DONOR STATES IN A GaAs/$Ga_{1-x}Al_xAs$ QUANTUM WELL WIRE OF CIRCULAR CROSS SECTION

By

Hannington Odhiambo Oyoko

B.Sc. University of Nairobi, Kenya, 1974

M.S. Fairleigh Dickinson University, New Jersey, 1987

A THESIS

Submitted in Partial Fulfillment of the

Requirements for the Degree of

Doctor of Philosophy

(in Physics)

The Graduate School

University of Maine

May, 1991

Advisory Committee:

Peter Csavinszky, Professor of Physics, Thesis Advisor

Kenneth R. Brownstein, Professor of Physics

Richard A. Morrow, Professor of Physics

Charles W. Smith, Professor of Physics

Paul L. Goodfriend, Professor of Chemistry

Leonard M. Scarfone, Professor of Physics, University of Vermont

In presenting this thesis in partial fulfillment of the requirements for an advanced degree at the University of Maine, I agree that the Library shall make it freely available for inspection. I further agree that permission for extensive copying of this thesis for scholarly purposes may be granted by the Librarian. It is understood that any copying or publication of this thesis for financial gain shall not be allowed without my written permission.

Signature [illegible]

Date April 9, 1991.

DONOR STATES IN A $GaAs/Ga_{1-x}Al_xAs$ QUANTUM WELL WIRE OF CIRCULAR CROSS SECTION

By Hannington Odhiambo Oyoko

Thesis Advisor: Peter Csavinszky, Ph.D.

An Abstract of the Thesis Presented in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy (in Physics).

May, 1991

The present work considers the donor states in a $GaAs/Ga_{1-x}Al_xAs$ QWW of circular cross section. Several trial wave functions are used to describe the ground state of the donor impurity. Using these trial wave functions the binding energy of the donor impurity in the ground state is determined for the hydrogenic case $\epsilon(o)$, and for the non-hydrogenic case, $\epsilon(r)$.

The binding energy for the first excited state is also determined using a trial wave function which is orthogonal to the ground state trial wave function. Here again the calculation is carried out for the hydrogenic case $\epsilon(o)$, and for the non-hydrogenic case $\epsilon(r)$.

It is found that in the ground state the binding energy increases with decreasing QWW radius for both the hydrogenic ($\epsilon(o)$) and non-hydrogenic ($\epsilon(r)$) cases. However, the binding energy increases much more rapidly with QWW radius

in the non-hydrogenic than in the hydrogenic case. The spatial dielectric function leads to substantially enhanced binding energy.

For the first excited state the binding energy also increases with decreasing QWW radius but here the screening effect of $\epsilon(r)$ is negligible.

It is seen from the present work that the binding energy of a donor in a $GaAs/Ga_{1-x}Al_xAs$ increases with decreasing QWW radius and that for the ground state binding energy it is sensitive to the screening effect of $\epsilon(r)$. This is because in the first excited state the donor electron does not approach the impurity ion as closely as in the ground state.

ACKNOWLEDGMENTS

I wish to express my sincere appreciation to my advisor, Professor Peter Csavinszky for the advice and guidance he has given me over the past two and a half years. I could not have asked for more.

I would also like to express my gratitude to members of my committee, Kenneth R. Brownstein, Richard A. Morrow, Charles W. Smith, Paul L. Goodfriend and Leonard M. Scarfone. They have all given me their time, suggestions and comments whenever I called on them, which was quite often.

I would like to thank my parents for all their prayers and encouragement.

To my wife goes my heartfelt gratitude for her support, understanding and encouragement and for taking the best care of our children, Inger Achieng, Joanne Akinyi and Yuri Omondi. To her I say "Erokamano Osiepa".

I wish to express my heartfelt thanks to my three children for their understanding, love and kindness. From now on you will have all my attention.

Lastly, my thanks go to the Physics Department at the University of Maine, the faculty and staff, especially Patricia Heal, Drs. Susan McKay, Gerald Harmon, and George Krueger, and to the two very kind ladies at the Computer Center (CAPS), Eloise Kleban and Betty Johnson.

TABLE OF CONTENTS

PAGE

LIST OF TABLES

LIST OF FIGURES

I. INTRODUCTION

In recent years, the development of thin film growth techniques, such as molecular beam epitaxy [1,2,3], liquid phase epitaxy [4], and metal organic chemical vapor deposition [3,4] have made it possible to fabricate quasi-two and quasi-one dimensional structures. An example of the quasi-two dimensional structure is a GaAs layer sandwiched between two thick slabs of $Ga_{1-x}Al_xAs$. This structure is called a quantum well (QW) since the (x-dependent) discrepancy between the band gaps in the two semiconductors effectively confines a free electron to the GaAs layer. An example of the quasi-one dimensional structure is a GaAs wire of circular, rectangular or triangular cross section, embedded in a $Ga_{1-x}Al_xAs$ matrix. This structure is called a quantum well wire (QWW), and for the reason mentioned above, in this structure a free electron is confined to the GaAs wire.

An imperfection that is critical in the fabrication and performance of GaAs electronic devices is impurity substitution, where a foreign atom intentionally (by doping) or unintentionally replaces either a Ga or an As atom at a regular site. The foreign atoms may remain neutral, promote electrons as donors, acquire electrons as acceptors, or act as charge traps. The type of effect that an impurity exhibits in the GaAs lattice depends on its valence state and binding energy. Impurities lying at shallow energy levels can readily contribute to the conduction process.

The nature of impurity energy levels in a QW or in a QWW is of considerable interest. A number of potential device applications (see Sect. V.A.) such as photodetectors, fast pulse lasers, phototransistors solar cells, and fast electronic switches [4,5] are the motivating factors for research into the behavior of impurities in the QW and QWW structures.

A number of workers [4,7,8,9] have studied hydrogenic impurity states in GaAs QWW of various cross sections. Some of these workers have used variational calculations to determine the binding energy of a donor as a function of the QWW radius. In these calculations the image charges on the interfaces arising from the dielectric mismatch between GaAs and $Ga_{1-x}Al_xAs$ are neglected. In the variational calculations, a one-band spherically symmetric effective mass was assumed. This is reasonable since P. Sercel and K.J. Vahala [7] have shown that for infinite potential barrier, the effective mass of the charge carriers is independent of the QWW radius. In most of these calculations the donor impurity was located on the axis of the QWW (on-axis). Lee and Spector [8] performed a general calculation for an impurity located anywhere in the GaAs QWW but determined the binding energy only for an on-axis donor.

These binding energies of the donor have been calculated with the assumption that the depth of the potential well between GaAs and $Ga_{1-x}Al_xAs$ is infinite [8,9]. It is found in all these calculations using wires of circular cross sections that the binding energy increases as the QWW radius decreases. Calculations by Osorio, et al. [10], using a QWW of rectangular cross section, confirm this trend.

A non-hydrogenic donor in a $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ QW has been considered by Csavinszky and Elabsy both for infinite [11] and for finite [12] QW depths. In the non-hydrogenic calculations the static dielectric constant of GaAs is replaced by the spatial dielectric function of Resta [13], and Cornolti and Resta [14]. Weber et al. [15] considered a shallow on-axis hydrogenic impurity for an infinitely long QWW of rectangular cross section. These authors assumed an infinite potential barrier and replaced the static dielectric constant with the spatial dielectric function proposed by Hermanson [16]. This dielectric function is independent both of the location of the impurity and of the shape of the QWW cross section. The spatial dielectric function referred to possesses complete spherical symmetry. Weber et al. [17] have found that the effect of the spatially dependent screening of the donor ion becomes less pronounced as the impurity approaches the edges of the QWW.

In these calculations [17] they found a substantial increase in the on-axis acceptor binding energy with respect to the binding energies obtained with the static dielectric constant. The importance of the spatially dependent screening diminishes as the QWW cross section increases. This finding has its origin in the spreading out of the donor wave function. Thus, the effect of the spatially dependent dielectric function on the binding energy is important only for very small (less than 200 a.u.) QWW cross sections.

The objective of the present work is the determination of the binding energy of on-axis hydrogenic and non-hydrogenic donors in the ground and first excited states. The donor impurity is considered to be located in an infinitely long GaAs QWW of circular cross section, and the barrier potential is assumed to be infinite.

The objective stated above is achieved by using different types of trial wave functions for the ground state of hydrogenic and non-hydrogenic donors. In the case of the hydrogenic and non-hydrogenic donors in the first excited state, the trial wave function used is constructed from the sum of the ground state hydrogen atom wave function and the first excited state hydrogen atom wave function with an appropriate envelope wave function to satisfy the boundary conditions. The wave function for the first excited state is orthogonal to the ground state trial wave function.

In the present calculations the parabolic band effective mass Hamiltonian is used with $m^* = 0.067\ m_e$ [8]. The static dielectric constant used in the hydrogenic case is that of the bulk GaAs, $\epsilon(o) = 12.56$ [8], and the spatial dielectric function used is that first suggested by Hermanson [16]. The constant c represents the screening distance beyond which $\epsilon(r) = \epsilon(o)$ and is determined to be $c = 0.8$ a.u. The procedure leading to this c-value is discussed in Section A.2.

The organization of this work is as follows: Section II presents the theory; Section II.A. deals with the ground state binding energy of an on-axis donor with ordinary Bessel function as the envelope wave function. This section is divided into two parts: (1) hydrogenic donor, and (2) non-hydrogenic donor. In Section II.B., the binding energy of an on-axis donor is considered but here the envelope wave function is a spherical Bessel function. Again, this section is subdivided into two parts: (1) hydrogenic donor, and (2) non-hydrogenic donor. Section II.C. considers the binding energy of an on-axis donor but this time the envelope wave function is unity. This section is also divided into two parts: (1) hydrogenic donor, and (2) non-hydrogenic donor.

Finally, Section II.D. deals with the binding energy of an on-axis donor in the first excited state. This section is subdivided into two parts: (1) hydrogenic donor, and

(2) non-hydrogenic donor.

Section III presents the data obtained in tabular form. Section IV shows the plots of the binding energy as a function of the QWW radius for the on-axis hydrogenic and non-hydrogenic donors both in their ground and in their first excited states.

Section V is a presentation of the results and discussion of these results. Section VI gives the conclusions. Section VI consists of a brief summary of techniques used in the measurement of the binding energies of donor impurities in GaAs.

Section VII lists papers published and lectures presented which have resulted from this thesis. Literature citations by other researchers are given in Section VIII, and Section IX contains the Appendices which present the details of the calculations and discussion of the numerical integration techniques employed in this work.

II. THEORY

A. GROUND STATE DONOR IMPURITY

A.1. Ground State Binding Energy of an On-Axis Hydrogenic Donor Impurity with an Ordinary Bessel Function as the Envelope Wave Function.

In the present work, the variational method [18] is employed in calculating the ground state binding energy of an on-axis hydrogenic donor as a function of the QWW radius.

Assuming a parabolic conduction band with a corresponding scalar effective mass m* and neglecting image forces, the Hamiltonian in circular cylindrical coordinates is given by [19]

$$H = -\frac{\hbar^2}{2m*}\Delta - \frac{e^2}{\epsilon(o)\,[\rho^2 + z^2]^{1/2}} + V_B(\rho)$$

$$= -\frac{1}{2m*}\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\right] + \frac{\partial^2}{\partial z^2}\right\} - \frac{1}{\epsilon(o)[\rho^2 + z^2]^{1/2}} + V_B(\rho) \qquad \text{II-A.1}$$

after setting $\hbar^2 = 1$ and $e^2 = 1$ and where $m* = 0.0667\, m_e$ is the effective mass of an electron at the bottom of the conduction band of GaAs, $\epsilon(o) = 12.56$ is [8] the static dielectric constant of GaAs, while $V_B(\rho)$ is the potential energy barrier which confines the electron to the GaAs cylinder of radius a, such that

$$V_B(\rho) = \begin{cases} 0 & \rho < a \\ \infty & \rho > a \,. \end{cases}$$

The coordinate $\rho = (x^2 + y^2)^{\frac{1}{2}}$ measures the distance perpendicular to the axis of the QWW, and the coordinate z measures the distance along the axis of the QWW. Both ρ and z have their origin at the (point) donor ion. The geometry of the structure is illustrated in Figure 16.

The trial wave function used in the calculation, is that suggested but not used by Lee and Spector [8], namely

$$\Psi_{1s}(\rho, z) = N\, J_o(k_{10}\rho)\; e^{-\beta\sqrt{\rho^2 + z^2}} \qquad \text{II-A.2}$$

where N is the normalization constant, and β is a variational parameter. The function $J_o(k_{10}\rho)$ [20] is a Bessel function of order zero (called the envelope wave function) and argument $k_{10}\rho$. The quantity k_{10} is related [21] to the first zero of the Bessel function J_o.

In the present work, the function $J_o(k_{10}\rho)$ is replaced by $J_o(\alpha\rho)$, where $\alpha = k_{10}$ is given [22] by

$$k_{10} = \alpha = \frac{2.4048}{a}$$

Thus, when $\rho = a$

$$J_o(\alpha\rho) = J_o\left(\frac{2.4048}{a}.a\right) = J_o(2.4048) = 0$$

Similarly, when $\rho = 0$

$$J_o\left(\frac{2.4048}{a}\rho\right) = J_o(o) = 1$$

The detailed calculations of the normalization constant, and the expectation values of the kinetic, potential, and total energy operators, are given in Appendix A.

The above quantities are related by

$$< H > = < T > + < V > \qquad \text{II-A.3}$$

where $< T >$, $< V >$, and $< H >$ are, respectively, the expectation values of the kinetic, potential, and total energy operators, and are given by

$$< T > = \frac{\beta^2}{2m*} + \frac{\alpha^2}{2m*} \qquad \text{II-A.4}$$

$$< V > = - \frac{1}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho} \qquad \text{II-A.5}$$

$$< H > = \frac{\beta^2}{2m*} + \frac{\alpha^2}{2m*} - \frac{1}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho} \qquad \text{II-A.6}$$

The normalization constant is obtained from

$$N^2 = [4\pi\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho]^{-1} \qquad \text{II-A.7}$$

In Equations II-A.5 and II-A.6 the quantities K_o and K_1 are the modified Bessel functions [23] of order zero and one, respectively, and of argument $2\beta\rho$.

In the variational approach, the minimum energy, $E_{min}(a)$, is obtained by minimizing the expectation value of the total energy $< H >$ with respect to the variational parameter β,

$$\frac{\partial < H >}{\partial \beta} = 0 \qquad \text{II-A.8}$$

The minimizing value of β is then substituted back into Equation II-A.6, for a given value of the quantum well wire radius.

The expression for the expectation value of the total energy is not analytical. The minimization procedure involving β must be done numerically. The details of the numerical procedure and accuracy are given in Appendix IX.F. This procedure leads to the minimum energy $E_{min}(a)$ for each QWW radius a.

The binding energy $E_b(a,\beta)$ is then obtained by subtracting $E_{min}(a,\beta)$ from the "free" particle energy $E_{free}(a)$ [24]. $E_{free}(a)$ is the energy in the absence of the hydrogenic donor ion.

One can then write

$$E_b(a,\beta) = E_{free}(a) - E_{min}(a,\beta)$$

$$= \frac{\alpha^2}{2m*} - \{ \frac{\alpha^2}{2m*} + \frac{\beta^2}{2m*} \qquad \text{II-A.9}$$

$$- \frac{1}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho} \}$$

$$= - \frac{\beta^2}{2m*} + \frac{1}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho)} \qquad \text{II-A.10}$$

$$= - \frac{\beta^2}{2m*} + \frac{1}{\epsilon(o)} \frac{A}{B}$$

where

$$A = \int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho \qquad \text{II-A.11}$$

and

$$B = \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho . \qquad \text{II-A.12}$$

The calculation of the free particle energy $E_{free}(a)$ is given in Appendix E.

The numerical results for the binding energy $E_b(a,\beta)$, the minimizing values of the variational parameter β, and the respective QWW radius a, are presented in Table 1. The plot of $E_{min}(a,\beta)$ as a function of the QWW radius a is shown in Figure 1.

A.2. Ground State Binding Energy of an On-Axis Non-Hydrogenic Donor with an Ordinary Bessel Function as the Envelope Wave Function.

In the case of a non-hydrogenic donor in the ground state, the static dielectric constant of GaAs is replaced by the spatial dielectric function of GaAs. In the present work, the spatial dielectric function used is that suggested by Hermanson [16]. This function has recently been used by Oliveira and Falicov [17]. The analytical form of this function is

$$\frac{1}{\epsilon(r)} = \frac{1}{\epsilon(o)} + (1 - \frac{1}{\epsilon(o)}) e^{-\frac{r}{c}} \qquad \text{II-A.13}$$

The quantity $\epsilon(o)$ in Equation II-A.1 is replaced by $\epsilon(r)$ in Equation II-A.13. In Equation II-A.13, $r = \sqrt{\rho^2 + z^2}$ is the position of the electron, and c is a constant that is determined in the present work by requiring that, in the screening region, $\epsilon(r)$ should agree as well as possible with the spatial dielectric function of Resta [13]. In other words, $\epsilon(r)$ approaches 1 for small r and $\epsilon(o)$ for large r. The Fourier transform of II-A.13 also should fit the dielectric constant of GaAs, i.e., 12.56. It should also be noted that the dielectric function II-A.13 is independent of the location of the impurity in the z direction.

This goal is achieved by plotting $\epsilon(r)$ as a function of r for various values of c until the appropriate value of c is obtained. The value of c which is used in the present work is c = 0.8 $(a.u.)^{-1}$. The numerical results for $\epsilon(r)$ as a function of r are displayed in Table 15, and the graph of $\epsilon(r)$ against r is presented in Figure 15.

It can be seen from Equation II-A.13 that $\epsilon(r)$ becomes unity as the distance r from the (point) donor ion goes to zero. It is also seen from the same equation that $\epsilon(r)$ becomes $\epsilon(o)$ as the distance r from the (point) donor ion goes to about 9 a.u..

The expectation value of the total energy, < H >, is then calculated using the same method as in II-A.1. The expression for the expectation value of the total energy becomes:

$$
\begin{aligned}
\langle H' \rangle &= \langle T \rangle + \langle V' \rangle \\
&= \langle T \rangle + \langle V \rangle + \langle \Delta V \rangle \\
&= \langle H \rangle + \langle \Delta V \rangle
\end{aligned}
\qquad \text{II-A.14}
$$

$$
= \frac{\beta^2}{2m*} + \frac{\alpha^2}{2m*} - \frac{1}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho}
\qquad \text{II-A.15}
$$

$$
- \frac{(\epsilon_o - 1)}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o[(2\beta + \frac{1}{c})\rho]\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho}
$$

where < H' >, < T > and < V > have the same meaning as in II-A.4, II-A.5 and II-A.6, and < ΔV > is given by

$$\langle \Delta V \rangle = -\frac{(\epsilon(o) - 1)}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o[(2\beta + \frac{1}{C})\rho]\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho}.$$

II-A.16

The minimum energy $E_b(a,\beta)$, is then determined in a manner similar to that used for the hydrogenic donor, except that in this case there is an extra term in the potential energy due to the extra term in the dielectric function. The binding energy is then obtained by subtracting the new minimum energy $E_{min}(a,\beta)$ from the free particle energy $E_{free}(a)$.

The numerical values of $E_b(a,\beta)$, the minimizing value of β, together with the respective values of the QWW radii are presented in Table 2. A plot of $E_b(a,\beta)$ as a function of the QWW radius a, is displayed in Figure 2.

B.1. Ground State Binding Energy of an On-Axis Hydrogenic Donor with a Spherical Bessel Function as the Envelope Wave Function.

In this section, the ground state binding energy for an on-axis hydrogenic donor is calculated using (instead of the ordinary Bessel function) the spherical Bessel function [25] $j_o(\mu\rho)$.

The Hamiltonian for the total energy is the same as the one used in section II.A., that is:

$$H = -\frac{1}{2m*}\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\right] + \frac{\partial^2}{\partial z^2}\right\} - \frac{1}{\epsilon(o)\,[\rho^2 + z^2]^{1/2}} + V_B(\rho) \qquad \text{II-B.1}$$

where the terms retain their definitions as given in Equation II-A.1.

The trial wave function used in this calculation is given by

$$\Psi_{1s}(\rho, z) = N\, j_o(\mu\rho)\; e^{-\beta\sqrt{\rho^2 + z^2}} \qquad \text{II-B.2}$$

where [25]

$$j_o(\alpha\rho) = \frac{\sin\mu\rho}{\mu\rho} \qquad \text{II-B.3}$$

is the spherical Bessel function of order zero and argument $\mu\rho$, [26] where μ is given by

$$\mu = \frac{n\pi}{a} \quad , n = 1,2,3\;.\;.\;.$$

It is seen from II-B.3 that $j_o(\mu\rho)$ has the following properties:

$j_o(\mu\rho) = 0$ at $\rho = a$, i.e. at the radius of the QWW, and

$j_o(\mu\rho) = 1$ at $\rho = 0$.

The detailed calculations for the expectation value of the total energy < H > are presented in Appendix D. The expression for the expectation value of the total energy is non-analytical and the minimum energy $E_{min}(a,\beta)$ for each value of the QWW radius a is obtained by numerical techniques. The expression for the expectation value of the total energy is given by

$$< H > = < T > + < V >$$

$$= -\frac{2\pi h^2\beta^2N^2}{m*}\int_o^a \rho j_o^2(\mu\rho)K_1(2\beta\rho)\,d\rho$$

$$-\frac{2\pi N^2h^2}{m*}\int_o^a j_o^2(\mu\rho)K_1(2\beta\rho)\,d\rho$$

$$-\frac{2\pi h^2\mu N^2}{m*}\int_o^a \rho j_o(\mu\rho)\eta_o(\mu\rho)K_1(2\beta\rho)\,d\rho$$

$$-\frac{4\pi h^2\beta\mu N^2}{m*}\int_o^a \rho^2 j_o(\mu\rho)\eta_o(\mu\rho)K_o(2\beta\rho)\,d\rho$$

$$+\frac{2\pi h^2\mu^2N^2}{m*}\int_o^a \rho\, j_o^2(\mu\rho)K_1(2\beta\rho)\,d\rho$$

$$-\frac{4\pi N^2e^2}{\epsilon(o)}\int_o^a \rho\, j_o^2(\mu\rho)K_o(2\beta\rho)\,d\rho$$

II-B.4

where the normalization constant N can be expressed as

$$N^2 = \left[4\pi\int_o^a \rho^2 j_o^2(\mu\rho)K_1(2\beta\rho)\,d\rho\right]^{-1} \qquad \text{II-B.5}$$

and

$$\eta_o(\mu\rho) = -\frac{\cos\mu\rho}{\mu\rho} \qquad \text{II-B.6}$$

where $\eta_o(x)$ [26] is the spherical Neumann function of order one.

The binding energy is obtained by subtracting the minimum energy $E_{min}(a,\beta)$, obtained by minimizing < H > with respect to β, from the free particle energy $E_{free}(a)$. The result is a long complicated expression:

$$E_b(a,\beta) = \frac{h^2\alpha^2}{2m*} - \left\{ \frac{2\pi h^2\beta^2 N^2}{m*} \int_o^a \rho\, j_o^2(\mu\rho) K_1(2\beta\rho)\, d\rho \right.$$

$$- \frac{2\pi h^2 N^2}{m*} \int_o^a j_o^2(\mu\rho) K_1(2\beta\rho)\, d\rho$$

$$- \frac{2\pi h^2 \mu N^2}{m*} \int_o^a \rho\, j_o(\mu\rho) \eta_o(\mu\rho) K_1(2\beta\rho)\, d\rho$$

$$+ \frac{2\pi h^2 \mu^2 N^2}{m*} \int_o^a \rho\, j_o^2(\mu\rho) K_1(2\beta\rho)\, d\rho$$

$$- \frac{4\pi h^2 \beta\mu N^2}{m*} \int_o^a \rho^2\, j_o(\mu\rho) \eta_o(\mu\rho) K_o(2\beta\rho)\, d\rho$$

$$\left. - \frac{4\pi N^2 e^2}{\epsilon(o)} \int_o^a \rho\, j_o^2(\mu\rho) K_o(2\beta\rho)\, d\rho \right\} \qquad \text{II-B.7}$$

B.2. Ground State Binding Energy for an On-Axis Non-Hydrogenic Donor with a Spherical Bessel Function as the Envelope Wave Function.

