the iteration formula.

        FINT=FINT+FPR
        INT=INT+PR

              F1=F1+H*F2+(H**2)*F3/2.D0+
     +           (H**3)*F4/6.D0+(H**4)*F5/24.D0+(H**
     +           5)*F6/120.D0
              F2=F2+H*F3+(H**2)*F4/2.D0+(H**3)*F5/6.D0+(H**4)*
     +           F6/24.D0+(H**5)*F7/120.D0
 3      CONTINUE

 250          X=X-H
              H=250000.-X
        OPEN(4,'SS.DAT')
        WRITE(4,42)X,F1,F2

              F1=F1+H*F2+(H**2)*F3/2.D0+
     +           (H**3)*F4/6.D0+(H**4)*F5/24.D0+(H**
     +           5)*F6/120.D0
              F2=F2+H*F3+(H**2)*F4/2.D0+(H**3)*F5/6.D0+(H**4)*
     +           F6/24.D0+(H**5)*F7/120.D0
        X=X+H

        OPEN(1,'S.DAT')
        WRITE(1,42)X,F1,F2
 42     FORMAT(F15.4,3X,G16.9,G16.9,4X,G16.9,G16.9)

        V1=(1.44D6)/(X)-(2.*1.44d6*X**2)/R**3
        V2=(-1.44D6)/(X**2)-4.*1.44d6*X/R**3
        V3=(2.D0*1.44D6)/(X**3)-4.*1.44d6/R**3
        V4=(-6.D0*1.44D6)/(X**4)
        V5=(24.D0*1.44D0)/(X**5)
        V6=(-120.D0*1.44D6)/(X**6)
        F3=(-E+V1)*F1*Z
```

```
      F4=((-E+V1)*F2+V2*F1)*Z
      F5=((-E+V1)*F3+2.D0*V2*F2+V3*F1)*Z
      F6=((-E+V1)*F4+3.D0*V2*F3+3.D0*
     +  V3*F2+V4*F1)*Z
      F7=((-E+V1)*F5+4.D0*V2*F4+6.D0*
     +  V3*F3+4.D0*V4*F2+V5*F1)*Z
      F8=((-E+V1)*F6+5.D0*V2*F5+10.D0*
     +  V3*F4+10.D0*V4*F3+5.D0*V5*F2
     +  +V6*F1)*Z

      CV1=DCONJG(V1)
      CF1=DCONJG(F1)
      CF2=DCONJG(F2)
      CF3=DCONJG(F3)
      CF4=DCONJG(F4)
      CF5=DCONJG(F5)
      CF6=DCONJG(F6)

     FPR=(H*(F1*CF1)+(H**2)/2.*(F1*CF2+F2*CF1)+(H**3)/3.*((F1*CF3/2.D0
     +  )+F2*CF2+(F3*CF1/2.D0))+(H**4)/4.*((F1*CF4/6.D0)+(F2*CF3/
     +  2.D0)+(F3*CF2/2.D0)+(F4*CF1/6.D0))+(H**5)/5.*((F1*CF5/24
     + .D0)+(F2*CF4/6.D0)+(F3*CF3/4.D0)+(F4*CF2/6.D0)+(F5*CF1
     + /24.D0))+(H**6)/6.*((F1*CF6/120.D0)+(F2*CF5/24.D0)+(F3*CF
     + 4/12.D0)+(F4*CF3/12.D0)+(F5*CF2/24.D0)+(F6*CF1/120.D0)
     + )+(H**7)/7.*((F2*CF6/120.D0)+(F3*CF5/48.D0)+(F4*CF4/36.D0
     + )+(F5*CF3/48.D0)+(F6*CF2/120.D0))+(H**8)/8.*((F3*CF6/240.
     + D0)+(F4*CF5/144.D0)+(F5*CF4/144.D0)+(F6*CF3/240.D0))+(
     + H**9)/9.*((F4*CF6/720.D0)+(F5*CF5/576.D0)+(F6*CF4/720.D0))
     + +(H**10)/10.*((F6*CF5/2800.D0)+(F5*CF6/2800.D0))+(H**11)/11.*(F6
     + *CF6/14400.D0))

      PR=FPR*(V1-CV1)

      INT=INT+PR
      FINT=FINT+FPR

      CC=(2./9.6364E-8)*CF1*F2
      Y1=DBLE(CC)
      Y2=DBLE(FINT)
      Y3=DBLE(INT)
```

```
      Y4=INT-Y3

      WRITE(50,19)I
      WRITE(50,20)Y4
      WRITE(50,21)Y2
      WRITE(50,22)Y1
      DER=(Y3+Y1)/Y2
      DEI=Y4/Y2
      E=E+DER
      E=E+(0.D0,1.D0)*DEI
      LAMDA=2.*DEI/6.58217E-16
      WRITE(50,*)
      WRITE(50,8) E
      WRITE(50,9)DER
      WRITE(50,10)DEI
      WRITE(50,11) LAMDA
      IF(CDABS(DER).LT.1.D-15) GOTO 66
      IF(J.GT.2) GO TO 66
      GO TO 6
66
19    FORMAT(2X,'NO. OF ITERATIONS=',I8)
20    FORMAT(2X,'INT.=',G16.9,2X,G16.9)
21    FORMAT(2X,'FINT.='G16.9,2X,G16.9)
22    FORMAT(2X,'CC   ='G16.9,2X,G16.9)
9     FORMAT(4X,'DE REAL   =',G16.9,3X,G16.9)
8     FORMAT(4X,'THE ENERGY=',G16.9,3X,G16.9)
10    FORMAT(4X,'DEIMAG.   =',G16.9,3X,G16.9)
11    FORMAT(4X,'LAMDA     =',2G16.9)
      STOP
      END
```