As in II-A.2, the static dielectric constant $\epsilon(o)$ is replaced by the spatial dielectric function $\epsilon(r)$, which is given by Equation II-A.13 as

$$\frac{1}{\epsilon(o)} = \frac{1}{\epsilon(o)} + \left(1 - \frac{1}{\epsilon(o)}\right) e^{-\frac{r}{c}} \qquad \text{II-A.13}$$

The expectation value of the total energy now has an extra term compared with the hydrogenic donor case of Equation II-B.7. This expression is now given by

$$
\begin{aligned}
\langle H \rangle = & - \frac{2\pi h^2 \beta^2 N^2}{2m*} \int_o^a \rho \, j_o^2(\mu\rho) K_1(2\beta\rho) \, d\rho \\
& - \frac{2\pi h^2 N^2}{m*} \int_o^a j_o^2(\mu\rho) K_1(2\beta\rho) \, d\rho \\
& - \frac{2\pi h^2 \mu N^2}{m*} \int_o^a \rho \, j_o(\mu\rho) \eta_o(\mu\rho) K_1(2\beta\rho) \, d\rho \\
& + \frac{2\pi h^2 \mu^2 N^2}{m*} \int_o^a \rho \, j_o^2(\mu\rho) K_1(2\beta\rho) \, d\rho \\
& - \frac{4\pi h^2 \beta \mu N^2}{m*} \int_o^a \rho^2 \, j_o(\mu\rho) \eta_o(\mu\rho) K_o(2\beta\rho) \, d\rho \\
& - \frac{4\pi N e^2}{\epsilon(o)} \int_o^a \rho \, j_o^2(\mu\rho) K_o(2\beta\rho) \, d\rho \\
& - \frac{4\pi N^2 e^2 [\epsilon(o) - 1]}{\epsilon(o)} \int_o^a \rho \, j_o^2(\mu\rho) K_o[(2\beta + \frac{1}{c})\rho] \, d\rho
\end{aligned}
$$

II-B.8

The minimum energy is obtained by numerical methods. The result, $E_{min}(a,\beta)$, is then subtracted from the free particle energy $E_{free}(a)$ to obtain the binding energy $E_b(a,\beta)$. The numerical results for $E_b(a,\beta)$, the minimizing values of β, and the respective QWW radii a are displayed in Table 5. A plot of $E_b(a,\beta)$ as a function of the QWW radius a is presented in Figure 5.

C.1. Ground State Binding Energy of an On-Axis Hydrogenic Donor with an Envelope Wave Function of Unity.

The wave function used here is that of a simple isolated hydrogen atom embedded in a GaAs cylinder surrounded by a $Ga_{1-x}Al_xAs$ matrix. The wave function does not vanish at the boundary, namely at $\rho = a$, but is finite at $\rho = 0$. This is a drawback in this choice of trial wave function.

The Hamiltonian used is the same as that in Equation II-A.1, i.e.,

$$H = -\frac{1}{2m*}\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial z^2}\right\} - \frac{1}{\epsilon(o)\,[\rho^2 + z^2]^{1/2}} + V_B(\rho)$$

II-A.1

The trial wave function is given by

$$\Psi_{1s}(\rho, z) = N\, e^{-\beta\sqrt{\rho^2 + z^2}} \qquad \text{II-C.1}$$

The expectation value of the total energy is obtained by determining the expectation value of < H >. The details of the calculations are presented in Appendix C.

The result is given by

$$\langle H \rangle = -\frac{h\beta^2}{m*} - \frac{\int_o^a \rho K_o(2\beta\rho)\,d\rho}{\int_o^a \rho^2 K_1(2\beta\rho)\,d\rho} \qquad \text{II-C.2}$$

This is a non-analytical expression and the minimization is carried out using numerical techniques.

C.2. Ground State Binding Energy of an On-Axis Non-Hydrogenic Donor with an Envelope Wave Function of Unity.

The spatial dielectric constant in Eq. II-A.1 is replaced by the spatial dielectric function

$$\frac{1}{\epsilon(r)} = \frac{1}{\epsilon(o)} + \left(1 - \frac{1}{\epsilon(o)}\right)\exp\left[-\frac{1}{c}\sqrt{\rho^2 + z^2}\right]. \quad \text{II-A.13}$$

The resulting expression for the expectation value of the total energy is again non-analytical and the minimum energy is determined numerically from

$$\langle H' \rangle = \frac{\beta^2}{2m*} - \frac{1}{\epsilon(o)} \frac{\int_o^a \rho K_o(2\beta\rho)\,d\rho}{\int_o^a \rho^2 K_1(2\beta\rho)\,d\rho} - \frac{(\epsilon(o) - 1)}{\epsilon(o)} \frac{\int_o^a \rho K_o[(2\beta + \frac{1}{c})\rho]\,d\rho}{\int_o^a \rho^2 K_1(2\beta\rho)\,d\beta} \quad \text{II-C.3}$$

With the above expression, the binding energy becomes

$$E_b(a,\beta) = \frac{\alpha^2}{2m*} - \left\{ + \frac{\beta}{2m*} - \frac{1}{\epsilon(o)} \frac{\int_o^a \rho K_o(2\beta\rho)\,d\rho}{\int_o^a \rho^2 K_1(2\beta\rho)\,d\rho} - \frac{(\epsilon(o) - 1)}{\epsilon(o)} \frac{\int_o^a \rho K_o[(2\beta + \frac{1}{c})\rho]\,d\rho}{\int_o^a \rho^2 K_1(2\beta\rho)\,d\rho} \right\} \quad \text{II-C.4}$$

The numerical results for $E_b(a,\beta)$, β, as function of the QWW radius a are presented in Table 8, while a plot of the binding energy $E_b(a,\beta)$ as a function of the QWW radius a is shown in Figure 8.

D.1. Binding Energy of the First Excited State of an On-Axis Hydrogenic Donor Impurity with J_o as the Envelope Wave Function.

In this section the first excited state binding energy of an on-axis hydrogenic donor is calculated. The Hamiltonian is the same as in Equation II-A.1, and the quantities are as defined in Section II.A.1:

$$H = -\frac{1}{2m*}\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\right]+\frac{\partial^2}{\partial z^2}\right\} - \frac{1}{\epsilon(o)}\left[\rho^2+z^2\right]^{-1/2}+V_B(\rho) \qquad \text{II.A.1}$$

The trial wave function is given by

$$\Psi_{2s}(\rho,z) = NJ_o(\alpha\rho)\left[e^{-\beta\sqrt{\rho^2+z^2}}+K\left[2-\lambda\sqrt{\rho^2+z^2}\right]e^{-\lambda\sqrt{\rho^2+z^2}}\right] \qquad \text{II-D.1}$$

Here K is an orthogonality constant and λ is a variational parameter which is determined when the minimization of the expectation value of the total energy is done. This expectation value is given by

$$\langle H \rangle = \langle \psi_{2s} \mid H \mid \psi_{2s} \rangle \qquad \text{II-D.2}$$

The expression is very long and is given in Appendix E. The expectation value of the total energy is then minimized to obtain $E_{min}(a,\lambda)$ and the result is subtracted from the free particle energy $E_{free}(a)$ to obtain the binding energy $E_b(a,\beta)$. Most of the integrals in the expectation value of the total energy are non-analytical and therefore have been evaluated numerically.

D.2. Binding Energy of the First Excited State of an On-Axis Non-Hydrogenic Donor.

The Hamiltonian for the expectation value of the total energy now has an extra term and is given by

$$H = - \frac{1}{2m*} \left\{ \frac{1}{\rho} \frac{\partial}{\partial \rho} \left[\rho \frac{\partial}{\partial \rho} \right] + \frac{\partial^2}{\partial z^2} \right\} - \frac{1}{\epsilon(o) \, [\rho^2 + z^2]^{1/2}}$$

$$- \frac{[\epsilon(o) - 1]}{\epsilon(o) \, [\rho^2 + z^2]^{1/2}} \, e^{-\frac{\sqrt{\rho^2 + z^2}}{c}} + V_B(\rho)$$

II-D.3

The expectation value is given by

$$< H > = < \psi_{2s} \mid H' \mid \psi_{2s} >$$

$$= < \psi_{2s} \mid H \mid \psi_{2s} > + < \psi_{2s} \mid \Delta V \mid \psi_{2s} >$$

II-D.4

The extra term in the expectation value of the total energy is due to the spatial dielectric function which has been substituted for the static dielectric constant.

Again, the expression for the expectation value of the total energy is non-analytical and the rest of the calculations are done numerically. The expression is given in Appendix E.

The minimum value of the expectation value of the total energy, $E_{min}(a,\lambda)$, is subtracted from the free particle energy $E_f(a)$ and the result is the binding energy $E_b(a,\lambda)$. In sections D.1 and D.2 the parameter β is determined by the technique presented in section A.

III. TABLE CAPTIONS

The extensive numerical results of this study are presented in this chapter as a sequence of tables. The unit of the QWW radius is the atomic unit, (a_o), those of the variational parameters β and λ are the inverse atomic unit, (a_o^{-1}) and the binding energy is given in millielectron volts, meV.

Table 1. This table shows the results for the on-axis hydrogenic donor with an ordinary Bessel function as the envelope wave function.

Table 2. This table shows the results for the non-hydrogenic on-axis donor with an ordinary Bessel function as the envelope wave function.

Table 3. This summary table shows data from Tables 1 and 2 on the same page for comparison.

Table 4. This table shows the results obtained with the spherical Bessel function as the envelope wave function for an on-axis hydrogenic donor.

Table 5. This table shows the results for the spherical Bessel function as the envelope wave function for the non-hydrogenic donor.

Table 6. This table shows the results for the hydrogenic and non-hydrogenic for comparison in the spherical Bessel function case.

Table 7. This table shows the results for the unit envelope wave function.

Table 8. This table shows the results for the case of non-hydrogenic donor with unit envelope wave function.

Table 9. This table shows the data for the hydrogenic and non-hydrogenic donor with unit envelope wave function.

Table 10. This table shows the results for the 2s excited state hydrogenic donor with the ordinary Bessel function as the envelope wave function.

Table 11. This table shows the results for the non-hydrogenic donor in its first excited (2s) state with the ordinary Bessel function as the envelope wave function.

Table 12. This table shows the results for the hydrogenic and non-hydrogenic donors in the first excited states.

Table 13. This table shows results for the ground state and first excited state hydrogenic donors (with an ordinary Bessel function as the envelope wave function).

Table 14. This table shows the results for the non-hydrogenic ground state and first excited state with the ordinary Bessel function as the envelope wave function.

Table 15. This table shows the data used [17] in the determination of c = 0.8 in the spatial dielectric function.

TABLE 1

a (a.u.)	$\beta \times 10^{-2}$ (a.u.)$^{-1}$	$E_b(a,\beta)$ (meV)
5.0	1.963	158.51
10.0	1.556	118.55
20.0	1.207	73.63
30.0	1.035	57.48
40.0	0.926	47.96
50.0	0.852	41.55
60.0	0.792	36.91
70.0	0.747	33.35
80.0	0.710	30.53
90.0	0.680	28.22
100.0	0.654	26.30
120.0	0.613	23.27
140.0	0.582	20.98
160.0	0.557	19.18
180.0	0.537	17.73
200.0	0.521	16.52
300.0	0.474	12.67
400.0	0.456	10.59
500.0	0.452	9.30
600.0	0.456	8.45
700.0	0.463	7.85
800.0	0.472	7.43
1000.0	0.488	6.88

TABLE 2

a (a.u.)	$\beta \times 10^{-2}$ (a.u.)$^{-1}$	$E_b(a,\beta)$ (meV)
5.0	3.219	343.73
10.0	1.918	147.44
20.0	1.306	81.07
30.0	1.080	60.38
40.0	0.953	49.45
50.0	0.868	42.45
60.0	0.806	37.50
70.0	0.757	33.77
80.0	0.719	30.84
90.0	0.687	28.46
100.0	0.660	26.49
120.0	0.618	23.40
140.0	0.585	21.08
160.0	0.560	19.25
180.0	0.539	17.76
200.0	0.523	16.55
300.0	0.574	12.68
400.0	0.456	10.59
500.0	0.452	9.31
600.0	0.456	8.45
700.0	0.464	7.86
800.0	0.473	7.43
1000.0	0.489	6.90

TABLE 3

HYDROGENIC DONOR			NON-HYDROGENIC DONOR	
a (a.u.)	$\beta \times 10^{-2}$ $(a.u.)^{-1}$	$E_b(a,\beta)$ (meV)	$\beta \times 10^{-2}$ $(a.u.)^{-1}$	$E_b(a,\beta)$ (meV)
5.0	1.963	158.51	3.219	343.73
10.0	1.556	118.55	1.918	147.44
20.0	1.207	73.63	1.306	81.07
30.0	1.035	57.48	1.080	60.38
40.0	0.926	47.96	0.953	49.45
50.0	0.852	41.55	0.868	42.45
60.0	0.792	36.91	0.806	37.50
70.0	0.747	33.35	0.757	33.77
80.0	0.710	30.53	0.719	30.84
90.0	0.680	28.22	0.687	28.46
100.0	0.654	26.30	0.660	26.49
120.0	0.613	23.27	0.618	23.40
140.0	0.582	20.98	0.585	21.08
160.0	0.557	19.18	0.560	19.25
180.0	0.537	17.73	0.539	17.76
200.0	0.521	16.52	0.523	16.55
300.0	0.474	12.67	0.574	12.68
400.0	0.456	10.59	0.456	10.59
500.0	0.452	9.30	0.452	9.31
600.0	0.456	8.45	0.456	8.45
700.0	0.463	7.85	0.464	7.86
800.0	0.472	7.43	0.473	7.43
1000.0	0.488	6.88	0.489	6.90

TABLE 4

a (a.u.)	$\beta \times 10^{-3}$ (a.u.)$^{-1}$	$E_b(a,\beta)$ (meV)
20.0	6.026	1911.55
30.0	5.602	1015.40
40.0	5.217	618.37
50.0	4.910	418.02
60.0	4.656	302.99
70.0	4.446	230.89
80.0	4.257	182.68
90.0	4.091	148.80
100.0	3.957	124.04
120.0	3.728	90.95
140.0	3.539	70.35
160.0	3.386	56.60
180.0	3.252	46.93
200.0	3.144	39.84
300.0	2.767	22.03
400.0	2.551	15.08
500.0	2.423	11.53
600.0	2.341	9.52
700.0	2.288	7.90
800.0	2.257	7.06
1000.0	2.272	5.80

TABLE 5

a (a.u.)	$\beta \times 10^{-3}$ (a.u.)$^{-1}$	$E_b(a,\beta)$ (meV)
20.0	6.356	1969.64
30.0	5.754	1016.61
40.0	5.306	619.17
50.0	4.970	418.43
60.0	4.697	303.26
70.0	4.473	231.09
80.0	4.277	182.82
90.0	4.116	148.91
100.0	3.975	124.16
120.0	3.740	90.01
140.0	3.550	70.39
160.0	3.390	56.63
180.0	3.260	46.96
200.0	3.150	39.86
300.0	2.770	22.04
400.0	2.555	15.08
500.0	2.425	11.53
600.0	2.340	9.41
700.0	2.290	8.03
800.0	2.260	7.06
1000.0	2.245	5.80

TABLE 6

HYDROGENIC DONOR			NON-HYDROGENIC DONOR	
a (a.u.)	$\beta \times 10^{-2}$ $(a.u.)^{-1}$	$E_b(a,\beta)$ (meV)	$\beta \times 10^{-2}$ $(a.u.)^{-1}$	$E_b(a,\beta)$ (meV)
20.0	6.026	1911.55	6.356	1969.64
30.0	5.602	1015.40	5.754	1016.61
40.0	5.217	618.37	5.306	619.17
50.0	4.910	418.02	4.970	418.43
60.0	4.656	302.99	4.697	303.26
70.0	4.446	230.89	4.473	231.09
80.0	4.257	182.68	4.277	182.82
90.0	4.091	148.80	4.116	148.91
100.0	3.957	121.04	3.975	124.16
120.0	3.728	90.95	3.740	91.01
140.0	3.539	70.35	3.550	70.39
160.0	3.386	56.60	3.90	56.63
180.0	3.252	46.93	3.260	46.96
200.0	3.144	39.84	3.150	39.86
300.0	2.767	22.03	2.770	22.04
400.0	2.551	15.08	2.555	15.08
500.0	2.423	11.53	2.425	11.53
600.0	2.341	9.52	2.340	9.41
700.0	2.288	7.90	2.290	8.03
800.0	2.257	7.06	2.260	7.06
1000.0	2.272	5.80	2.45	5.80

TABLE 7

a (a.u.)	$\beta \times 10^{-3}$ (a.u.)$^{-1}$	$E_b(a,\beta)$ (meV)
20.0	9.761	787.10
30.0	8.268	367.11
40.0	7.333	217.26
50.0	6.696	146.45
60.0	6.219	107.15
70.0	5.841	82.91
80.0	5.542	66.81
90.0	5.284	55.52
100.0	5.085	47.25
120.0	4.746	36.12
140.0	4.468	29.08
160.0	4.328	24.30
180.0	4.169	20.88
200.0	4.069	18.32
300.0	3.831	11.62
400.0	3.990	8.86
500.0	4.408	7.51
600.0	4.484	6.82
700.0	5.105	6.47
800.0	5.224	6.27
1000.0	5.304	6.07

TABLE 8

a (a.u.)	$\beta \times 10^{-3}$	$E_b(a,\beta)$ (meV)
20.0	9.980	788.47
30.0	8.837	367.65
40.0	7.393	217.54
50.0	6.736	146.71
60.0	6.239	107.25
70.0	5.861	82.98
80.0	5.562	66.87
90.0	5.303	55.57
100.0	5.105	47.29
120.0	4.766	36.14
140.0	4.525	29.10
160.0	4.328	24.32
180.0	4.189	20.87
200.0	4.070	18.33
300.0	3.831	11.62
400.0	3.990	8.87
500.0	4.428	7.51
600.0	4.846	6.83
700.0	5.104	5.88
800.0	5.241	5.82
1000.0	5.3515	6.08

TABLE 9

HYDROGENIC DONOR			NON-HYDROGENIC DONOR	
a (a.u.)	$\beta \times 10^{-3}$ $(a.u.)^{-1}$	$E_b(a,\beta)$ (meV)	$\beta \times 10^{-3}$	$E_b(a,\beta)$ (meV)
20.0	9.761	787.10	9.980	788.47
30.0	8.268	367.11	8.837	367.65
40.0	7.333	217.26	7.393	217.54
50.0	6.696	146.45	6.736	146.71
60.0	6.219	107.15	6.239	107.25
70.0	5.841	82.91	5.861	82.98
80.0	5.542	66.81	5.562	66.87
90.0	5.284	55.52	5.303	55.57
100.0	5.085	47.25	5.105	47.29
120.0	4.746	36.12	4.766	36.14
140.0	4.468	29.08	4.525	29.10
160.0	4.328	24.30	4.328	24.32
180.0	4.169	20.88	4.189	20.87
200.0	4.069	18.32	4.070	18.33
300.0	3.831	11.62	3.831	11.62
400.0	3.990	8.86	3.990	8.87
500.0	4.408	7.51	4.428	7.51
600.0	4.484	6.82	4.846	6.83
700.0	5.105	6.47	5.104	5.88
800.0	5.224	6.27	5.241	5.82
1000.0	5.304	6.07	5.3515	6.08

TABLE 10

a (a.u.)	$\lambda \times 10^{-2}$ (a.u.)$^{-1}$	$E_b(a,\lambda)$ (meV)
20.0	0.6875	735.42
30.0	0.5940	327.86
40.0	0.5330	185.12
50.0	0.4900	119.03
60.0	0.4543	83.10
70.0	0.4256	61.40
80.0	0.4023	47.31
90.0	0.3826	37.64
100.0	0.3656	30.84
120.0	0.3379	21.68
140.0	0.3164	16.23
160.0	0.2994	12.67
180.0	0.2851	10.23
200.0	0.2735	8.49
300.0	0.2338	4.35
400.0	0.2128	2.91
500.0	0.1993	2.26
600.0	0.1895	1.91
700.0	0.1816	1.70
800.0	0.1748	1.53
1000.0	0.1619	1.27

TABLE 10

a (a.u.)	$\lambda \times 10^{-2}$ (a.u.)$^{-1}$	$E_b(a,\lambda)$ (meV)
20.0	0.6875	735.42
30.0	0.5940	327.86
40.0	0.5330	185.12
50.0	0.4900	119.03
60.0	0.4543	83.10
70.0	0.4256	61.40
80.0	0.4023	47.31
90.0	0.3826	37.64
100.0	0.3656	30.84
120.0	0.3379	21.68
140.0	0.3164	16.23
160.0	0.2994	12.67
180.0	0.2851	10.23
200.0	0.2735	8.49
300.0	0.2338	4.35
400.0	0.2128	2.91
500.0	0.1993	2.26
600.0	0.1895	1.91
700.0	0.1816	1.70
800.0	0.1748	1.53
1000.0	0.1619	1.27

TABLE 11

a (a.u.)	$\lambda \times 10^{-2}$ (a.u.)$^{-1}$	$E_b(a,\lambda)$ (meV)
20.0	0.7459	735.96
30.0	0.62112	328.11
40.0	0.54938	185.28
50.0	0.49971	119.13
60.0	0.46170	83.17
70.0	0.43155	61.46
80.0	0.40683	47.36
90.0	0.38638	37.68
100.0	0.36882	30.76
120.0	0.34040	21.71
140.0	0.31860	16.24
160.0	0.301100	12.69
180.0	0.28621	10.25
200.0	0.27404	8.50
300.0	0.27197	4.95
400.0	0.21309	2.92
500.0	0.19934	2.26
600.0	0.18957	1.92
700.0	0.182045	1.70
800.0	0.17520	1.54
1000.0	0.16225	1.27

TABLE 12

HYDROGENIC DONOR			NON-HYDROGENIC DONOR	
a (a.u.)	$\lambda \times 10^{-3}$ $(a.u.)^{-1}$	$E_b(a,\lambda)$ (meV)	$\lambda \times 10^{-3}$ $(a.u.)^{-1}$	$E_b(a,\lambda)$ (meV)
20.0	6.87	735.42	7.46	735.96
30.0	5.94	327.86	6.21	328.11
40.0	5.33	185.12	5.49	185.28
50.0	4.90	119.03	4.99	119.13
60.0	4.54	83.10	4.62	83.17
70.0	4.26	61.40	4.32	61.46
80.0	4.02	47.31	4.68	47.36
90.0	3.83	37.64	3.86	37.68
100.0	3.66	30.84	3.69	30.76
120.0	3.38	21.68	3.40	21.71
140.0	3.16	16.23	3.18	16.24
160.0	2.99	12.67	3.11	12.69
180.0	2.85	10.23	2.86	10.25
200.0	2.73	8.49	2.74	8.50
300.0	2.34	4.35	2.72	4.95
400.0	2.13	2.91	2.13	2.92
500.0	1.99	2.26	1.99	2.26
600.0	1.89	1.91	1.89	1.92
700.0	1.82	1.70	1.82	1.70
800.0	1.75	1.53	1.75	1.54
1000.0	1.62	1.27	1.62	1.27

TABLE 12

HYDROGENIC DONOR			NON-HYDROGENIC DONOR	
a (a.u.)	$\lambda \times 10^{-3}$ $(a.u.)^{-1}$	$E_b(a,\lambda)$ (meV)	$\lambda \times 10^{-3}$ $(a.u.)^{-1}$	$E_b(a,\lambda)$ (meV)
20.0	6.87	735.42	7.46	735.96
30.0	5.94	327.86	6.21	328.11
40.0	5.33	185.12	5.49	185.28
50.0	4.90	119.03	4.99	119.13
60.0	4.54	83.10	4.62	83.17
70.0	4.26	61.40	4.32	61.46
80.0	4.02	47.31	4.68	47.36
90.0	3.83	37.64	3.86	37.68
100.0	3.66	30.84	3.69	30.76
120.0	3.38	21.68	3.40	21.71
140.0	3.16	16.23	3.18	16.24
160.0	2.99	12.67	3.11	12.69
180.0	2.85	10.23	2.86	10.25
200.0	2.73	8.49	2.74	8.50
300.0	2.34	4.35	2.72	4.95
400.0	2.13	2.91	2.13	2.92
500.0	1.99	2.26	1.99	2.26
600.0	1.89	1.91	1.89	1.92
700.0	1.82	1.70	1.82	1.70
800.0	1.75	1.53	1.75	1.54
1000.0	1.62	1.27	1.62	1.27

TABLE 13

GROUND STATE HYDROGENIC DONOR			1ST EXCITED STATE HYDROGENIC DONOR	
a (a.u.)	$\beta \times 10^{-2}$ $(a.u.)^{-1}$	$E_b(a,\beta)$ (meV)	$\lambda \times 10^{-2}$ $(a.u.)^{-1}$	$E_b(a,\lambda)$ (meV)
5.0	1.963	158.51		
10.0	1.556	118.55		
20.0	1.207	73.63	0.6875	735.42
30.0	1.035	57.48	0.5940	327.86
40.0	0.926	47.96	0.5330	185.12
50.0	0.852	41.55	0.4900	119.03
60.0	0.792	36.91	0.4543	83.10
70.0	0.747	33.35	0.4256	61.40
80.0	0.710	30.53	0.4023	47.31
90.0	0.680	28.22	0.3826	37.64
100.0	0.654	26.30	0.3656	30.84
120.0	0.613	23.27	0.3379	21.68
140.0	0.582	20.98	0.3164	16.23
160.0	0.557	19.18	0.2994	12.67
180.0	0.537	17.73	0.2851	10.23
200.0	0.521	16.52	0.2735	8.49
300.0	0.474	12.67	0.2338	4.35
400.0	0.456	10.59	0.2128	2.91
500.0	0.452	9.30	0.1993	2.26
600.0	0.456	8.45	0.1895	1.91
700.0	0.463	7.85	0.1816	1.70
800.0	0.472	7.43	0.1748	1.53
1000.0	0.488	6.88	0.1619	1.27

TABLE 13

GROUND STATE HYDROGENIC DONOR			1ST EXCITED STATE HYDROGENIC DONOR	
a (a.u.)	$\beta \times 10^{-2}$ $(a.u.)^{-1}$	$E_b(a,\beta)$ (meV)	$\lambda \times 10^{-2}$ $(a.u.)^{-1}$	$E_b(a,\lambda)$ (meV)
5.0	1.963	158.51		
10.0	1.556	118.55		
20.0	1.207	73.63	0.6875	735.42
30.0	1.035	57.48	0.5940	327.86
40.0	0.926	47.96	0.5330	185.12
50.0	0.852	41.55	0.4900	119.03
60.0	0.792	36.91	0.4543	83.10
70.0	0.747	33.35	0.4256	61.40
80.0	0.710	30.53	0.4023	47.31
90.0	0.680	28.22	0.3826	37.64
100.0	0.654	26.30	0.3656	30.84
120.0	0.613	23.27	0.3379	21.68
140.0	0.582	20.98	0.3164	16.23
160.0	0.557	19.18	0.2994	12.67
180.0	0.537	17.73	0.2851	10.23
200.0	0.521	16.52	0.2735	8.49
300.0	0.474	12.67	0.2338	4.35
400.0	0.456	10.59	0.2128	2.91
500.0	0.452	9.30	0.1993	2.26
600.0	0.456	8.45	0.1895	1.91
700.0	0.463	7.85	0.1816	1.70
800.0	0.472	7.43	0.1748	1.53
1000.0	0.488	6.88	0.1619	1.27

TABLE 14

GROUND STATE NON-HYDROGENIC DONOR			1ST EXCITED STATE NON-HYDROGENIC DONOR	
a $(a.u.)^{-1}$	$\beta \times 10^{-2}$ $(a.u.)^{-1}$	$E_b(a,\beta)$ (meV)	$\lambda \times 10^{-2}$ $(a.u.)^{-1}$	$E_b(a,\lambda)$ (meV)
5.0	3.219	343.73		
10.0	1.918	147.44		
20.0	1.306	81.07	0.7459	735.96
30.0	1.080	60.38	0.6211	328.11
40.0	0.953	49.45	0.5494	185.28
50.0	0.868	42.45	0.4997	119.13
60.0	0.806	37.50	0.4617	83.17
70.0	0.757	33.77	0.4315	61.46
80.0	0.719	30.84	0.4068	47.38
90.0	0.687	28.46	0.3864	37.68
100.0	0.660	26.49	0.3688	38.76
120.0	0.618	23.40	0.3404	21.71
140.0	0.585	21.08	0.3186	16.28
160.0	0.560	19.25	0.3011	12.68
180.0	0.539	17.76	0.2862	10.25
200.0	0.523	16.55	0.2740	8.50
300.0	0.474	12.68	0.2719	4.95
400.0	0.456	10.59	0.2131	2.92
500.0	0.452	9.31	0.1993	2.26
600.0	0.456	8.45	0.1896	1.92
700.0	0.464	7.86	0.1820	1.70
800.0	0.473	7.43	0.1752	1.54
1000.0	0.489	6.90	0.1622	1.27

TABLE 15

$c = 0.8$

r	ϵ(r)
0.0	1.0
0.25	1.3280497
0.50	1.747448
0.75	2.2724965
1.00	2.91280
1.25	3.66918
1.50	4.5297
1.75	5.468
2.00	6.4446
2.50	8.3294
3.00	9.87526
3.50	10.96446
4.00	11.6523877
4.50	12.057308
5.00	12.2858288
5.50	12.41174
6.00	12.4802058
6.50	12.5171628
7.00	12.5370344
7.50	12.547696998
8.00	12.553411678
9.00	12.55811
10.00	12.5594589
12.00	12.55995558

IV. FIGURE CAPTIONS

The following figures show the plots of the data given in the tables Chapter III. The same system of units is employed, that is the unit of the QWW radius is the atomic unit, (a_o), those of the variational parameters β, and λ the inverse atomic unit, (a_o^{-1}) and the binding energy is in meV.

Figure 1. This figure shows the plot of the results for the on-axis ground state hydrogenic donor with an ordinary Bessel function as an envelope wave function.

Figure 2. This figure shows the plot of the results for the on-axis ground state non-hydrogenic donor with an ordinary Bessel function as the envelope wave function.

Figure 3. This figure shows the plot of the results of the on-axis ground state hydrogenic and non-hydrogenic donors with an ordinary Bessel function as the envelope wave function.

Figure 4. This figure shows the plot of the results of the on-axis ground state hydrogenic donor with a spherical Bessel function as the envelope wave function.

Figure 5. This figure shows the plot of the results of the on-axis ground state non-hydrogenic donor with a spherical Bessel functions as the envelope wave function.

Figure 6. This summary figure compares the plots of the results of Tables 5 and 6.

Figure 7. This figure shows the plot of the results for on-axis ground state hydrogenic donor with unit envelope wave function.

Figure 8. This figure shows the plot of the results for on-axis ground state non-hydrogenic donor with unit envelope wave function.

Figure 9. Figure 9 compares the plots of the results of Table 8 and 9.

Figure 10. This figure shows the plot of the results of the on-axis first excited state of a hydrogenic donor.

Figure 11. Figure 11 shows the plot of the results of the on-axis first excited state of a non-hydrogenic donor.

Figure 12. This figure shows the comparative plot of the data of Table 11 and 12.

Figure 13. This figure shows the plot of the data of Table 2 and Table 11.

Figure 14. Figure 14 shows the plot of the data of Tables 2 and 12.

Figure 15. This figure shows the plot of the data obtained in the determination of c = 0.8 for the spatial dielectric function [17].

Figure 16. Figure 16 shows the geometrical configuration of the quantum well wire studied in this thesis.

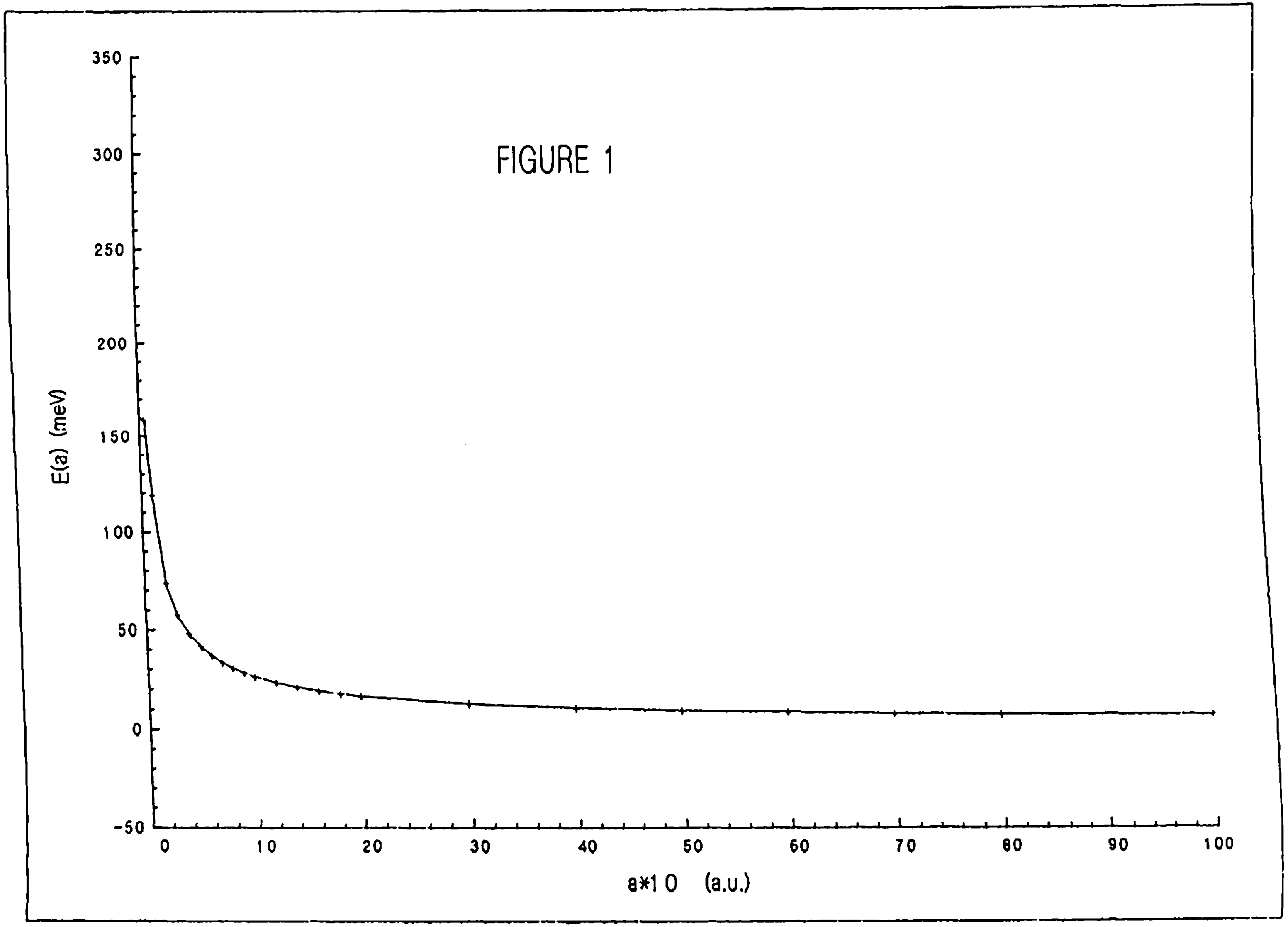

350
300
250
200
150
100
50
0
-50
E(a) (meV)
0
10
20
30
40
50
60
70
80
90
100
a*10 (a.u.)

FIGURE 1

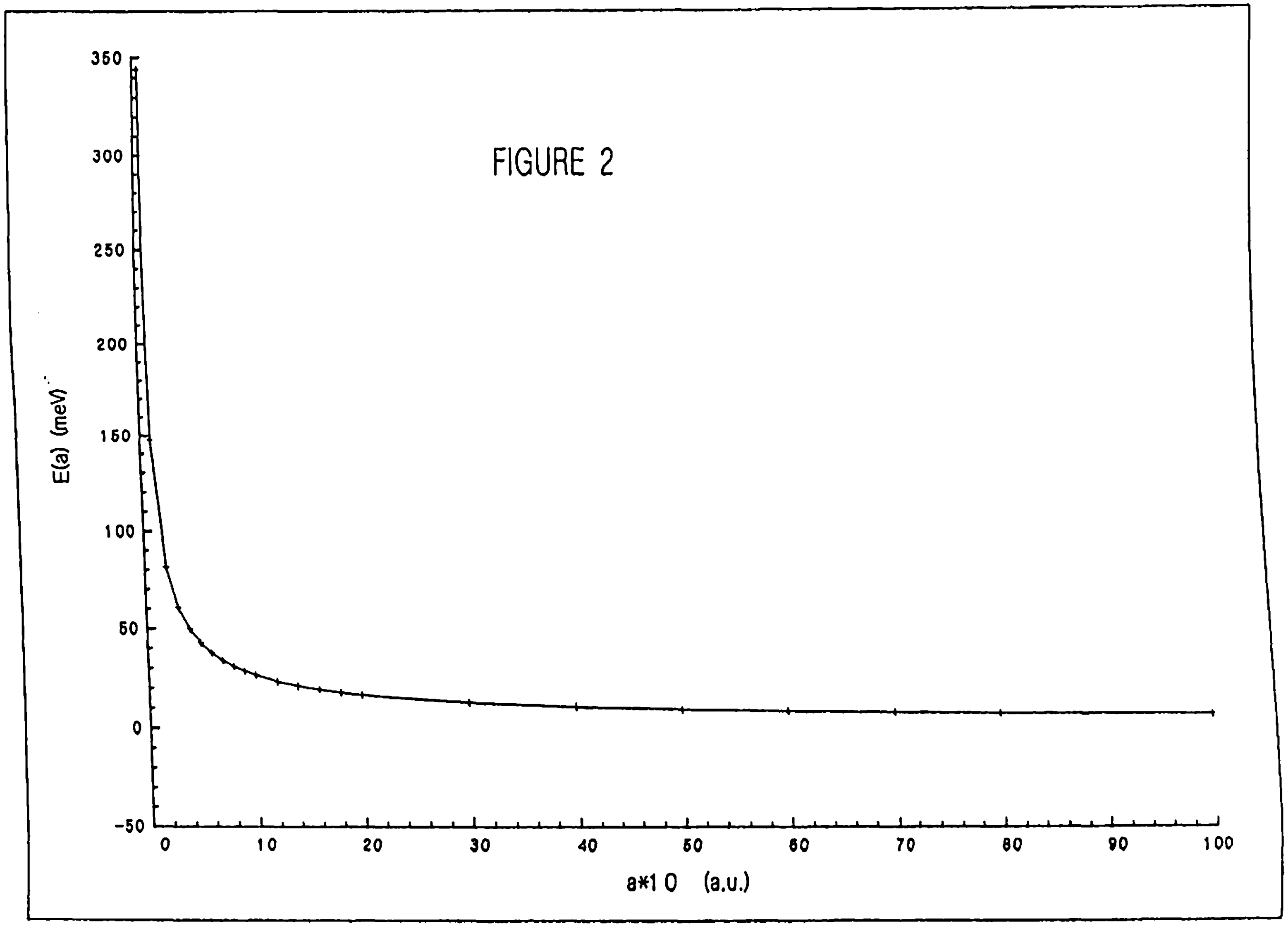

E(a) (meV)
350
300
250
200
150
100
50
0
-50
0
10
20
30
40
50
60
70
80
90
100
a*10 (a.u.)

FIGURE 2

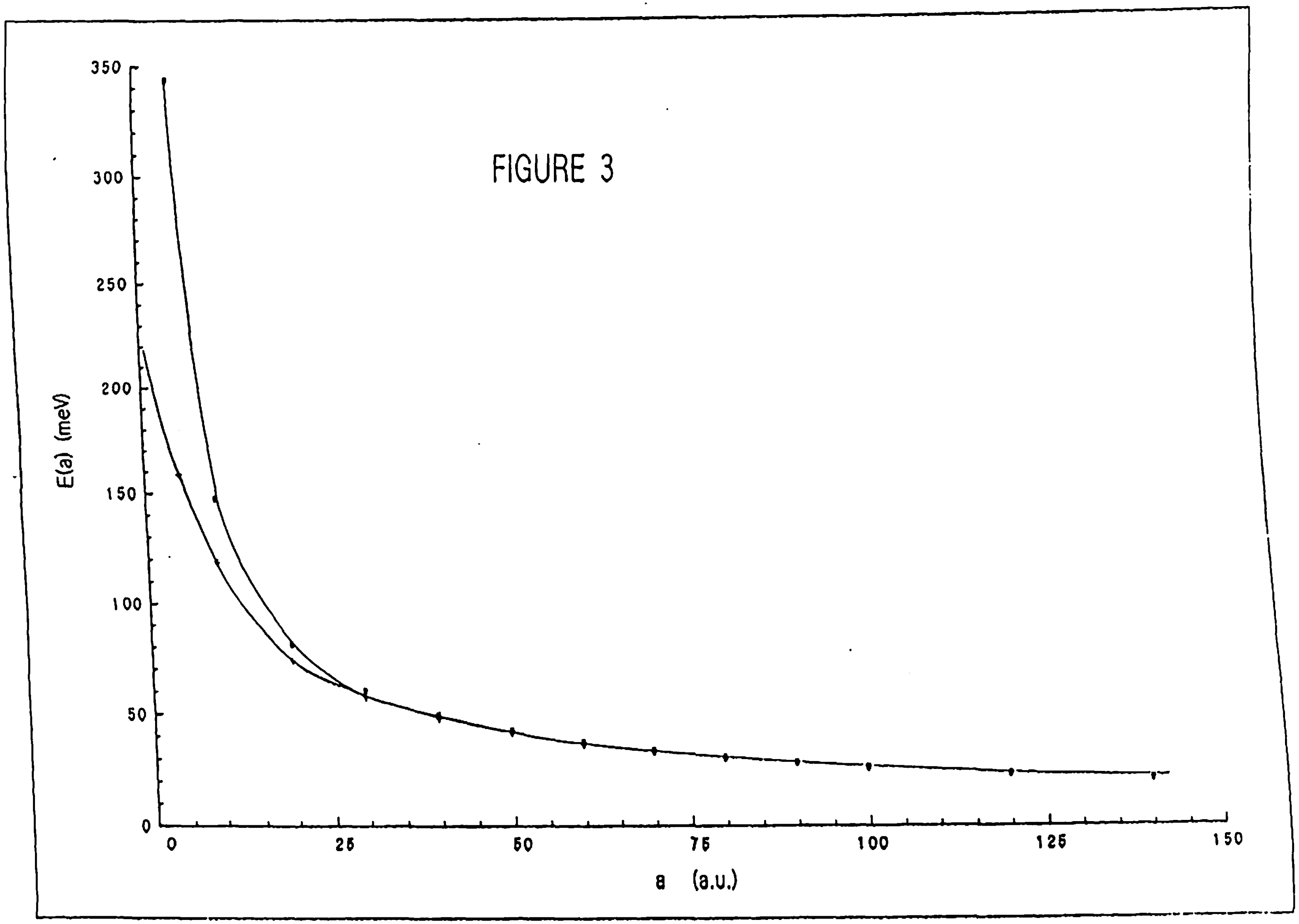


FIGURE 3

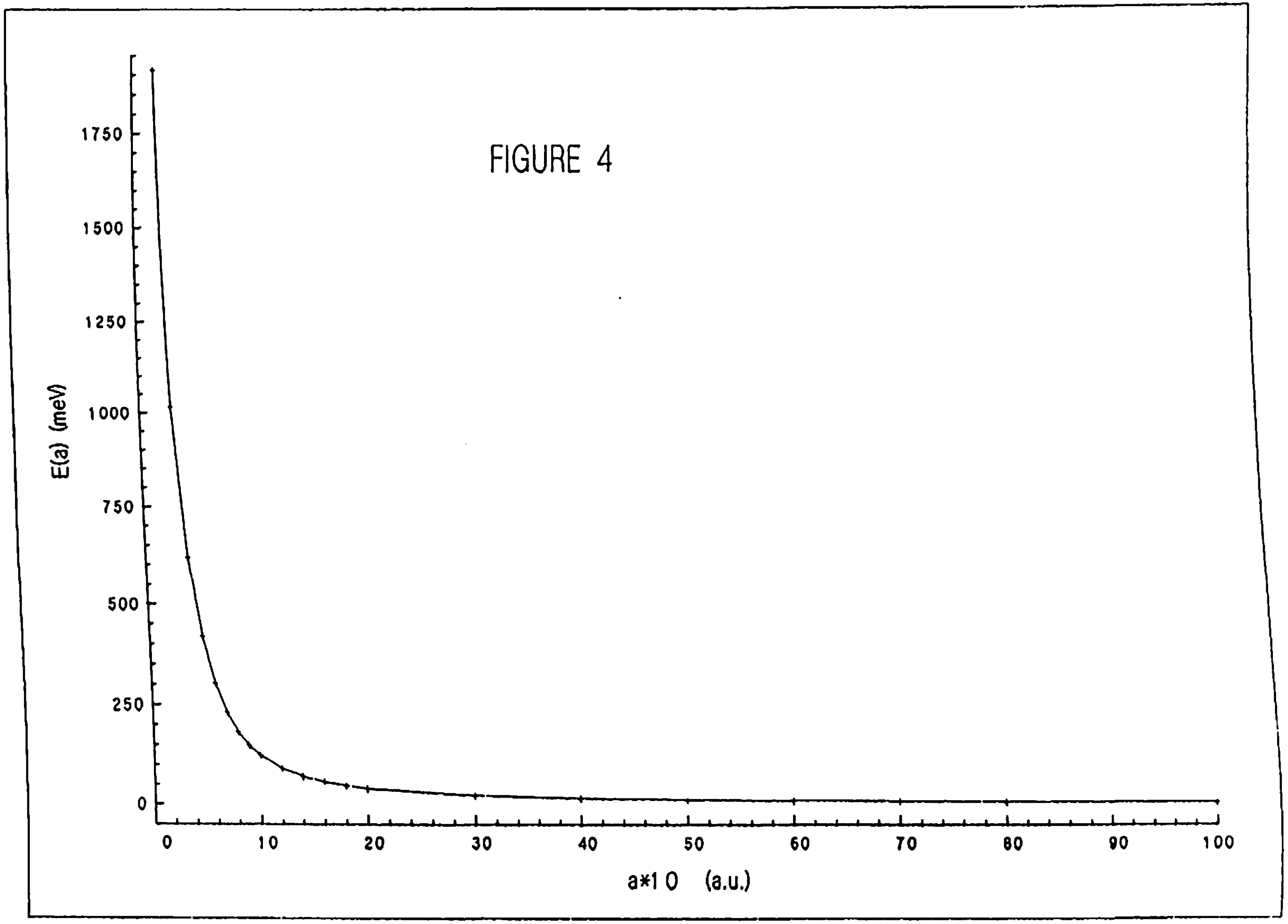

1750
1500
1250
1000
750
500
250
0
E(a) (meV)
0
10
20
30
40
50
60
70
80
90
100
a*10 (a.u.)

FIGURE 4

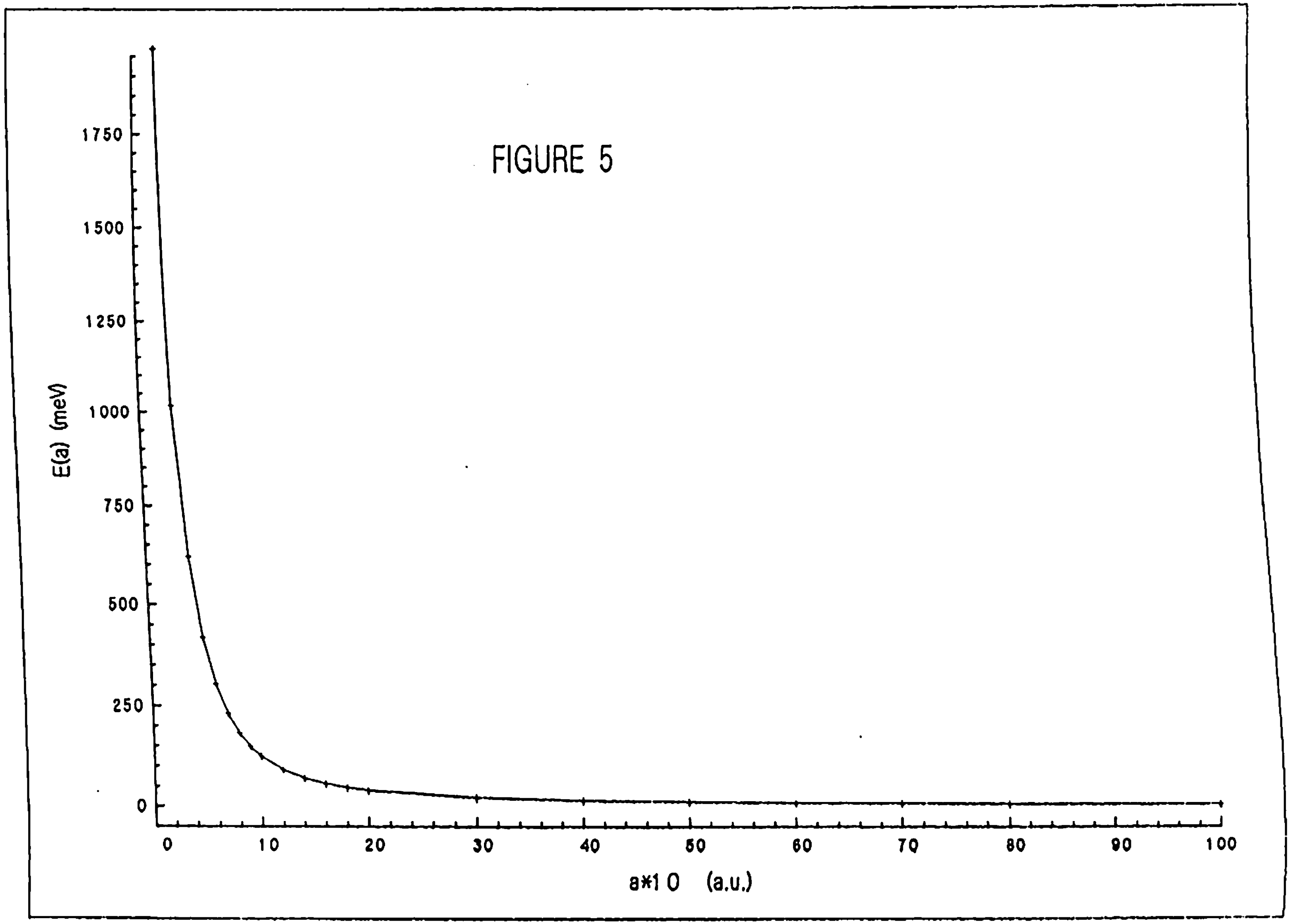

E(a) (meV)
1750
1500
1250
1000
750
500
250
0
0
10
20
30
40
50
60
70
80
90
100
a*10 (a.u.)

FIGURE 5

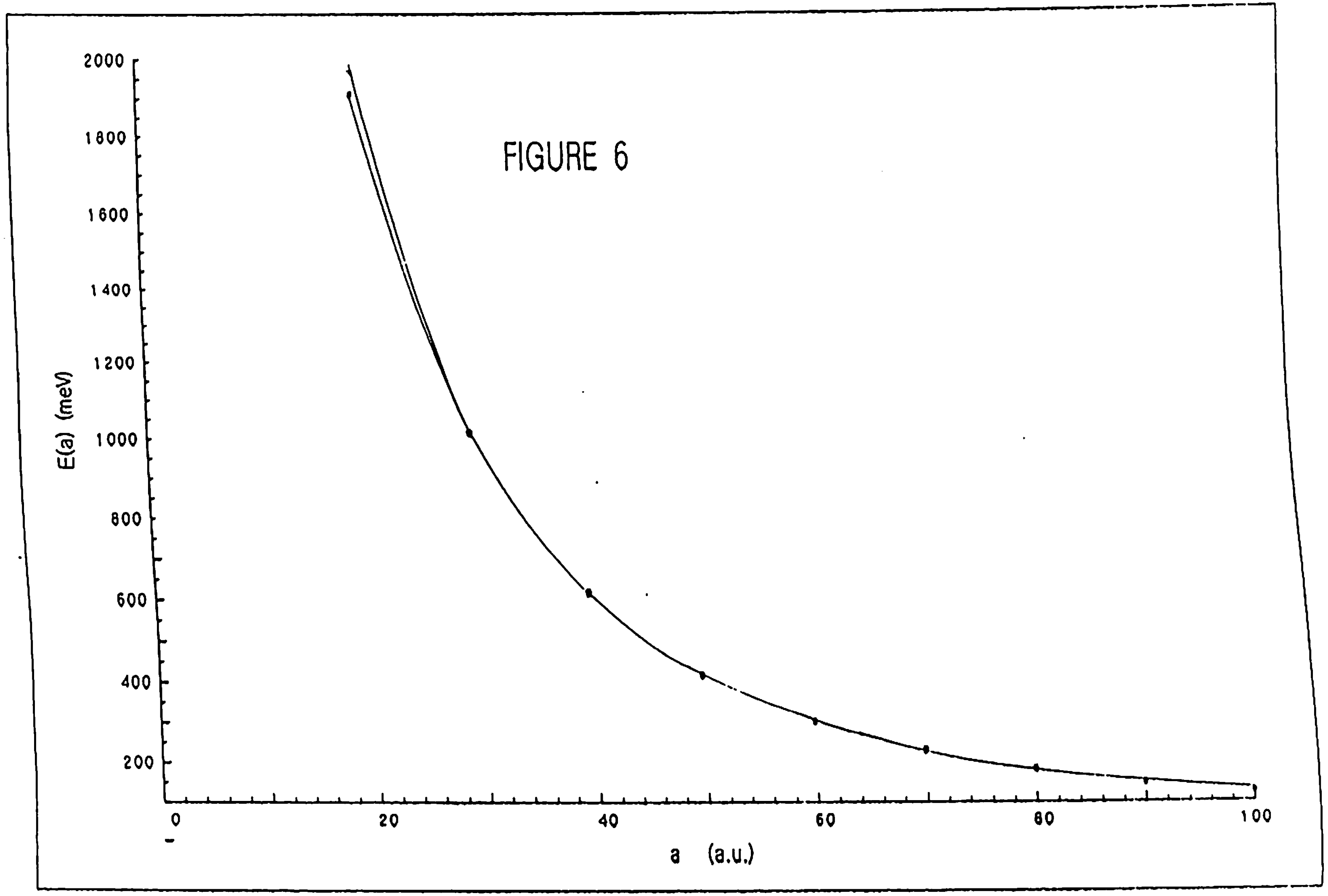

2000
1800
1600
1400
1200
1000
800
600
400
200
E(a) (meV)
0
20
40
60
80
100
a (a.u.)

FIGURE 6

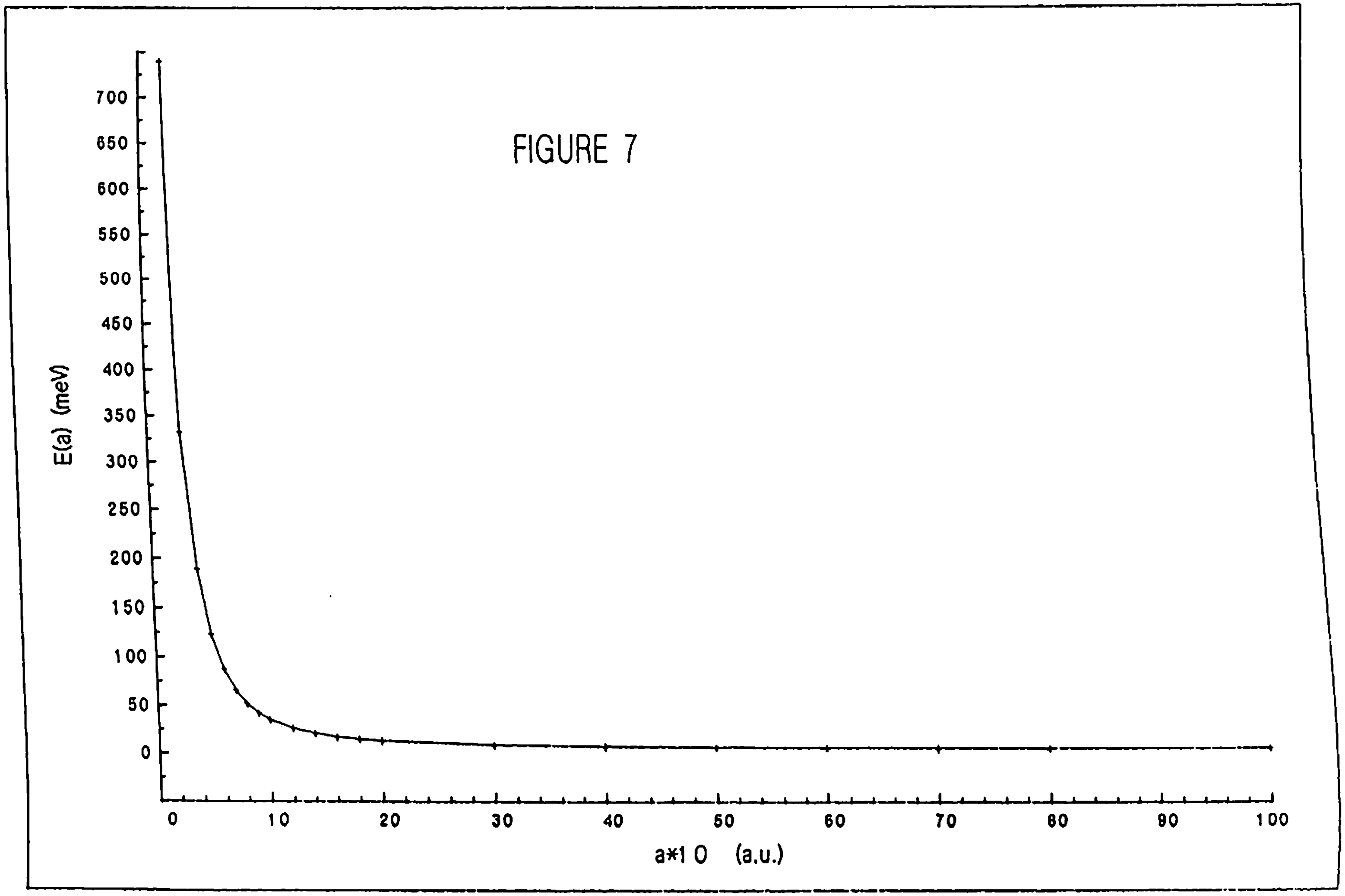

E(a) (meV)
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
0
10
20
30
40
50
60
70
80
90
100
a*10 (a.u.)

FIGURE 7

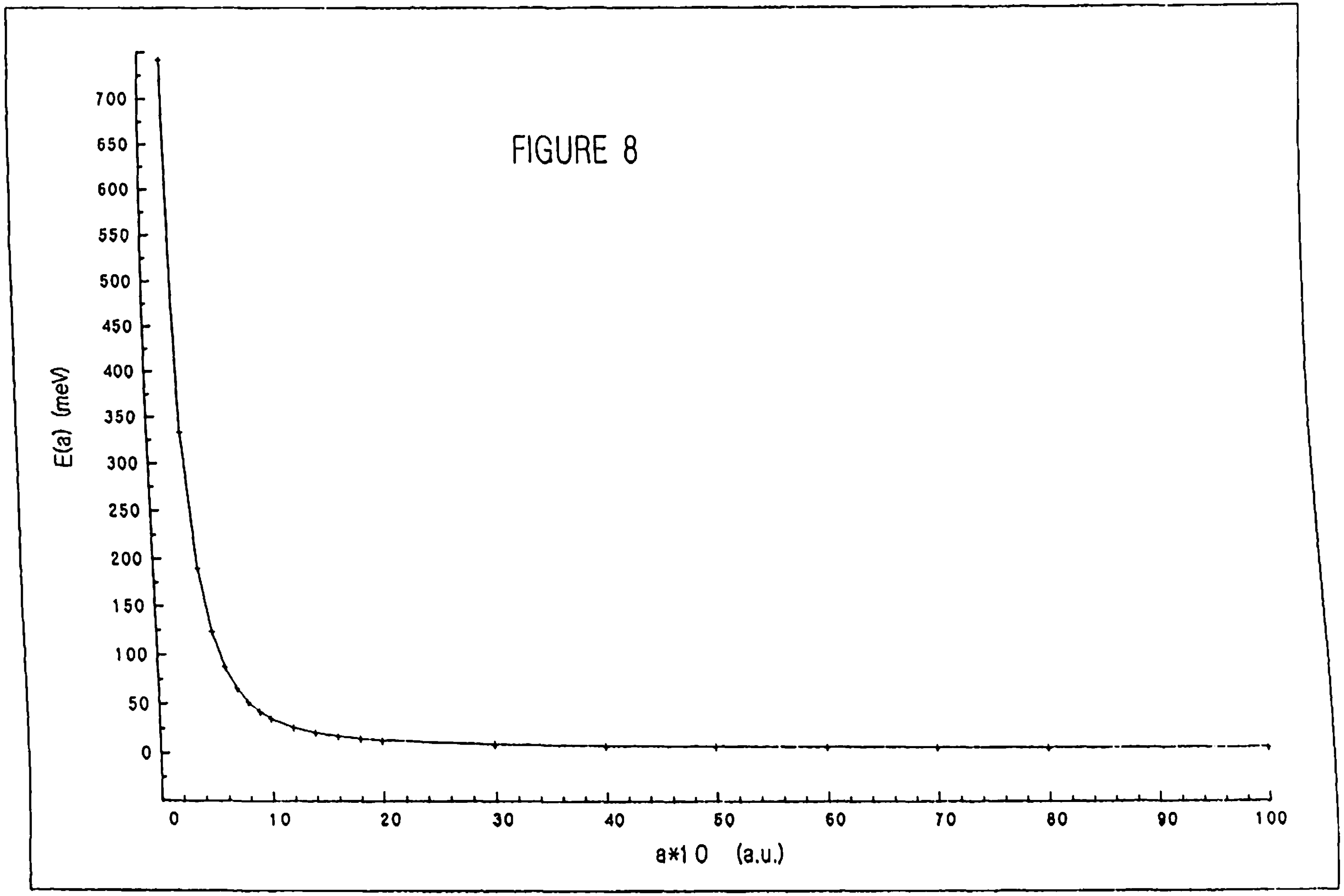

E(a) (meV)
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
0
10
20
30
40
50
60
70
80
90
100
a*10 (a.u.)

FIGURE 8

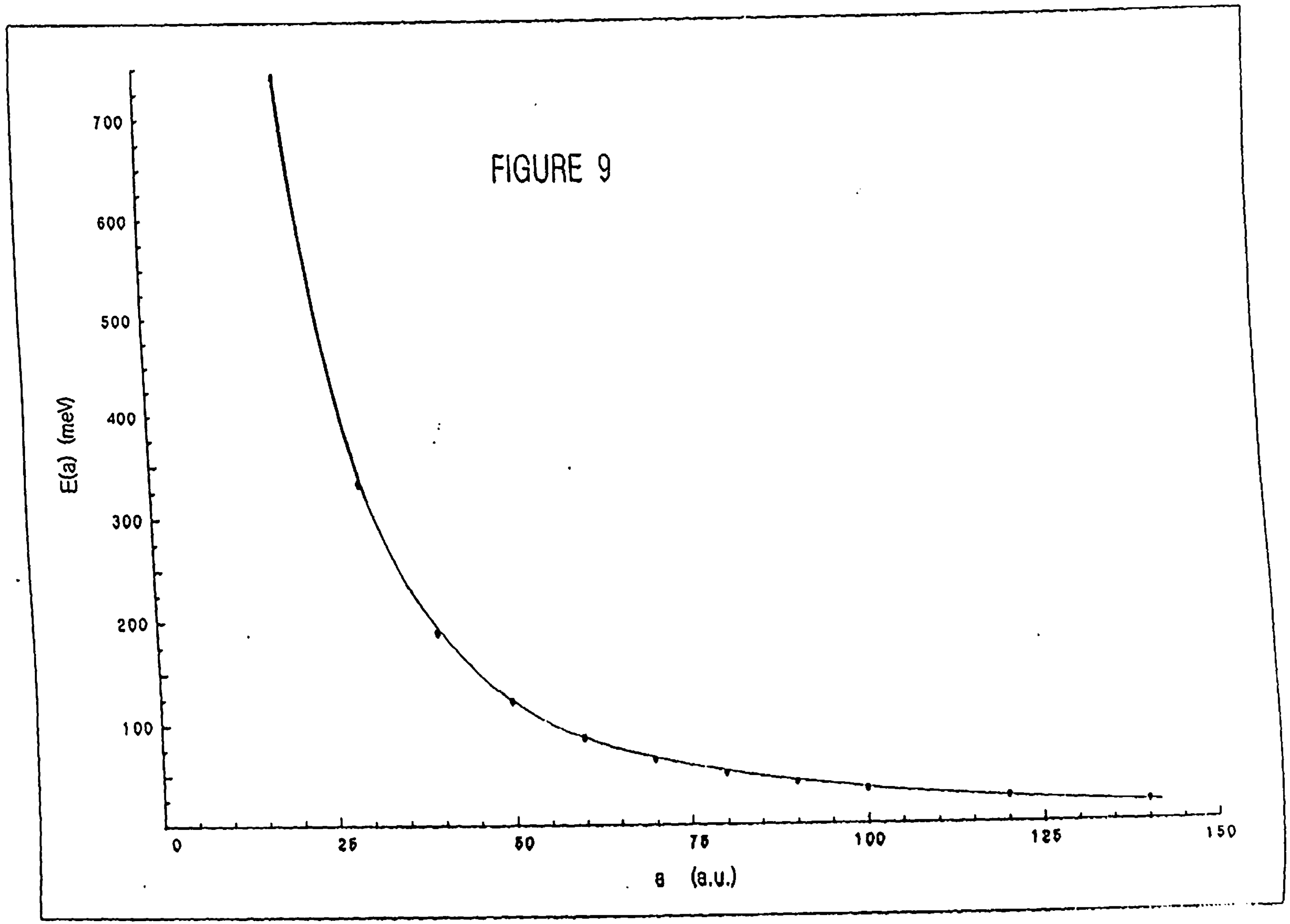


FIGURE 9

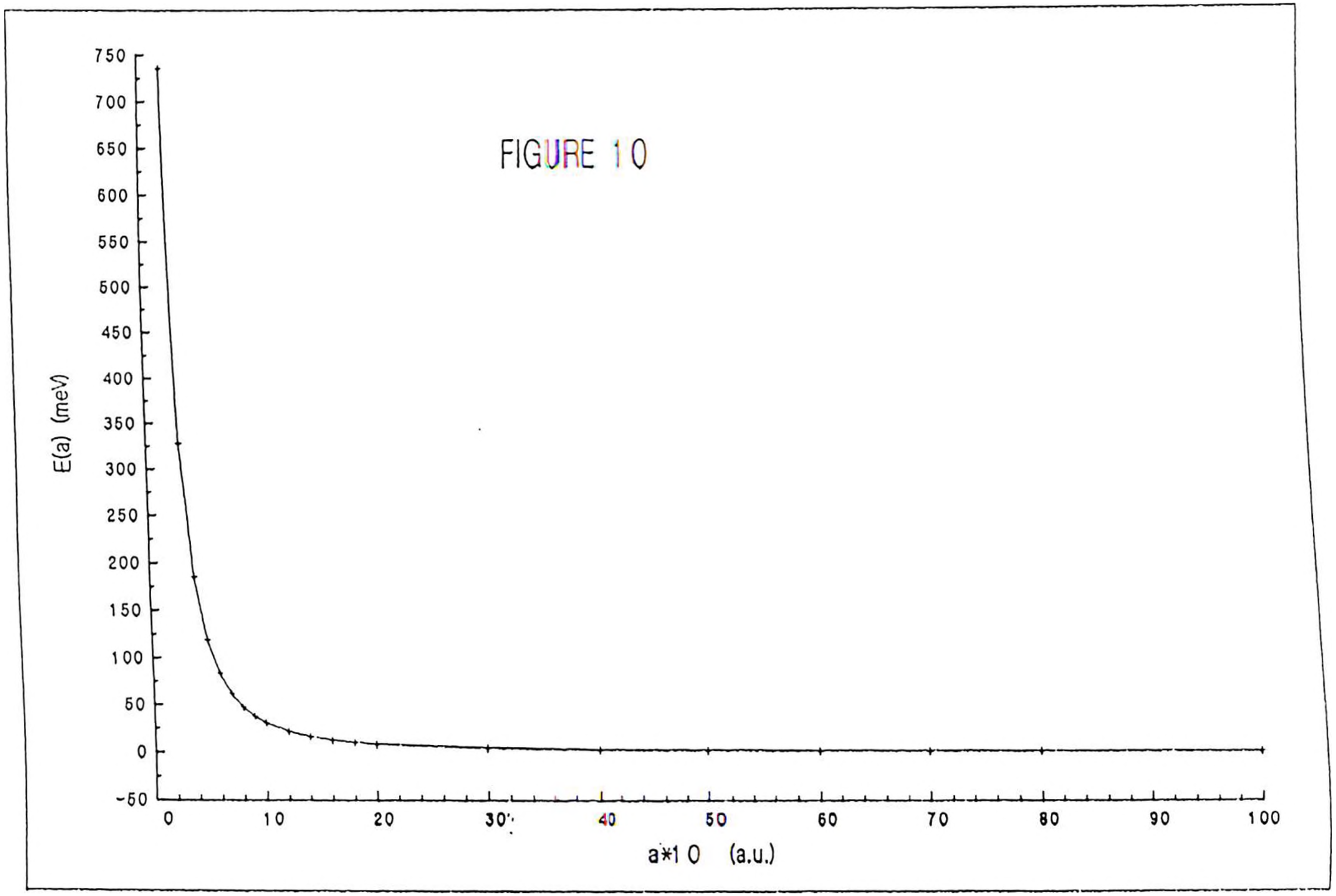

E(a) (meV)
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
0
10
20
30
40
50
60
70
80
90
100
a*10 (a.u.)

FIGURE 10

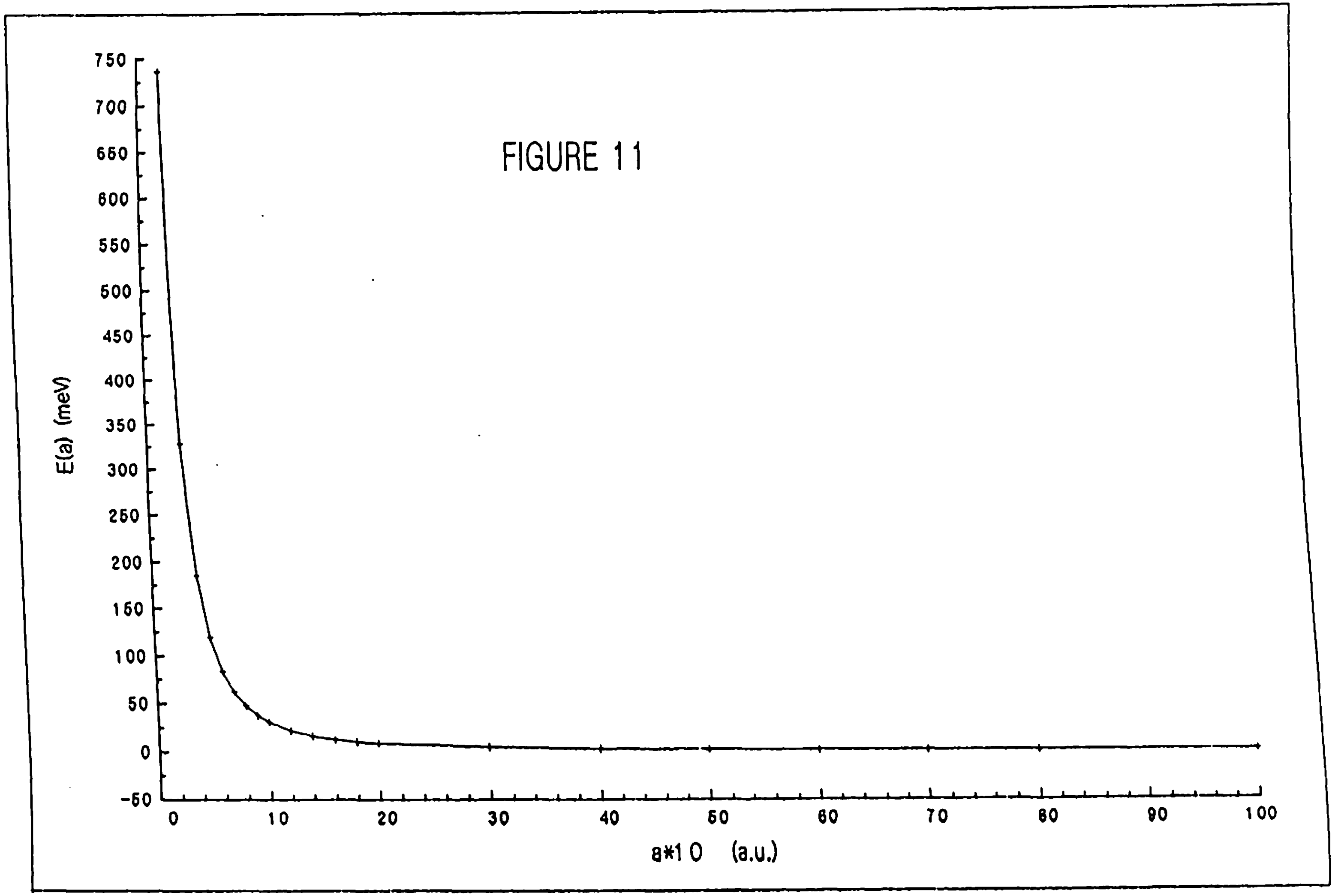

E(a) (meV)
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
0
10
20
30
40
50
60
70
80
90
100
a*10 (a.u.)

FIGURE 11

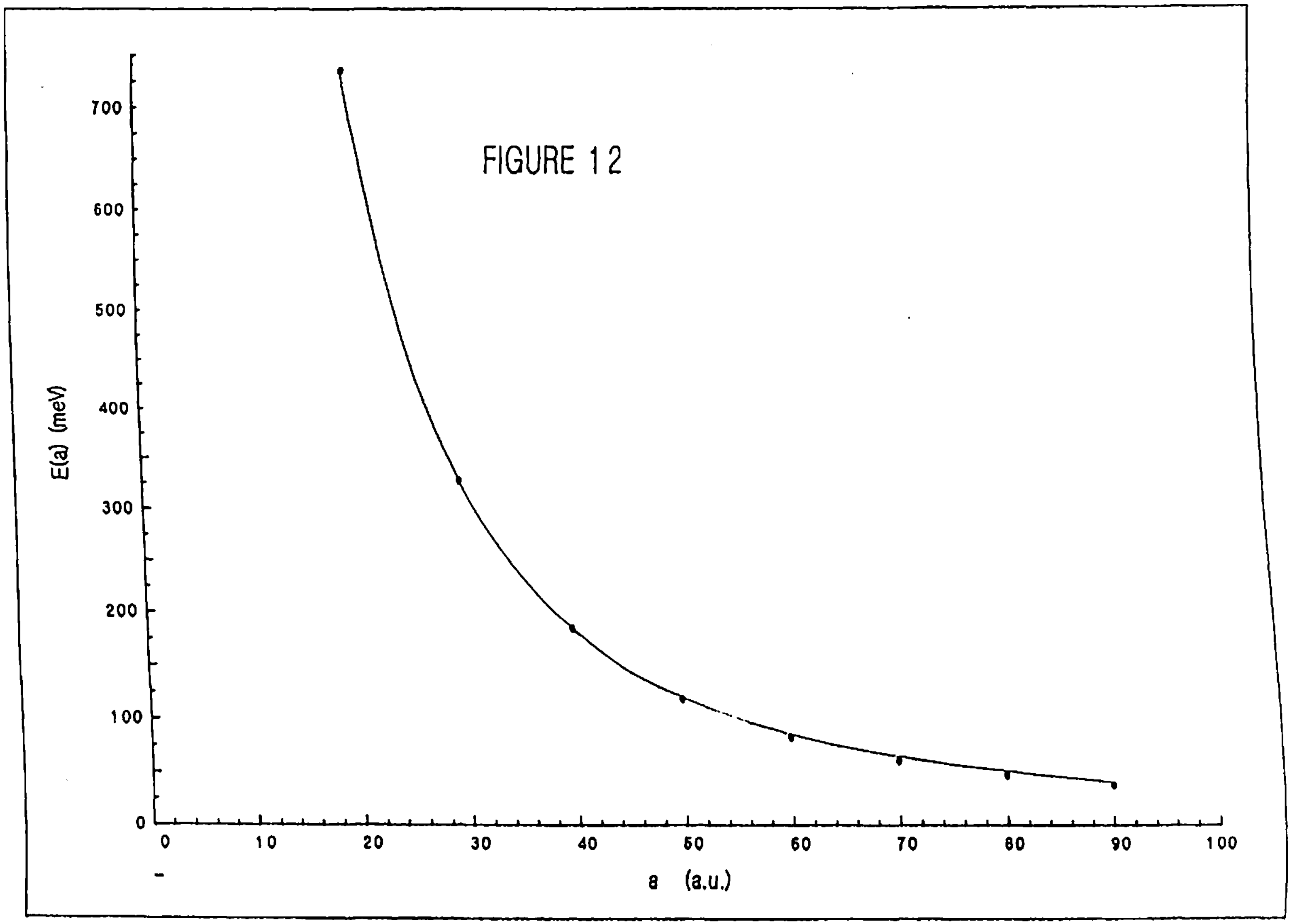

E(a) (meV)
700
600
500
400
300
200
100
0
0
10
20
30
40
50
60
70
80
90
100
a (a.u.)

FIGURE 12

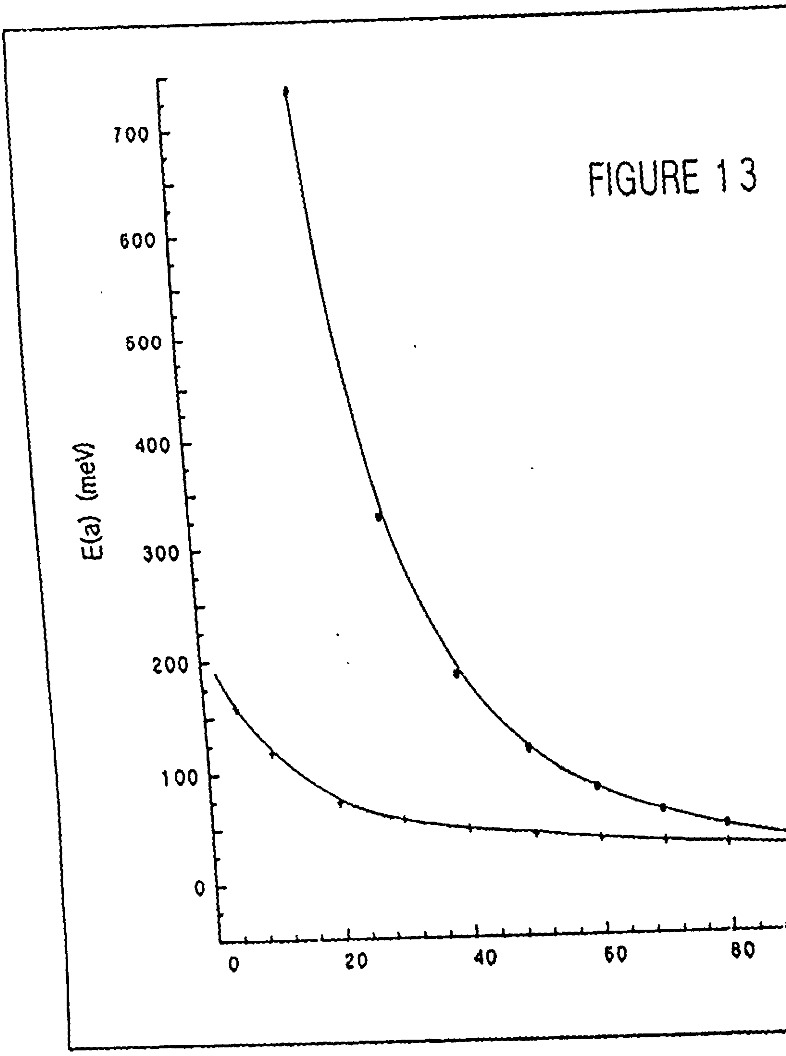
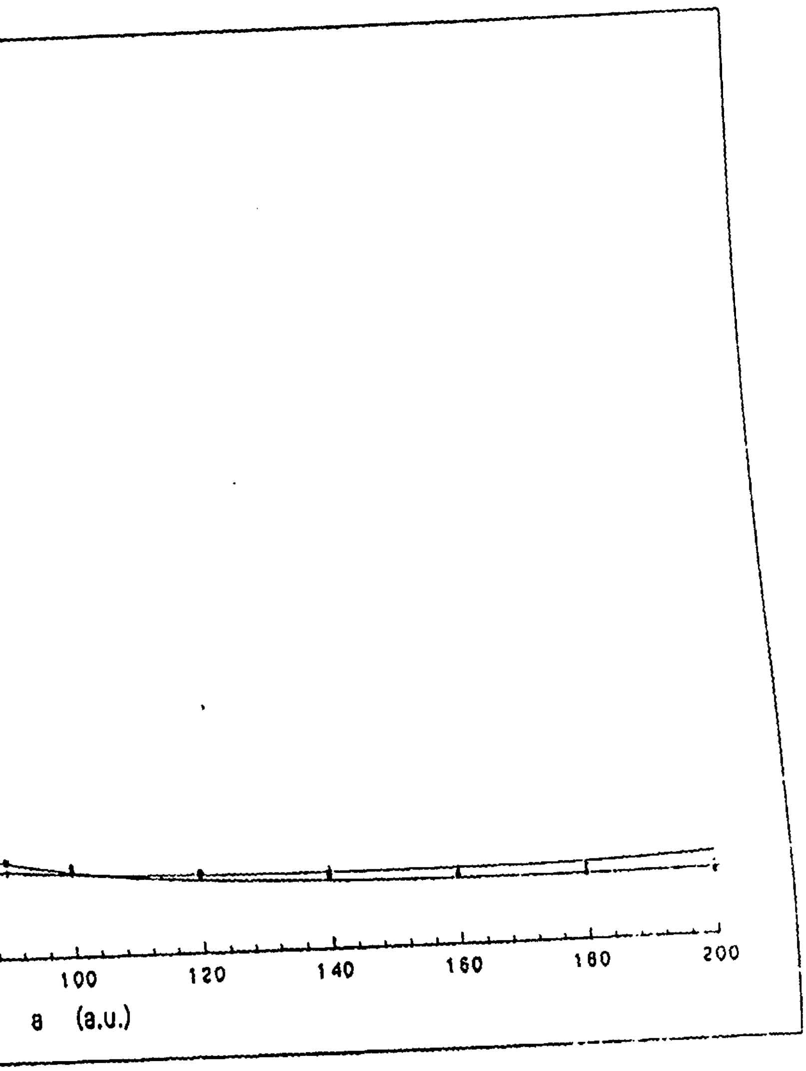


FIGURE 13



100
120
140
160
180
200
a (a.u.)

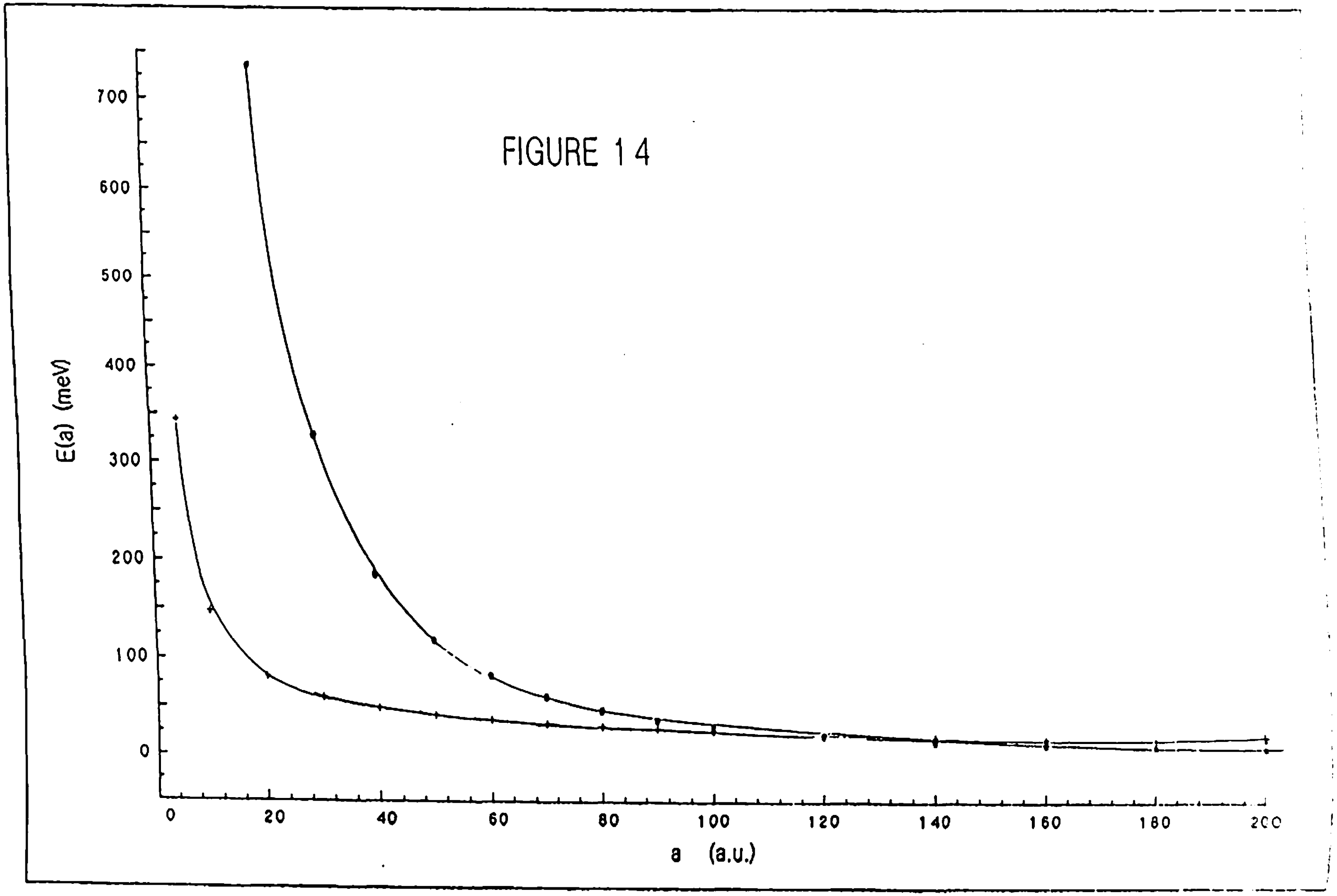

E(a) (meV)
700
600
500
400
300
200
100
0
0
20
40
60
80
100
120
140
160
180
200
a (a.u.)

FIGURE 14

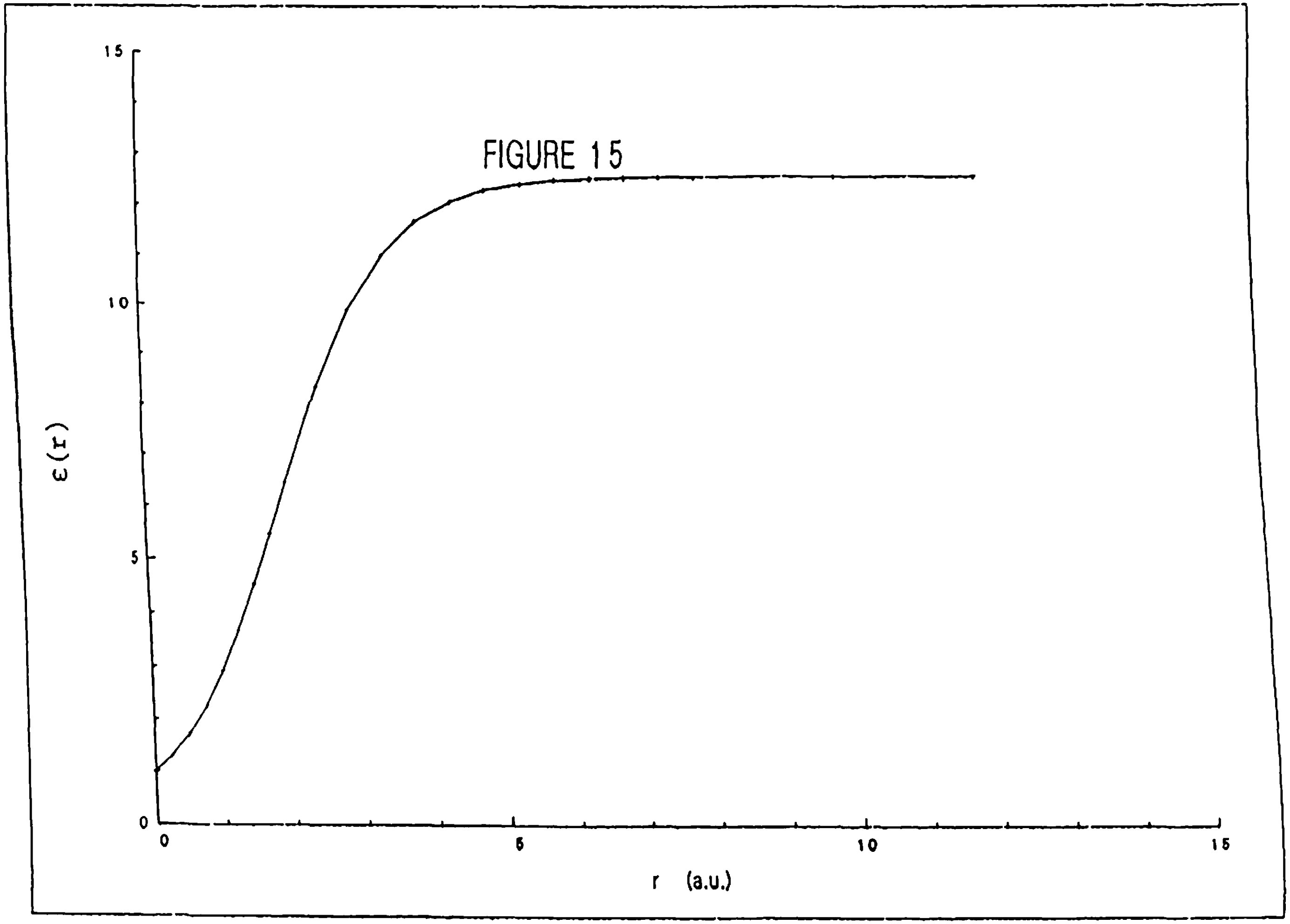
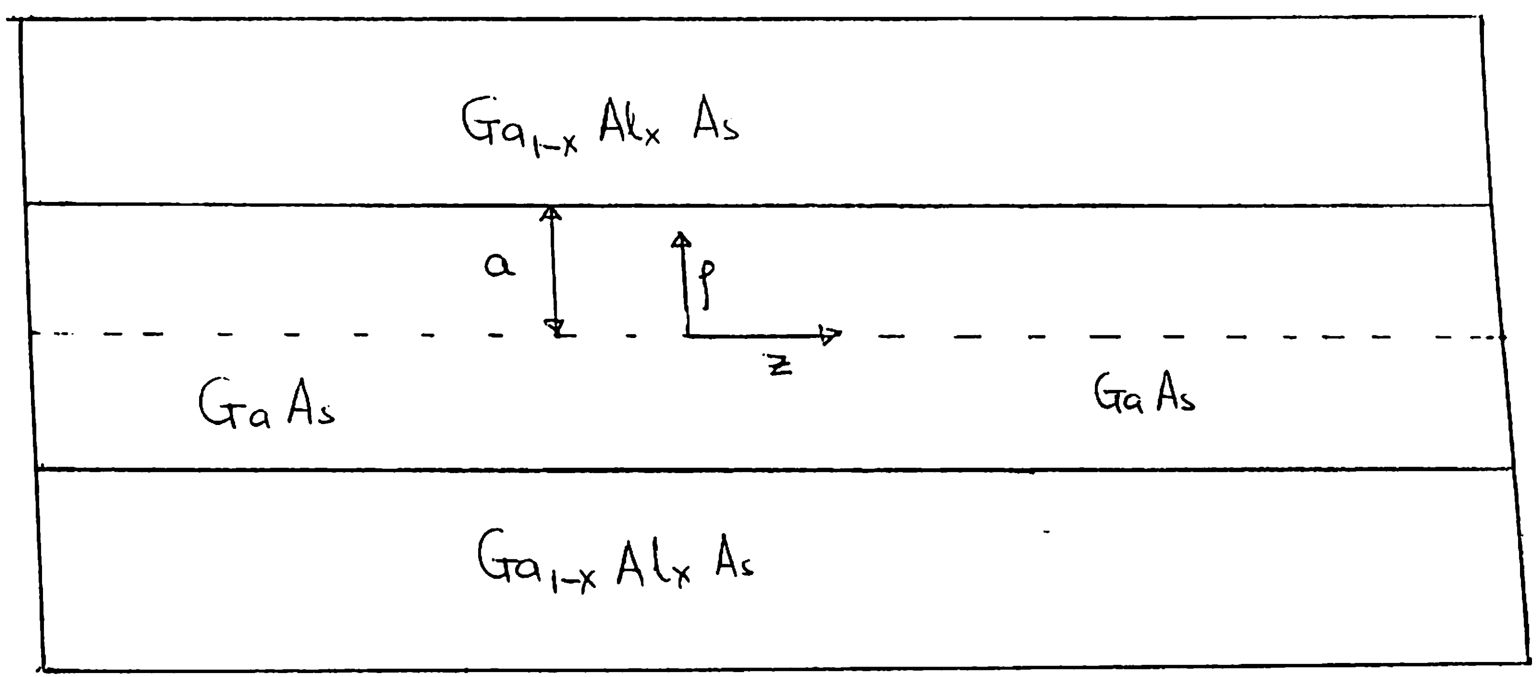


FIGURE 15

FIGURE 16



V. RESULTS AND DISCUSSION

A. Ground State Binding Energy of On-Axis Hydrogenic and Non-Hydrogenic Donors with an Ordinary Bessel Function as an Envelope Wave Function.

A.1. Ground State Energy of an On-Axis Hydrogenic Donor.

In this sub-section the results for the ground state energy of on-axis hydrogenic and non-hydrogenic donors are presented. A comparison is also made of the two results. These results were obtained using a trial wave function with the ordinary Bessel function of Equation II-A.2 as an envelope wave function.

Table 1 shows the numerical results of the binding energy $E_b(a,\beta)$ of Equation II-A.6 as a function of the QWW radius, a, of a hydrogenic donor. Also shown are the minimizing values of the variational parameter β. The binding energy, as a function of the QWW radius, a, is plotted in Figure 1.

It is seen from both Table 1 and Figure 1 that the binding energy $E_b(a,\beta)$ for large QWW radii, a, is constant at a value of 6.88 meV. This compares favorably with the bulk value given by D.R. Wright [27].

As the QWW radius decreases, the binding energy increases. At a QWW radius a, smaller than twice the GaAs Bohr radius [8], the increase in the binding energy with decreasing QWW radius becomes more and more pronounced and reaches a value that is about twenty three times the bulk value at a radius of about 5 a.u.

A.2. Ground State Binding Energy of an On-Axis Non-Hydrogenic Donor.

The results shown in Table 2 were obtained with the static dielectric constant replaced by the spatial dielectric function of Equation II-A.13. This changes the calculation of the expectation value of the potential energy.

Table 2 shows the variation of the binding energy $E_b(a,\beta)$, with the QWW radius a. In Table 2, the minimizing values of the variational parameter β are also shown. As in the case of A.1, the envelope wave function is the ordinary Bessel function.

Figure 2 shows the dependence of the binding energy $E_b(a,\beta)$ on the QWW radius a. Here, again, the binding energy for a large QWW radius has about the same value as that in bulk [27] GaAs. It is seen from Figure 2 that the binding energy increases with decreasing QWW radius until at about a radius of 5 a.u. it becomes about fifty times the bulk value.

A.3. Comparison of the Results for Hydrogenic and Non-Hydrogenic Donors.

Table 3 compares the hydrogenic and non-hydrogenic donor binding energies $E_b(a,\beta)$ as functions of the QWW radius a. The minimizing values of the variational parameter β are also shown.

Figure 3 shows the plots of the binding energy $E_b(a,\beta)$ as a function of the QWW radius a for both hydrogenic and non-hydrogenic donors. It is seen from both Table 3 and Figure 3, that the binding energies for both the hydrogenic and non-hydrogenic donors are about the same at a large QWW radius but begin to show significant differences at about a $\leq$ 80 a.u.. When the QWW radius becomes much smaller than 5 a.u., the binding energy for the non-hydrogenic donor is about twice that of the hydrogenic donor.

Thus, Table 3 and Figure 3 reveal that the screening of the donor ion by the spatial dielectric function displayed in Equation II-A.13 begins to be important for a QWW radius of a $\leq$ 80 a.u..

The finding that the binding energies of both the hydrogenic and non-hydrogenic donors are sensitive functions of the QWW radius, and increase as the radius decreases, is in agreement with the results by Lee and Spector [8] who used a different trial wave function with one variational parameter. It should be mentioned, however, that Bryant [28] has found that the binding energy first increases and then decreases as the QWW radius decreases. This is attributed to the fact that in the calculations by Bryant a finite potential barrier was used, while in the present calculations by Bryant a finite potential barrier was used, while in the present calculations, and in those by Lee and Spector [8], an infinite barrier height is assumed. Furthermore, Bryant used a Gaussian donor wave function.

In the calculations of References [8] and [28] and in the present work, the non-parabolicity of the GaAs conduction band is not considered. This effect, for on-center donors, in a $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ QW has been considered by Chaudhuri [28] and Bajaj [29], while in the same effect for off-center donors has been investigated by Csavinszky and Elabsy [30].

B. Ground State Binding Energy of On-Axis Hydrogenic and Non-Hydrogenic Donors with a Spherical Bessel Function as Envelope Wave Function.

B.1. Ground State Binding Energy of an On-Axis Hydrogenic Donor.

In this sub-section the results for the ground state energy of on-axis hydrogenic and non-hydrogenic donors are presented. The results were obtained by a trial wave function with spherical Bessel function of Equation II.b.2. as envelope wave function.

Table 4 shows the numerical values of the binding energy $E_b(a,\beta)$, as a function of the QWW radius a, for an on-axis hydrogenic donor. The minimizing values of the variational parameter β are also shown. The binding energy, $E_b(a,\beta)$, as a function of the QWW radius a, is plotted in Figure 4.

It is seen from both Table 4 and Figure 4, that the binding energy for a large QWW radius is 5.80 meV which compares favorably with that given by Wright [27]. As the QWW radius decreases, the binding energy increases until at very small QWW radii the binding energy tends to infinity.

B.2. Ground State Energy of an On-Axis Non-Hydrogenic Donor.

The data shown in Table 5 were obtained with the static dielectric constant $\epsilon(o)$ replaced by the spatial dielectric function $\epsilon(r)$ in the calculation of the expectation value of the potential energy. The values listed in Table 5 are plotted in Figure 5.

It is seen from both Table 5 and Figure 5, that the binding energy approaches the bulk value for a large QWW radii. As in the case of the hydrogenic donor, the binding energy increases with decreasing QWW radius, ultimately approaching infinity for very small QWW radii.

B.3. Comparison of the Results for Hydrogenic and Non-Hydrogenic Donors.

Table 6 presents a comparison of the binding energies, as functions of the QWW radius, of hydrogenic and non-hydrogenic donors. Figure 6 shows plots for the two cases. It is seen from both Table 6 and Figure 6, that the binding energies are about the same at a large QWW radius and compare favorably with the bulk value [27]. However, as the QWW radius decreases below about $a \leq 100$ a.u., the results begin to differ markedly, with the binding energy for the non-hydrogenic donor becoming bigger than that of the hydrogenic donor. Thus binding energies of both the hydrogenic and non-hydrogenic donors are again sensitive functions of the QWW radius, as was seen to be the case when the ordinary Bessel function was used as an envelope wave function. The binding energies obtained with the spherical Bessel function as envelope wave function are, however, much larger than those obtained with the ordinary Bessel function as the envelope wave function.

C. Ground State Binding Energy of On-Axis Hydrogenic and Non-Hydrogenic Donors with Unit Envelope Wave Function.

C.1. Ground State Binding Energy of an On-Axis Hydrogenic Donor.

In this sub-section the results for the ground state energy of an on-axis hydrogenic donor are presented. Table 7 shows the variation of the binding energy, $E_b(a,\beta)$, with the QWW radius a. The variational parameter β assumes only one value. This is calculated from the expectation value of the total energy, that is given by an analytical expression. In this case too, the binding energy assumes the bulk value for a large QWW radius. The binding energy then increases with decreasing QWW radii and approaches very large values at very small QWW radii, $a \leq 20$ a.u.

Figure 7 shows the plot of the binding energy as a function of the QWW radius.

C.2. Ground State Binding Energy of an On-Axis Non-Hydrogenic Donor.

Table 8 shows the values of the binding energy, $E_b(a,\beta)$, as a function of the QWW radius a. With the use of the spatial dielectric function in the calculation of the expectation of the potential energy, the expectation value of the total energy is no longer analytical.

The plot of the binding energy as a function of the QWW radius is given in Figure 8. It is seen from both Table 8 and Figure 8, that at large QWW radii the binding energy is about that of the bulk value. Again, as in the case of other trial functions, the binding energy for the non-hydrogenic donor becomes much larger with decreasing QWW radius, then the binding energy for the hydrogenic case.

C.3. Comparison of the Results for the Ground State of Hydrogenic and Non-Hydrogenic Donor Binding Energies.

Table 9 shows a comparison of the binding energies as functions of QWW radii for the on-axis ground state of hydrogenic and non-hydrogenic donors. The minimizing values of the variational parameter β are also shown in Table 9 for comparison.

Both Table 9 and Figure 9 show that for large Qww radius the binding energies of the hydrogenic and non-hydrogenic donors are about the same and approach the bulk value. However, for a QWW radius of $a \leq 90$ a.u., the binding energy of the non-hydrogenic donor increases more rapidly with decreasing QWW radius than that of the hydrogenic donor. This effect has been observed in all three cases that have been presented in this work. In addition, the binding energy as a function of QWW radius determined with unit envelope wave function is observed to be intermediate between the values obtained with the ordinary and with the spherical Bessel functions as envelope wave functions.

D. First Excited State Binding Energy of On-Axis Hydrogenic and Non-Hydrogenic Donors with Ordinary Bessel Function as the Envelope Wave Function.

In this section the calculated binding energies, as functions of the QWW radii, are given for the first excited state of on-axis hydrogenic and non-hydrogenic donors.

D.1. First Excited State Binding Energy of an On-Axis Hydrogenic Donor.

Table 10 shows the numerical results for the binding energy $E_b(a,\lambda)$, the optimal values of the variational parameter λ, and the respective QWW radius a, for the first excited state of an on-axis hydrogenic donor.

Figure 10 shows a plot of the binding energy as a function of the QWW radius. It is seen from both Table 10 and Figure 10, that the binding energy increases with decreasing QWW radius.

D.2. First Excited State for an On-Axis Non-Hydrogenic Donor.

Table 11 shows the numerical values for the binding energy when in the calculation of the expectation value of the potential energy the static dielectric constant $\epsilon(o)$ is replaced by the spatial dielectric function $\epsilon(r)$. Also shown are the corresponding values of the QWW radius a, and the minimizing values of the variational parameter λ.

Figure 11 shows the plot of the binding energy $E_b(a,\lambda)$, as a function of the QWW radius a. It is seen from both Table 11 an Figure 11, that the binding energy increases with decreasing QWW radius until for a small wire radius it approaches infinity.

D.3. Comparison of the Results for the First Excited State Hydrogenic and Non-Hydrogenic Donor Binding Energies.

Table 12 presents values of the binding energy as a function of the QWW radius in both the hydrogenic and non-hydrogenic cases. Figure 12 shows the plot of the binding energy as a function of the QWW radius both for the hydrogenic and non-hydrogenic cases.

It is seen from both Table 12 and Figure 12, that there is very little difference between the binding energies for the hydrogenic and non-hydrogenic cases at the same QWW radius, although the respective variational parameter values are different. This indicates that the binding energy, while sensitive to the QWW radius, is not too sensitive to the spatial dielectric function $\epsilon(r)$. Furthermore, in the 2s state the donor electron does not approach the impurity ion as closely as in the ground state.

E. Comparison of the Binding Energies for the Ground State and First Excited State of On-Axis Hydrogenic Donors.

Table 13 shows a comparison of the binding energies as functions of the QWW radius for the ground state, and for the first excited state of on-axis hydrogenic donors. Figure 13 compares the plots of the binding energies for the two cases.

It is seen from both Table 13 and Figure 13, that the binding energy, at a large QWW radius, is much smaller in the first excited state than in the ground state. As the QWW radius decreases, the binding energy in both cases increases. The binding energy of the first excited state is, however, still less than that of the ground state until a QWW radius of $a \leq 120$ a.u. is reached. In this region, the binding energy for the first excited state begins to increase much faster with decreasing QWW radius, than the binding energy in the ground state hydrogenic case.

F. Comparison of the Binding Energies for On-Axis Ground State and First-Excited State Non-Hydrogenic Donors.

Table 14 shows a comparison of the binding energy as a function of the QWW radius for the non-hydrogenic ground state and for the first-excited state. Figure 14 shows plots of the respective binding energies as functions of the QWW radius. It is seen both from Table 14 and Figure 14, that the binding energy for the first excited state is much smaller than that for the ground state at a large QWW radius. Again, as the QWW radius decreases below a ≤ 120 a.u., the binding energy for the first excited state increases much faster than that for the ground state. This may be an indication that the 2s trial wave function is not very good.

G. Concluding Discussion.

(a) The type of impurity donors studied here are the shallow level type. They can be identified by Zeeman splitting [31]. Furthermore, hydrogen and hydrogenic type of impurity are important in GaAs because hydrogen is the normal environment in which GaAs is heated to remove other impurities.

(b) The lattice constant mismatch [32] between GaAs and $Ga_{1-x}Al_xAs$ ($x \approx 0.5$) is very small and this makes it easier to grow them by molecular beam epitaxy. The MBE is used to fabricate layered quantum wells which are then etched, for example, by photolithography, into quantum well wires.

VI. CONCLUSION

A. Binding Energy of the Ground State of On-Axis Hydrogenic and Non-Hydrogenic Donors.

(1) From the results obtained in the present work, one concludes that (a) the binding energies of both the hydrogenic and non-hydrogenic donors approach the bulk value for a very large QWW radius but (b) as the QWW radius decreases, the binding energy increases. The increase in the binding energy becomes more and more rapid as the QWW radius decreases below about $a \leq 80$ a.u. and thereafter approaches infinity.

(2) As the QWW radius decreases below about $a \leq 80$ a.u., the binding energy of the non-hydrogenic donor begins to increase more rapidly than that of the hydrogenic donor. This indicates that below about $a \leq 80$ a.u. the screening effect by the spatial dielectric function begins to be more and more important.

(3) The above two conclusions apply to all trial wave functions used in the present work except that the values of the binding energies are different in each case and that the screening effect of spatial dielectric function also begins to become more important at much larger QWW radii.

B. Binding Energy of the First Excited State of On-Axis Hydrogenic and Non-Hydrogenic Donors.

(1) In the case of the first excited state, the binding energy for both the hydrogenic and non-hydrogenic donors is much smaller than in the ground state at large QWW radii. However, the binding energy is still a sensitive function of the QWW radius. The increase in the binding energy with decreasing QWW radius is less rapid than in the case of the ground state. It is found that at a QWW radius of $a \leq 120$ a.u., the rate of increase of the binding energy for the first excited state begins to exceed that of the ground state. This finding may be an indication of the breakdown of the quality of the 2s state wave function.

(2) There is no significant difference between the binding energy of the on-axis first excited state hydrogenic donor and that of the non-hydrogenic donor. This conclusion pertains to all QWW radii. This means that the screening by the spatial dielectric function is less important for the first excited state than for the ground state. This is expected since an excited-state wave function is more spread out than a ground-state wave function.

C. General Conclusion from the Study.

The study finds that the binding energy of a hydrogenic and non-hydrogenic donor impurity generally increases with decreasing QWW radius. This leads to the phenomenon of quantum confinement which was first observed by Sakaki et al. [33] in the form of negative differential resistance.

Furthermore, this purely quantum mechanical effect can be explained in the following way. The band gap Δ of a GaAs is much less than the band gap of $Ga_{1-x}Al_xAs$. In the $GaAs/Ga_{1-x}Al_xAs$ boundary, the conduction band edge in GaAs lies at a lower energy then the conduction band edge of $Ga_{1-x}Al_xAs$ and the valence band edge of GaAs lies at a higher energy than the valence band edge of $Ga_{1-x}Al_xAs$. Thus the GaAs acts as a quantum well and the $Ga_{1-x}Al_xAs$ acts as a potential barrier. Thus a donor electron in a $Ga_{1-x}Al_xAs$ on making the $Ga_{1-x}Al_xAs/GaAs$ boundary would literally drop into the GaAs well and effect can be exploited to construct quantum well wire lasers with very precise energy (wavelength).

One other advantage of the quantum confinement of the donor impurity is that it is then localized, thus reducing its effectiveness in terms of range as a scattering center. Thus the quantum confinement of the donor impurity reduces its effectiveness to degrade conduction.

D. Measurement of the Donor Binding Energies.

Some of the techniques that have been used in the measurement of the impurity binding energies are photoluminescence [34,35,36], Raman scattering [36] and farinfrared magnetic spectroscopy [36] of intra-impurity transitions on a series of center-doped QW's. However, there are as yet no reliable experimental data on impurities on QWW [38,39,40] although experiments of references [34,35,36] have confirmed the increase in binding energy with decreasing width of QW.

E. Applications.

GaAs has certain electrical and physical properties which makes it more attractive than silicon in certain device applications. Some of these are discussed below.

(a) The transferred electron effect [41]: This is a property of quantum wells and quantum well wires, in which photoexcited electrons diffuse towards the surface. They acquire enough kinetic energy to promore them to the valleys of the conduction band. Exploitation of this effect has resulted in more efficient photoemission with quantum efficiences as high as 5% out to 1.6 μm, although this operation requires a temperature of 125 K.

(b) GaAs is a direct band gap material and because of the high electron mobilities in it (typically 3500 - 4000 (cm^2/vs) [45]. It has useful optoelectronic properties. It is expected that the QWW will be important in device applications because of their potential as QWW lasers [44]. These lasers can operate continuously at heat-sink temperatures. Furthermore, one expects as in quantum well lasers, that the QWW lasers will have other advantages over other lasers used for electronic and communication devices, because of their small size, simple structure and ease of operation [44].

(c) Woodall et al. [45] have developed heterojunction solar cells which show higher power conversion efficiencies than corresponding silicon solar cells.

(d) Others [46] have developed a $GaAs/Ga_{1-x}Al_xAs$ heterostructure phototransistor of relatively high optical gain and short response time. These have been extensively used in optical fiber communication systems [47].

VII. Papers Published and Lectures Presented (which have resulted from this study to date).

1. "Variational Calculation of the binding energy of hydrogenic donors located on the axis of a quantum well wire". (Lowell, Massachusetts, April 1990) (with P. Csavinszky). Bulletin of the American Physical Society 35, 1546 (1990).

2. "A variational approach to the binding energy of a donor in a gallium arsenide quantum well wire". (with P. Csavinszky). (The Third Atlantic Theoretical Chemistry Symposium, Orono, Maine, May 1990).

3. "Dielectric response of a $GaAs/Ga_{1-x}Al_xAs$ quantum well wire to the presence of a donor ion located on the axis of the QWW of circular cross section". (with P. Csavinszky). (New Haven, Connecticut, October 1990). Bulletin of the American Physical Society (to be published).

4. "Binding energy of on-axis hydrogenic and non-hydrogenic donors in a $GaAs/Ga_{1-x}Al_xAs$ quantum well wire of circular cross section". (with P. Csavinszky). Physical Review B (accepted for publication, January 17, 1991).

VIII. REFERENCES

[1] A.Y. Cho, J. Appl. Phys. 42, 2074 (1971).

[2] E.H.C. Parker, Technol. and Physics of Molecular Beam Epitaxy (Plenum Press, New York, 1985).

[3] H.M. Manasevit, J. Electrochem. Soc. 118, 647 (1971).

[4] D.K. Kerry, Gallium Arsenide Technology (H.W. Sams, (1985).

[5] R. Dingle, in Festor perprobleme, Advances in Solid State Physics, edited by H.J. Quessner (Pergamon Press, Braunschweig, 1975), Vol. 15.

[6] H.C. Casey and B.M. Panish, Heterostructure and Lasers (Academic Press, New York, 1978) part A.

[7] P.C. Sercel and K.J. Vahala, Phys. Rev. B 42, 3690 (1990)-II.

[8] J. Lee and H.N. Spector, J. Vac. Sci. Technol. B, 2(1), Jan.-Mar. 1984.

[9] R. Dingle, et al., Phys. Rev. Lett. 33, 825 (1974).

[10] F.A.P. Osorio et al., Phys. Rev. B 37, 1402 (1988)-II.

[11] P. Csavinszky and A.M. Elabsy, Phys. Rev. B 32, 6498 (1985).

[12] P. Csavinszky and A.M. Elabsy, Int. J. Quantum Chem: Quant. Chem. Symposium 20, 325 (1986).

[13] R. Resta, Phys. Rev. B 16, 2727 (1977).

[14] F. Cornolti and R. Resta, Phys. Rev. B 17, 3239 (1978).

[15] G. Weber et al., Phys. Rev. B 37, 1402 (1988)-II.

[16] J. Hermanson, Phys. Rev. B 150, 660 (1966).

[17] L.E. Oliveira and L.M. Falicov, Phys. Rev. B 34, 8676 (1986).

[18] L. Schiff, Quantum Mechanics, 3rd Edition (McGraw, 1968).

[19] G. Weber, et al., Materials Science Forum Vol. 38-41, 1415-1420 (1989).

[20] I.S. Gradshteyn and I.M. Ryzhik (Academic Press, 1980).

[21] Private discussion with K. Brownstein (University of Maine), and my graduate level mathematical physics text.

[22] C.R.C. Standard Mathematical Tables, 28th edition 1987.

[23] E. Butkov, Mathematical Physics (Addison-Wesley, Reading, MA, 1966).

[24] Private discussion with K. Brownstein (University of Maine) and any standard mathematical physics textbook.

[25] See references [23], [22], etc.

[26] Private discussion with Dr. Flory (Fairleigh-Dickinson University) and any standard text in Mathematical Physics e.g., P. Morse and H. Feshbach, Methods of Theoretical Physics, Vol. I, (McGraw, 1953).

[27] M.J. Howes and D.V. Morgan, Gallium Arsenide (John Wiley, 1985).

[28] G.W. Bryant, Phys. Rev. B 29, 6632 (1984).

[29] S. Chaudhuri and K.K. Bajaj, Phys. Rev. B 29, 1803 (1984).

[30] P. Csavinszky and A.M. Elabsy, Int. J. Quantum Chem.: Quantum Chem. Symposium 22, 25 (1988).

[31] M. Schur, GaAs Devices and Circuits, Plenum, 1987.

[32] D.L. Smith and C. Mailhiot, Review of Modern Physics, 163, 1, 173 Jan. 1990.

[33] H. Sakaki, Jpn. J. Appl. Phy. 19, L 735 (1980).

[34] B.V. Shanabrook and J. Comas, Surf. Sci. 142, 504 (1984).

[35] R.C. Miller, et al., Phys. Rev. B 25, 3871 (1982).

[36] N.C. Jaroski et al., Phys. Rev. Lett. 54, 1283 (1985).

[37] B.V. Shanabrook et al., Phys. Rev. B 29, 7096 (1984).

[38] E.A. Gold et al., Phys. Rev. B 41, 7626 (1990)-II.

[39] E.A. de Andrada e Silva et al., Phys. Rev. B 37, 853 (1987).

[40] P.M. Petroff et al., Appl. Phys. Lett. 41, 635 (1982).

[41] M.J. Howes, GaAs Materials, Devices and Circuits (Wiley, 1985).

[42] Science, Volume 247, 5 January 1990.

[43] I. Hayaski and M.B. Panish, J. Appl. Phys. 41, 150 (1970).

[44] Y. Arakawa and T. yamaguchi, Phys. Rev. B 43, 4732 (1991 II).

[45] J.M. Woodall and H.J. Hovel, Appl. Phys. Lett. 21, 379 (1972).

[46] M. Shur, GaAs Devices and Circuits (Plenum, 1987).

[47] D. Hartman and C.C. Shen, Gallium Arsenide Technology edited by D.K. Ferry (H.W. Sams Publishing, Co., 1985).

[48] R. Gradshteyn and Ryzhik, Table of Integrals, Series, Products (Academic Press, 1980).

[49] P. Morse and H. Feshbach, Methods of Theoretical Physics, Vol. I (McGraw, 1953).

[50] Private discussion with K. Brownstein, also see any standard text on Mathematical Physics.

[51] Math/Library, IMSL, Inc. Houston, Texas (1987).

IX. APPENDICES

A. Details of the Calculations of the Ground State Binding Energy with J_o as the Envelope Wave Function.

In the wave function of the 1s state, the normalization constant is determined as follows:

$$\Psi_{1s}(\rho, z) = N J_o(\alpha\rho)\, e^{-\beta\sqrt{\rho^2 + z^2}}$$

the integral

$$\int_{all\ space} \Psi^*_{1s}\, \Psi_{1s}\, d\tau = 1 \qquad \text{A.1}$$

is evaluated as:

$$N^2 \int_o^{2\pi} d\theta \int_o^a \rho\, J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\, e^{-2\beta\sqrt{\rho^2 + z^2}} = 1 \qquad \text{A.2}$$

The integrations are now done as follows:

$$\int_{-\infty}^{\infty} dz\, e^{-2\beta\sqrt{\rho^2 + z^2}} = 2 \int_o^{\infty} dz\, e^{-2\beta\sqrt{\rho^2 + z^2}} \qquad \text{A.3}$$

Let A.4

$$r^2 = \rho^2 + z^2$$

therefore

$$z^2 = r^2 - \rho^2$$

$$2z\, dz = 2r\, dr$$

$$dz = rdr = \frac{rdr}{\sqrt{z}} = \frac{rdr}{\sqrt{r^2 - \rho^2}} \qquad \text{A.5}$$

Substituting A.4 and A.5 into A.3, with a change of limits from 0 to ∞ to ρ to ∞, gives

$$2\int_{o}^{\infty} dz\, e^{-2\beta\sqrt{\rho^2 + z^2}} = 2\int_{\rho}^{\infty} \frac{dr\, re^{-2\beta r}}{\sqrt{r^2 - \rho^2}} \qquad A.6$$

Use is made of the formula [44]

$$\int_{\rho}^{\infty} r(r^2 - \rho^2)^{\upsilon-1} e^{-\mu r} dr = \frac{2^{\upsilon-1/2}}{\sqrt{\pi}} \rho^{1/2+\upsilon} \mu^{1/2-\upsilon} \Gamma(\upsilon) K_{\upsilon+1/2}(\mu\rho) \qquad A.7$$

which for $\nu = \frac{1}{2}$ and $\mu = 2\beta$, as in A.6, becomes:

$$2\int_{\rho}^{\infty} \frac{dr re^{-2\beta r}}{\sqrt{r^2 - \rho^2}} = 2\rho K_1(2\beta\rho) \qquad A.8$$

Therefore, the normalization A.2 becomes:

$$2N^2\int_{o}^{2\pi} d\theta \int_{o}^{a} \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho = 1$$

$$4\pi N^2 \int_{o}^{a} \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho = 1$$

and the normalization constant N is finally given by

$$N^2 = [4\pi\int_{o}^{a} \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho]^{-1}$$

A.9

Calculation of the Binding Energy $E_b(a,\beta)$ in the 1s (Ground) State in Cylindrical Coordinates with the Trial Function

$$\Psi_{1s}(\rho, z) = N J_o(\alpha\rho) e^{-\beta\sqrt{\rho^2 + z^2}}$$

Here the detailed calculations for the binding energy $E_b(a,\beta)$ as a function of the wire radius for the 1s (ground) state is shown.

The Hamiltonian operator H is defined by Equation A.1 and the trial wave function is defined by Equation A.2. The expectation value of H is given by

$$H = T + V \qquad \text{A.10}$$

where T is the kinetic energy operator and V is the potential energy operator. These quantities are given in cylindrical coordinates by:

$$T = -\frac{1}{2m*}\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial z^2}\right]\right\} \qquad \text{A.11}$$

and

$$V = -\frac{1}{\epsilon(r)\,[\rho^2 + z^2]^{1/2}} \qquad \text{A.12}$$

where $\epsilon(r)$, the spatial dielectric function of GaAs is defined by Equation II-A.13.

Now

$$\frac{1}{\rho}\ \frac{\partial}{\partial\rho}\left[\rho\ \frac{\partial}{\partial\rho}\right] + \frac{\partial^2}{\partial z^2} = \frac{1}{\rho}\ \frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial\rho^2} + \frac{\partial^2}{\partial z^2}$$

Then

$$\frac{1}{\rho}\ \frac{\partial}{\partial\rho}\ \Psi_{1s}(\rho, z) = \frac{N}{\rho}\left\{\frac{\partial}{\partial\rho}\ J_o(\alpha\rho)\right\} e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$+ \frac{NJ_o(\alpha\rho)}{\rho}\ \frac{(-\beta\rho)}{\sqrt{\rho^2 + z^2}}\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= -\frac{\alpha NJ_1(\alpha\rho)}{\rho}\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$- \frac{\beta NJ_o(\alpha\rho)\rho}{\rho\sqrt{\rho^2 + z^2}}\ e^{-\beta\sqrt{\rho^2 + z^2}} \qquad \text{A.13}$$

Therefore,

$$\frac{\partial}{\partial\rho} NJ_o(\alpha\rho)\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= -\frac{\alpha NJ_1(\alpha\rho)}{\rho}\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$\frac{-\beta N\rho J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}}\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

A.14

Consideration of the first term in Equation A.14, leads to:

$$N \frac{\partial}{\partial \rho} \left\{ -\alpha J_1(\alpha\rho) \; e^{-\beta\sqrt{\rho^2 + z^2}} \right\}$$

$$= -\alpha N \left\{ \frac{\partial}{\partial \rho} J_1(\alpha\rho) \right\} e^{-\beta\sqrt{\rho^2 + z^2}} - \alpha N J_1(\alpha\rho) \left\{ \frac{\partial}{\partial \rho} e^{-\beta\sqrt{\rho^2 + z^2}} \right\}$$

$$= -\alpha N \left\{ \frac{1}{2} \alpha \; J_{1-1}(\alpha\rho) - \frac{1}{2} \alpha \; J_{1+1}(\alpha\rho) \right\} e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$- \alpha N J_1(\alpha\rho) \left\{ \frac{-\beta\rho}{\sqrt{\rho^2 + z^2}} \right\} e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= -\alpha N \left\{ \frac{\alpha J_o(\alpha\rho)}{2} - \frac{\alpha J_2(\alpha\rho)}{2} \right\} e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$+ \frac{\alpha\beta N J_1(\alpha\rho)\rho}{\sqrt{\rho^2 + z^2}} e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= -\frac{\alpha^2 N J_o(\alpha\rho)}{2} e^{-\beta\sqrt{\rho^2 + z^2}} + \frac{\alpha^2 N J_2(\alpha\rho)}{2} e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$+ \frac{\alpha\beta\rho J_1(\alpha\rho)}{\sqrt{\rho^2 + z^2}} e^{-\beta\sqrt{\rho^2 + z^2}}$$

Using the relation [45]

$$J_2(\alpha\rho) = \frac{2}{\alpha\rho} J_1(\alpha\rho) - J_o(\alpha\rho)$$

The result for the first term A.14 becomes:

$$\left\{ -\frac{\alpha^2 N J_o(\alpha\rho)}{2} + \frac{\alpha N J_1(\alpha\rho)}{\rho} - \frac{\alpha^2 N J_o(\alpha\rho)}{2} \right.$$

$$\left. + \frac{\alpha\beta N\rho J_1(\alpha\rho)}{\sqrt{\rho^2 + z^2}} \right\} x\, e^{-\beta\sqrt{\rho^2 + z^2}}$$

A.15

Performing the same operation on the second term in Equation A.14 leads to:

$$N \frac{\partial}{\partial\rho} \left\{ \frac{-\beta\rho J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} e^{-\beta\sqrt{\rho^2 + z^2}} \right\}$$

$$= N \left\{ \frac{-\beta J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} e^{-\beta\sqrt{\rho^2 + z^2}} + \frac{\alpha\beta\rho J_1(\alpha\rho)}{\sqrt{\rho^2 + z^2}} e^{-\beta\sqrt{\rho^2 + z^2}} \right.$$

$$\left. + \frac{\beta\rho^2 J_o(\alpha\rho)}{[\rho^2 + z^2]^{3/2}} e^{-\beta\sqrt{\rho^2 + z^2}} + \frac{\beta^2\rho^2 J_o(\alpha\rho)}{[\rho^2 + z^2]} e^{-\beta\sqrt{\rho^2 + z^2}} \right\}$$

A.16

Now

$$\frac{\partial^2}{\partial z^2}\Psi_{1s}(\rho, z) = \frac{\partial^2}{\partial z^2} N\, J_o(\alpha\rho)\, e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= NJ_o(\alpha\rho)\ \frac{\partial}{\gamma z}\left\{ - \frac{\beta z e^{-\beta\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2 + z^2}} \right\}$$

$$= NJ_o(\alpha\rho)\left\{ \frac{-\beta}{\sqrt{\rho^2 + z^2}} + \frac{\beta z^2}{[\rho^2 + z^2]^{3/2}} \right.$$

$$\left. + \frac{\beta^2 z^2}{[\rho^2 + z^2]} \right\} x\ e^{-\beta\sqrt{\rho^2+z^2}}$$

A.17

Addition of A.13, A.15, A.16 and A.17 yields $\nabla^2\psi_{1s}(\rho,z)$.

The detailed expression for this quantity is

$$\nabla^2\Psi_{1s}(\rho, z) + \left\{ \frac{-\alpha NJ_1(\alpha\rho)}{\rho} - \frac{\beta NJ_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} \right.$$

$$- \frac{\alpha^2 NJ_o(\alpha\rho)}{2} + \frac{\alpha NJ_1(\alpha\rho)}{\rho}$$

$$- \frac{\beta NJ_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} - \frac{\alpha^2 NJ_o(\alpha\rho)}{2}$$

$$+ \frac{\alpha\beta NJ_1(\alpha\rho)\rho}{\sqrt{\rho^2 + z^2}} + \frac{\alpha\beta NJ_1(\alpha\rho)\rho}{\sqrt{\rho^2 + z^2}}$$

$$+ \frac{\beta N J_o(\alpha\rho)\,\rho^2}{[\rho^2 + z^2]^{3/2}} + \frac{\beta^2 N J_o(\alpha\rho)\,\rho^2}{[\rho^2 + z^2]}$$

$$- \frac{\beta N J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \frac{\beta N J_o(\alpha\rho)\,z^2}{[\rho^2 + z^2]^{3/2}}$$

$$+ \left. \frac{\beta^2 N J_o(\alpha\rho)\,z^2}{[\rho^2 + z^2]} \right\} x\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= \left\{ - \frac{3\beta N J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \frac{\beta N J_o(\alpha\rho)}{[\rho^2 + z^2]^{3/2}} (\rho^2 + z^2) \right.$$

$$+ \frac{\beta^2 N J_o(\alpha\rho)}{[\rho^2 + z^2]} (\rho^2 + z^2) - \alpha^2 N J_o(\alpha\rho)$$

$$+ \left. \frac{2\alpha\beta N J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}}\ \rho \right\} x\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= \left\{ - \frac{2\beta N J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \beta^2 N J_o(\alpha\rho) - \alpha^2 N J_o(\alpha\rho) \right.$$

$$+ \left. \frac{2\alpha\beta N J_1(\alpha\rho)\,\rho}{\sqrt{\rho^2 + z^2}} \right\} x\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

A.18

$$\Psi_{1s} \nabla^2 \Psi_{1s} = NJ_o(\alpha\rho)\, e^{-\beta\sqrt{\rho^2 + z^2}} \left\{ \frac{-2\beta NJ_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} \right.$$

$$\left. + \beta^2 NJ_o(\alpha\rho) - \alpha^2 NJ_o(\alpha\rho) + \frac{2\beta\alpha NJ_1(\alpha\rho)\rho}{\sqrt{\rho^2 + z^2}} \right\}$$

$$x\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= \left\{ - 2\beta N^2 J_o^2(\alpha\rho) + \beta^2 N^2 J_o^2(\alpha\rho) \right.$$

$$\left. - \alpha^2 N^2 J_o^2(\alpha\rho) + 2\alpha\beta N^2 J_o(\alpha\rho) J_1(\alpha\rho)\rho \right\}$$

$$x\ e^{-2\beta\sqrt{\rho^2 + z^2}} \qquad \text{A.19}$$

Multiplication of this equation by $- \frac{\hbar^2}{2m*}$ gives

$$- \frac{h^2}{2m*} \Psi_{1s} \nabla^2 \Psi_{1s}$$

$$= \left\{ \frac{h^2\beta N^2 J_o^2(\alpha\rho)}{m*\sqrt{\rho^2 + z^2}} - \frac{h^2\beta^2 N^2 J_o^2(\alpha\rho)}{2m*} \right.$$

$$\left. + \frac{h^2\alpha^2 N^2 J_o^2(\alpha\rho)}{2m*} - \frac{h^2\alpha\beta N^2 J_o(\alpha\rho) J_1(\alpha\rho)\rho}{m*\sqrt{\rho^2 + z^2}} \right\} \qquad \text{A.20}$$

$$x\ e^{-2\beta\sqrt{\rho^2 + z^2}}$$

The calculation of expectation value of the kinetic energy operator T proceeds as follows:

$$< T > = \int_\tau \psi_{1s}\, T\, \psi_{1s}\, d\tau$$

$$= \frac{h^2\beta N^2}{m*}\int_o^{2\pi} d\theta \int_o^a \rho J_o^2(\alpha\rho)\,d\rho \int_{-\infty}^{\infty} \frac{dz\; e^{-2\beta\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}}$$

$$- \frac{h^2\beta^2N^2}{2m*}\int_o^{2\pi} d\theta \int_o^a \rho J_o^2(\alpha\rho)\,d\rho \int_{-\infty}^{\infty} dz\; e^{-2\beta\sqrt{\rho^2+z^2}}$$

$$+ \frac{h^2\alpha^2N^2}{2m*}\int_o^{2\pi} d\theta \int_o^a \rho J_o^2(\alpha\rho)\,d\rho \int_{-\infty}^{\infty} dz\; e^{-2\beta\sqrt{\rho^2+z^2}}$$

$$- \frac{h^2\alpha\beta N^2}{m*}\int_o^{2\pi} d\theta \int_o^a \rho^2 J_o(\alpha\rho)J_1(\alpha\rho)\,d\rho \int_{-\infty}^{\infty} dz\; e^{-2\beta\sqrt{\rho^2+z^2}}$$

A.21

The θ integration gives 2π, and < T > becomes

$$< T > = \left(\frac{h^2\alpha^2}{2m*} - \frac{h^2\beta^2}{2m*}\right) 2\pi N^2 \int_o^a \rho J_o^2(\alpha\rho)\,d\rho \int_{-\infty}^{\infty} dz\; e^{-2\beta\sqrt{\rho^2+z^2}}$$

$$+ \frac{h^2\beta N^2}{m*}2\pi \int_o^a \rho J_o^2(\alpha\rho)\,d\rho \int_{-\infty}^{\infty} \frac{dz\; e^{-2\beta\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}}$$

$$- \frac{h^2\alpha\beta 2\pi N^2}{m*}\int_o^a \rho^2 J_o(\alpha\rho)J_1(\alpha\rho)\,d\rho$$

$$x \int_{-\infty}^{\infty} \frac{dz\; e^{-2\beta\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}}$$

A.22

Of the z integrals

$$I_1(z) = \int_{-\infty}^{\infty} \frac{dz\ e^{-2\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

and

$$I_2(z) = \int_{-\infty}^{\infty} dz\ e^{-2\beta\sqrt{\rho^2 + z^2}}$$

the second one $I_2(z)$ has already been evaluated in the calculation of the normalization constant, and the first one is evaluated as follows

$$\int_{-\infty}^{\infty} \frac{dz\ e^{-2\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} = 2\int_{\rho}^{\infty} \frac{r\ e^{-2\beta r} dr}{r(r^2\rho^2)^{1/2}}$$

$$= 2\int_{\rho}^{\infty} e^{-2\beta r}\ (r^2 - \rho^2)^{1/2} dr \qquad \text{A.25}$$

$$= 2K_o(2\beta\rho)$$

In obtaining A.25, the same procedure and substitutions have been used as in Equations A.3, A.4, A.5, A.6 and A.7.

Then < T > becomes

$$< T > = \frac{4\pi h^2 \beta N^2}{m*} \int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho$$

$$- \frac{4\pi h^2 \beta^2 N^2}{2m*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

$$+ \frac{4\pi h^2 \alpha^2 N^2}{2m*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

$$- \frac{4\pi h^2 \alpha\beta N^2}{m*} \int_o^a \rho^2 J_o^2(\alpha\rho) J_1(\alpha\rho) K_o(2\beta\rho)\, d\rho$$

A.26

Now

$$\int_o^a \rho^2 J_o(\alpha\rho) J_1(\alpha\rho) K_o(2\beta\rho)\, d\rho$$

can be further integrated by parts to yield

$$\int_o^a \rho^2 J_o(\alpha\rho) J_1(\alpha\rho) K_o(2\beta\rho)\, d\rho$$

$$= - \frac{1}{2\alpha} \int_o^a \left[\frac{d}{d\rho} J_o^2(\alpha\rho) \right] \rho^2 K_o(2\beta\rho)\, d\rho$$

$$+ \frac{1}{2}\alpha \int_o^a J_o^2(\alpha\rho) \{ 2\rho K_o(2\beta\rho) - 2\beta\rho^2 K_1(2\beta\rho) \}\, d\rho$$

$$= - \frac{1}{2\alpha} J_o^2(\alpha\rho)\, \rho^2 K_o(2\beta\rho) \Big|_o^a$$

$$+ \frac{2}{2\alpha} \int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho - \frac{2\beta}{2\alpha} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

$$= - \frac{1}{2\alpha} J_o^2(\alpha\rho)\, \rho^2 K_o(2\beta\rho) \Big|_o^a$$

$$+ \frac{1}{\alpha} \int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho - \frac{\beta}{\alpha} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

A.27

Considering that the integrated part vanishes at the boundaries, the whole integral becomes:

$$\int_o^a \rho^2 J_o(\alpha\rho)\, J_1(\alpha\rho)\, K_o(2\beta\rho)\, d\rho$$

$$= \frac{1}{\alpha}\int_o^a \rho\ J_o^2(\alpha\rho)\, K_o(2\beta\rho)$$

$$- \frac{\beta}{\alpha}\int_o^a \rho^2\ J_o^2(\alpha\rho)\, K_1(2\beta\rho)\, d\rho$$

A.28

Substituting A.26 back into the expression for the kinetic energy Equation A.26 leads to the following results:

$$\langle T \rangle = \frac{4\pi h^2 \beta N^2}{m*} \int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho$$

$$- \frac{2\pi h^2 \beta^2 N^2}{m*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

$$+ \frac{2\pi h^2 \alpha^2 N^2}{m*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

$$- \frac{4\pi h^2 \alpha\beta N^2}{m*} \frac{1}{\alpha} \int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho$$

$$+ \frac{4\pi h^2 \beta^2 N^2}{m*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

$$= \frac{4\pi h^2 \beta N^2}{m*} \int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho$$

$$- \frac{4\pi h^2 \beta^2 N^2}{2m*} \int_o^a \rho J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

$$+ \frac{4\pi h^2 \alpha^2 N^2}{2m*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

$$- \frac{4\pi h^2 \beta N^2}{m*} \int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho$$

$$+ \frac{4\pi h^2 \beta^2 N^2}{m*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

A.27

Now

$$N^2 = \left[4\pi \int_o^2 \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho\right]^{-1}$$

Equation II-A.7

Substituting this into Equation A.27 leads to

$$< T > = \frac{h^2\alpha^2}{2m*} + \frac{h^2\beta^2}{2m*}$$

A.28

The expectation value of the potential energy is now calculated as follows:

$$< V > = \int_\tau \Psi_{1s}^* \, V \, \Psi_{1s} d\tau$$

$$= - \frac{e^2N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} \frac{dz \; e^{-2\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

$$= - \frac{4\pi e^2N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho J_o^2(\alpha\rho)\, K_o(2\beta\rho)\, d\rho$$

Which on substitution of

$$N^2 = \left[4\pi \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\beta\rho)\, d\rho\right]^{-1}$$

becomes

$$< V > = - \frac{e^2}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho)\, K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\beta\rho)\, d\rho}$$

A.29

The rest of the integrals are non-analytical and therefore are carried out numerically. Here the static dielectric constant $\epsilon(o)$ has been used instead of the spatial dielectric function $\epsilon(r)$.

The expression for the expectation value of the total energy now becomes:

$$< H > = < T > + < V >$$

$$= \frac{h^2\alpha^2}{2m*} + \frac{h^2\beta^2}{2m*}$$

$$- \frac{e^2}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho}$$

The expectation value of the total energy is now minimized with respect to the variational parameter β. The result, $E_{min}(a,\beta)$, is subtracted from the free particle energy $E_f(a)$ to yield the binding energy $E_b(a,\beta)$. Thus, one arrives at

$$E_b(a,\beta) = \frac{h^2\alpha^2}{2m*} - \left\{ \frac{h^2\alpha^2}{2m*} + \frac{h^2\beta^2}{2m*} \right.$$

$$\left. - \frac{e^2}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho} \right\}$$

$$= - \frac{h^2\beta^2}{2m*} + \frac{e^2}{\epsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho} \qquad \text{A.30}$$

Calculation of the expectation value of the potential energy, using the spatial dielectric function, proceeds as follows:

$$\frac{1}{\epsilon(r)} = \frac{1}{\epsilon(o)} + \left(1 - \frac{1}{\epsilon(o)}\right) e^{-\frac{\sqrt{\rho^2 + z^2}}{c}}$$

II.A.13

The expectation value of the potential energy now becomes

$$\langle V \rangle = -e^2 \int_\tau \Psi^*_{1s} \frac{1}{\epsilon(r)\,[\rho^2 + z^2]^{1/2}} \Psi_{1s}\, d\tau$$

$$= - e^2 N^2 \int_o^{2\pi} d\theta \int_o^a \rho\, d\rho \int_{-\infty}^{\infty} dz\, \Psi^*_{1s} \left\{ \frac{1}{\epsilon(o)} + \left(\frac{\epsilon(o) - 1}{\epsilon(o)} \right) e^{-\frac{\sqrt{\rho^2 + z^2}}{c}} \right.$$

$$x \frac{\Psi_{1s}}{[\rho^2 + z^2]^{1/2}}\, d\tau$$

$$= - \frac{e^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho\, d\rho \int_{-\infty}^{\infty} dz \frac{\Psi^*_{1s}\Psi_{1s}}{[\rho^2 + z^2]^{1/2}}$$

$$- \frac{e^2(\epsilon(o) - 1)}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho\, d\rho \int_{-\infty}^{\infty} dz \frac{e^{-\frac{\sqrt{\rho^2 + z^2}}{c}} \Psi^*_{1s}\Psi_{s}}{[\rho^2 + z^2]^{1/2}}$$

A.31

Let $(2\beta + (1/c) = \gamma$ and $r^2 = \rho^2 + z^2$

then $z^2 = r^2 - \rho^2$

$$zdz = rdr$$

$$dz = \frac{rdr}{z}$$

$$= \frac{rdr}{\sqrt{r^2 - \rho^2}} \qquad \text{A.32}$$

Therefore,

$$\Delta V = - \frac{e^2}{\epsilon(0)} (\epsilon(o) - 1) 2\pi N^2$$

$$x \int_o^a \rho J_o^2(\alpha\rho) d\rho \; 2 \int_\rho^\infty \frac{dr e^{-\gamma r}}{\sqrt{\rho^2 + z^2}}$$

$$= - \frac{e^2 (\epsilon(o) - 1}{\epsilon(o)} 4\pi N^2$$

$$x \int_o^a \rho J_o^2(\alpha\rho) K_o(\gamma\rho) d\rho \qquad \text{A.33}$$

This expression is now added to the expression for the expectation value of the total energy in Equation A.30. The result is:

$$E_b(a,\beta) = -\frac{h^2\beta^2}{2m*} + \frac{e^2}{\varepsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho}$$

$$+ \frac{e^2(\varepsilon(o) - 1)}{\varepsilon(o)} \frac{\int_o^a \rho J_o^2(\alpha\rho) K_o(\gamma\rho)\, d\rho}{\int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho}$$

A.34

B. Details of the Calculations of the Ground State Binding Energy with j_o as the Envelope Wave Function.

The normalization constant is obtained as follows:

$$1 = N^2 \int_\tau \Psi_{1s}^* \Psi_{1s} \, d\tau$$

$$= N^2 \int_o^{2\pi} d\theta \int_o^a \rho \, j_o^2(\mu\rho) \, d\rho \int_{-\infty}^{\infty} dz \, e^{-2\beta\sqrt{\rho^2 + z^2}}$$

$$= 4\pi N^2 \int_o^a \rho^2 j_o^2(\mu\rho) K_1(2\beta\rho) \, d\rho$$

B.1

Therefore, the normalization constant becomes

$$N^2 = \frac{1}{4\pi \int_o^a \rho^2 j_o^2(\mu\rho) K_1(2\beta\rho) \, d\rho}$$

$$= \frac{\alpha^2}{4\pi \int_o^a \sin^2\mu\rho K_1(2\beta\rho) \, d\rho}$$

$$= \mu^2 [4\pi \int_o^a \sin^2\mu\rho K_1(2\beta\rho) \, d\rho]^{-1}$$

B.2

Calculation of the Expectation Value of the Kinetic Energy $< T >$.

$$\Psi_{1s}(\rho, z) = N j_o(\mu\rho)\, e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$\nabla^2 \Psi_{1s}(\rho, z) = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho \frac{\partial}{\partial\rho}\right]\Psi_{1s}(\rho, z) + \frac{\partial^2}{\partial z^2}\Psi_{1s}(\rho, z)$$

B.3

The first ρ differentiation gives:

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho \frac{\partial}{\partial\rho}\right] N \frac{\sin\mu\rho}{\mu\rho}\, e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= \frac{N}{\rho}\frac{\partial}{\partial\rho}\left[\rho \frac{\partial}{\partial\rho}\frac{\sin\mu\rho}{\mu\rho}\, e^{-\beta\sqrt{\rho^2 + z^2}}\right]$$

$$= \frac{N}{\mu\rho}\frac{\partial}{\partial\rho}\left\{\rho\left[\frac{-\sin\mu\rho}{\rho^2} + \frac{\mu\cos\mu\rho}{\rho}\right.\right.$$

B.4

$$\left.\left. - \frac{\beta\rho\sin\mu\rho}{\rho\sqrt{\rho^2 + z^2}}\right]\right\} x\, e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= \frac{N}{\mu\rho}\frac{\partial}{\partial\rho}\left\{\frac{-\sin\mu\rho}{\rho} + \mu\cos\mu\rho\right.$$

$$\left. - \frac{\beta\sin\mu\rho}{\sqrt{\rho^2 + z^2}}\right\} x\, e^{-\beta\sqrt{\rho^2 + z^2}}$$

The second ρ differentiation leads to

$$\frac{N}{\mu\rho}\left\{\frac{\sin\mu\rho}{\rho^2} - \frac{\mu\cos\mu\rho}{\rho}\right.$$

$$- \frac{\sin\mu\rho}{\rho}\frac{(-\beta\rho)}{\sqrt{\rho^2 + z^2}} - \mu^2\sin\mu\rho$$

$$+ \mu\cos\mu\rho\frac{(-\beta\rho)}{\sqrt{\rho^2 + z^2}} - \frac{\beta\sin\mu\rho}{\sqrt{\rho^2 + z^2}}$$

$$- \frac{\mu\beta\rho\cos\mu\rho}{\sqrt{\rho^2 + z^2}} - \frac{\beta\rho\sin\mu\rho(-\rho)}{[\rho^2 + z^2]^{3/2}}$$

$$\left. - \frac{\beta\rho\sin\mu\rho}{[\rho^2 + z^2]}(-\beta\rho)\right\} x\ e^{-\beta\sqrt{\rho^2 + z^2}} \qquad \text{B.5}$$

$$= \left\{\frac{N\sin\mu\rho}{\mu\rho^3} - \frac{N\cos\mu\rho}{\rho^2} + \frac{\beta N\sin\mu\rho}{\mu\rho\sqrt{\rho^2 + z^2}} + \frac{\beta N\cos\mu\rho}{\sqrt{\rho^2 + z^2}}\right.$$

$$- \frac{\beta N\cos\mu\rho}{\sqrt{\rho^2 + z^2}} - \frac{\beta N\sin\mu\rho}{\mu\rho\sqrt{\rho^2 + z^2}} - \frac{\beta N\cos\mu\rho}{\sqrt{\rho^2 + z^2}}$$

$$\left. + \frac{\beta N\rho\sin\mu\rho}{[\rho^2 + z^2]^{3/2}} + \frac{\beta^2 N\rho\sin\mu\rho}{[\rho^2 + z^2]}\right\} x\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

B.5'

$$\nabla_z^2 \, \Psi_{1s}(\rho, z) = \frac{N sin\mu\rho}{\mu\rho} \frac{\partial^2}{\partial z^2} e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= \frac{N sin\mu\rho}{\mu\rho} \frac{\partial}{\partial\rho} \left\{ - \frac{\beta \; z \; e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} \right\}$$

$$= \frac{N sin\mu\rho}{\mu\rho} \left\{ - \frac{\beta}{\sqrt{\rho^2 + z^2}} + \frac{\beta z^2}{[\rho^2 + z^2]^{3/2}} \right.$$

$$\left. + \frac{\beta^2 z^2}{[\rho^2 + z^2]} \right\} x \; e^{-\beta\sqrt{\rho^2 + z^2}}$$

B.6

$$= \left\{ - \frac{\beta N sin\mu\rho}{\mu\rho\sqrt{\rho^2 + z^2}} + \frac{\beta N sin\mu\rho \; z^2}{\mu\rho\,[\rho^2 + z^2]^{3/2}} \right.$$

$$\left. + \frac{\beta^2 N sin\mu\rho \; z^2}{\mu\rho\,[\rho^2 + z^2]} \right\} x \; e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= - \frac{\beta N sin\mu\rho}{\mu\rho\sqrt{\rho^2 + z^2}} e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$+ \frac{\beta N sin\mu\rho \; z^2}{\mu\rho\,[\rho^2 + z^2]^{3/2}} e^{-\beta\sqrt{\rho^2 + z^2}} + \frac{\beta^2 N sin\mu\rho}{\mu\rho\,[\rho^2 + z^2]} e^{-\beta\sqrt{\rho^2 + z^2}}$$

B.6'

Adding Equation B.5 and B.6' gives the following expression for $\nabla^2 \psi_{1s}(\rho,z)$

$$\nabla^2 \Psi_{1s}(\rho,z) = \frac{N}{\mu} e^{-\beta\sqrt{\rho^2+z^2}} \left\{ \frac{\sin\mu\rho}{\rho^3} - \frac{\mu\cos\mu\rho}{\rho^2} \right.$$

$$+ \frac{\beta\sin\mu\rho}{\rho\sqrt{\rho^2+z^2}} - \frac{\mu^2\sin\mu\rho}{\rho} - \frac{\mu\beta\cos\mu\rho}{\sqrt{\rho^2+z^2}}$$

$$- \frac{\beta\sin\mu\rho}{\rho\sqrt{\rho^2+z^2}} - \frac{\mu\beta\cos\mu\rho}{\sqrt{\rho^2+z^2}} + \frac{\beta\rho^2\sin\mu\rho}{\rho[\rho^2+z^2]^{3/2}}$$

$$+ \frac{\beta^2\rho^2\sin\mu\rho}{\rho[\rho^2+z^2]} - \frac{\beta\sin\mu\rho}{\rho\sqrt{\rho^2+z^2}} + \frac{\beta\sin\mu\rho}{\rho[\rho^2+z^2]^{3/2}} z^2$$

$$\left. + \frac{\beta^2\sin\mu\rho}{\rho[\rho^2+z^2]} z^2 \right\}$$

B.7

$$= \frac{N e^{-\beta\sqrt{\rho^2+z^2}}}{\mu} \left\{ \frac{\beta\sin\mu\rho(\rho^2+z^2)}{\rho[\rho^2+z^2]^{3/2}} + \frac{\beta^2\sin\mu\rho(\rho^2+z^2)}{\rho[\rho^2+z^2]} \right.$$

$$- \frac{2\mu\beta\cos\mu\rho}{\sqrt{\rho^2+z^2}} + \frac{\sin\mu\rho}{\rho^3} - \frac{\mu\cos\mu\rho}{\rho^2}$$

$$\left. - \frac{\mu^2\sin\mu\rho}{\rho} - \frac{\beta\sin\mu\rho}{\rho\sqrt{\rho^2+z^2}} \right\}$$

B.7'

$$= \frac{N}{\rho} e^{-\beta\sqrt{\rho^2 + z^2}} \left\{ \frac{\beta^2 \sin\mu\rho}{\rho^2} - \frac{2\mu\beta\cos\mu\rho}{\sqrt{\rho^2 + z^2}} + \frac{\sin\mu\rho}{\rho^3} \right.$$

$$\left. - \frac{\mu\cos\mu\rho}{\rho^2} - \frac{\mu^2 \sin\mu\rho}{\rho} \right\}$$

$$= \frac{N}{\rho} \left\{ \frac{\beta^2 \sin\mu\rho}{\rho^2} - \frac{2\mu\beta\cos\mu\rho}{\sqrt{\rho^2 + z^2}} + \frac{\sin\mu\rho}{\rho^3} \right.$$

$$\left. - \frac{\mu\cos\mu\rho}{\rho^2} - \frac{\mu^2 \sin\mu\rho}{\rho} \right\} x\, e^{-\beta\sqrt{\rho^2 + z^2}}$$

B.8

The result in Equation B.8 is now multiplied by ψ_{1s} to obtain:

$$\Psi^*_{1s} \nabla^2 \Psi_{1s} = \frac{N\sin\mu\rho}{\mu\rho} \frac{N}{\mu} e^{-2\beta\sqrt{\rho^2 + z^2}}\, x$$

$$\left\{ \frac{\beta^2 \sin\mu\rho}{\rho^2} - \frac{2\mu\beta\cos\mu\rho}{\sqrt{\rho^2 + z^2}} + \frac{\sin\mu\rho}{\rho^3} - \frac{\mu\cos\mu\rho}{\rho^2} \right.$$

$$\left. - \frac{\mu^2 \sin\mu\rho}{\rho} \right\}$$

B.9

This expression is further multiplied by $\frac{-\hbar^2}{2m*}$. This gives

$$\Psi^*_{1s}\left(-\frac{h^2}{2m*}\nabla^2\Psi_{1s}\right)$$

$$= -\frac{h^2N^2}{2\mu^2m^*}\left\{\frac{\beta^2\sin^2\mu\rho}{\rho^3} - 2\mu\beta\sin\mu\rho\cos\mu\rho + \frac{\sin^2\mu\rho}{\rho^4}\right.$$

$$\left. - \frac{\mu\sin\mu\rho\cos\mu\rho}{\rho^3}\right\} x\ e^{-2\beta\sqrt{\rho^2+z^2}}$$

B.10

$$= \left\{-\frac{h^2\beta^2N^2\sin^2\mu\rho}{2\mu^2m^*\rho^2} + \frac{h^2\beta N^2\sin\mu\rho\cos\mu\rho}{\mu m\rho\sqrt{\rho^2+z^2}}\right.$$

$$- \frac{h^2N^2\sin^2\mu\rho}{2\mu^2m^*\rho^4} + \frac{h^2N^2\sin\mu\rho\cos\mu\rho}{2\mu m^*\rho^3}$$

$$\left. + \frac{h^2N^2\sin^2\mu\rho}{2m^*\rho^2}\right\} x\ e^{-\beta\sqrt{\rho^2+z^2}}$$

B.11

The expectation value of the kinetic energy is now obtained by integrating the terms in B.11 one by one:

$$< T > = - \frac{h^2\beta^2N^2}{2m^*\mu^2} \int_o^{2\pi} d\theta \int_o^a \frac{\rho\sin^2\mu\rho}{\rho^3} \, d\rho \int_{-\infty}^{\infty} dz \; e^{-2\beta\sqrt{\rho^2 + z^2}}$$

$$+ \frac{h^2\beta N^2}{m^*\mu} \int_o^{2\pi} d\theta \int_o^a \frac{\rho\sin\mu\rho\cos\mu\rho}{\rho} \, d\rho \int_{-\infty}^{\infty} \frac{dz \; e^{-2\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

$$- \frac{h^2N^2}{2m^*\mu^2} \int_o^{2\pi} d\theta \int_o^a \frac{\rho\sin^2\mu\rho}{\rho^4} \, d\rho \int_{-\infty}^{\infty} dz \; e^{-2\beta\sqrt{\rho^2 + z^2}}$$

$$+ \frac{h^2N^2}{2m^*\mu^2} \int_o^{2\pi} d\theta \int_o^a \frac{\rho\sin\mu\rho\cos\mu\rho}{\rho^3} \, d\rho \int_{-\infty}^{\infty} dz \; e^{-2\beta\sqrt{\rho^2 + z^2}}$$

$$+ \frac{h^2N^2}{2m^*} \int_o^{2\pi} d\theta \int_o^a \frac{\rho\sin^2\mu\rho}{\rho^2} \, d\rho \int_{-\infty}^{\infty} dz \; e^{-2\beta\sqrt{\rho^2 + z^2}} \qquad \text{B.12}$$

Using the integrals

$$\int_{-\infty}^{\infty} dz \; e^{-2\beta\sqrt{\rho^2 + z^2}} = 2\rho K_1(2\beta\rho)\, d\rho$$

and

$$\int_{-\infty}^{\infty} \frac{dz \; e^{-2\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} = 2 \; K_o(2\beta\rho)\, d\rho$$

the final expression for the expectation value of the kinetic energy is:

$$< T > = -\frac{2\pi h^2\beta^2N^2}{m^*\mu^2}\int_o^a \frac{\sin^2\mu\rho}{\rho} K_1(2\beta\rho)\,d\rho$$

$$+\frac{4\pi h^2\beta N^2}{m^*\mu}\int_o^a \sin\mu\rho\,\cos\mu\rho\; K_o(2\beta\rho)\,d\rho$$

$$-\frac{2\pi h^2N^2}{m^*\mu^2}\int_o^a \frac{\sin^2\mu\rho}{\rho^2} K_1(2\beta\rho)\,d\rho$$

$$+\frac{2\pi h^2N^2}{m^*\mu}\int_o^a \frac{\sin\mu\rho\,\cos\mu\rho}{\rho} K_1(2\beta\rho)\,d\rho$$

$$+\frac{2\pi h^2N^2}{m^*}\int_o^a \sin^2\mu\rho\; K_1(2\beta\rho)\,d\rho$$

$$= -\frac{2\pi h^2\beta^2N^2}{m^*\mu^2}\int_o^a \frac{\sin^2\mu\rho}{\rho} K_1(2\beta\rho)\,d\rho$$

$$+\frac{4\pi h2\beta N^2}{m^*\mu}\int_o^a \sin\mu\rho\,\cos\mu\rho\; K_o(2\beta\rho)\,d\rho$$

$$-\frac{2\pi h^2N^2}{m^*\mu^2}\int_o^a \frac{\sin^2\mu\rho}{\rho^2} K_1(2\beta\rho)\,d\rho$$

$$+\frac{2\pi h^2N^2}{m^*\mu}\int_o^a \frac{\sin\mu\rho\,\cos\mu\rho}{\rho} K_1(2\beta\rho)\,d\rho$$

$$+\frac{h^2\mu^2}{2m^*}$$

B.13

where

$$N^2 + \mu^2[4\pi\int_o^a \sin^2\mu\rho\; K_1(2\beta\rho)\,d\rho]^{-1}$$

B.14

has been used in the last term.

The determination of the expectation value of the potential energy with the spatial dielectric function is done as follows:

$$\frac{1}{\epsilon(r)} = \frac{1}{\epsilon(o)} + \left(1 - \frac{1}{\epsilon(o)}\right) e^{-\frac{\sqrt{\rho^2 + z^2}}{c}}$$

II-A.13

where

$$\left(1 - \frac{1}{\epsilon(o)}\right) e^{-\frac{\sqrt{\rho^2 + z^2}}{c}}$$

is treated as a small quantity in the expectation value of the total energy:

$$< H > = < T > + < V > + \Delta V$$

B.17

where < T > and < V > have already been determined in Equations B.13 and B.15.

$$\Delta V = - \frac{e^2}{\epsilon(o)} (\epsilon(o) - 1) N^2 \int_o^{2\pi} d\theta \int_o^a \frac{\rho \sin^2\mu\rho}{\mu^2\rho^2} d\rho \ x$$

$$\int_{-\infty}^{\infty} \frac{dz \ e^{-(2\beta + \frac{1}{c})\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

B.17'

$$= - \frac{4\pi e^2 N^2 (\epsilon(o) - 1)}{\epsilon(o) \mu^2} \int_o^a \frac{\sin^2\mu\rho}{\rho} K_o\left[\left(2\beta + \frac{1}{c}\right)\rho\right] d\rho$$

B.17''

Therefore, with the spatial dielectric function, the expectation value of the total energy becomes:

$$
\begin{aligned}
\langle H \rangle = & - \frac{2\pi h^2\beta^2 N^2}{m^*\mu^2} \int_o^a \frac{\sin^2\mu\rho}{\rho} K_1(2\beta\rho)\,d\rho \\
& + \frac{4\pi h^2\beta N^2}{m^*\mu} \int_o^a \sin\mu\rho \cos\mu\rho\, K_o(2\beta\rho)\,d\rho \\
& - \frac{2\pi h^2 N^2}{m^*\mu^2} \int_o^a \frac{\sin^2\mu\rho}{\rho^2} K_1(2\beta\rho)\,d\rho \\
& + \frac{2\pi h^2 N^2}{m^*\mu} \int_o^a \frac{\sin\mu\rho \cos\mu\rho}{\rho} K_1(2\beta\rho)\,d\rho \\
& + \frac{h^2\mu^2}{2m^*} - \frac{4\pi e^2 N^2}{\epsilon(o)} \int_o^a \frac{\sin^2\mu\rho}{\rho} K_o(2\beta\rho)\,d\rho \\
& - \frac{4\pi e^2(\epsilon(o) - 1)N^2}{\epsilon(o)\mu^2} \int_o^a \frac{\sin^2\mu\rho}{\rho} K_o\left[\left(2\beta + \frac{1}{c}\right)\rho\right] d\rho \\
= & \langle H \rangle + \Delta V
\end{aligned}
$$

B.18

The binding energy $E_b(a,\beta)$ with static dielectric constant $\epsilon(o)$ is given by:

$$E_b(a,\beta) = \frac{h^2\alpha^2}{2m^*} - \langle H \rangle_{min}$$

$$= \frac{h^2\alpha^2}{2m^*} - \left\{ - \frac{2\pi h^2\beta^2 N^2}{m^*\mu^2} \int_o^a \frac{\sin^2\mu\rho}{\rho} K_1(2\beta\rho)\,d\rho \right.$$

$$+ \frac{4\pi h^2\beta N^2}{m^*\mu} \int_o^a \sin\mu\rho \cos\mu\rho \; K_o(2\beta\rho)\,d\rho$$

$$- \frac{2\pi h^2 N^2}{m^*\mu^2} \int_o^a \frac{\sin^2\mu\rho}{\rho^2} K_1(2\beta\rho)\,d\rho$$

$$+ \frac{2\pi h^2 N^2}{m^*\mu} \int_o^a \frac{\sin\mu\rho \cos\mu\rho}{\rho} K_1(2\beta\rho)\,d\rho$$

$$\left. + \frac{h^2\mu^2}{2m^*} - \frac{4\pi e^2 N^2}{\epsilon(o)} \int_o^a \frac{\sin^2\mu\rho}{\rho} K_o(2\beta\rho)\,d\rho \right\} \qquad \text{B.19}$$

The binding energy $E_b'(a,\beta)$, with the spatial dielectric function $\epsilon(r)$, is given by:

$$E_b'(a,\beta) = \frac{h^2\alpha^2}{2m^*} - \Bigg\{ - \frac{2\pi h^2\beta^2 N^2}{m^*\mu^2} \int_o^a \frac{\sin^2\mu\rho}{\rho} K_1(2\beta\rho)\,d\rho$$

$$+ \frac{4\pi h^2\beta N^2}{m^*\mu} \int_o^a \sin\mu\rho \cos\mu\rho\, K_o(2\beta\rho)\,d\rho$$

$$- \frac{2\pi h^2 N^2}{m^*\mu^2} \int_o^a \frac{\sin^2\mu\rho}{\rho^2} K_1(2\beta\rho)\,d\rho$$

$$+ \frac{2\pi h^2 N^2}{m^*\mu} \int_o^a \frac{\sin\mu\rho \cos\mu\rho}{\rho} K_1(2\beta\rho)\,d\rho$$

$$+ \frac{h^2\mu^2}{2m^*} - \frac{4\pi e^2 N^2}{\epsilon(o)} \int_o^a \frac{\sin^2\mu\rho}{\rho} K_o(2\beta\rho)\,d\rho$$

$$- \frac{4\pi e^2(\epsilon(o) - 1)N^2}{\epsilon(o)\mu^2} \int_o^a \frac{\sin^2\mu\rho}{\rho} K_o\left[\left(2\beta + \frac{1}{c}\right)\rho\right] d\rho \Bigg\}$$

B.20

$$= \langle H \rangle + \Delta V$$

B.20'

C. Details of the Calculations of the Ground State Binding Energy with Unity as the Envelope Wave Function.

Here the detailed calculation of the normalization constant is given.

$$1 = \int_\tau \Psi_{1s}^* \Psi_{1s} \, d\tau$$

$$= N^2 \int_o^{2\pi} d\theta \int_\rho^a \rho \, d\rho \int_{-\infty}^{\infty} dz \, e^{-2\beta\sqrt{\rho^2 + z^2}} \qquad \text{C.21}$$

$$= 4\pi N^2 \int_o^a \rho^2 K_1(2\beta\rho) \, d\rho$$

Therefore,

$$N^2 = \left[4\pi \int_o^a \rho^2 K_1(2\beta\rho) \, d\rho \right]^{-1}$$

The detailed calculation of the binding energy of an on-axis donor proceeds as follows:

$$\Psi_{1s}(\rho, z) = N \, e^{-\beta\sqrt{\rho^2 + z^2}} \qquad \text{II.C.1}$$

Now

$$\nabla^2 = \frac{1}{\rho} \frac{\partial}{\partial\rho} \left[\rho \frac{\partial}{\partial\rho} \right] + \frac{\partial^2}{\partial z^2} \qquad \text{C.22}$$

Operating on the wave function with ∇^2, first beginning with the ρ part, the result is:

$$\nabla_\rho^2 \; \Psi_{1s}(\rho, z)$$

$$= \frac{N}{\rho} \frac{\partial}{\partial \rho} \left\{ \rho \frac{\partial}{\partial \rho} e^{-\beta\sqrt{\rho^2 + z^2}} \right\}$$

C.23

$$= \frac{N}{\rho} \frac{\partial}{\partial \rho} \left\{ \rho \left[\frac{(-\beta\rho) \; e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} \right] \right\}$$

$$= \frac{N}{\rho} \frac{\partial}{\partial \rho} \left\{ - \frac{\beta\rho^2 \; e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} \right\}$$

$$= \frac{N}{\rho} \left\{ - \frac{2\beta\rho \; e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} + \frac{\beta\rho^3 \; e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]^{3/2}} \right.$$

$$\left. + \frac{\beta^2\rho^3 \; e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]} \right\}$$

$$= - \frac{2\beta N \; e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} + \frac{\beta N\rho^2 \; e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]^{3/2}}$$

$$+ \frac{\beta^2 N\rho^2 \; e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]}$$

C.24

The z part of the differentiation is performed as follows:

$$\nabla_z^2 \Psi_{1s}(\rho, z) = N \frac{\partial^2}{\partial z^2} e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= N \frac{\partial}{\partial z} \left\{ - \frac{\beta z \, e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} \right\}$$

$$= N \left\{ - \frac{\beta \, e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} + \frac{\beta \, z^2 \, e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]^{3/2}} \right.$$

$$\left. + \frac{\beta^2 z^2 \, e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]} \right\}$$

$$= - \frac{\beta \, N \, e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} + \frac{\beta \, N \, z^2 \, e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]^{3/2}}$$

$$+ \frac{\beta^2 \, N \, z^2 \, e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]}$$

$\nabla^2 \psi_{1s}(\rho, z)$ is obtained by adding Equations C.24 and C.25, resulting in:

$$\nabla^2 \Psi_{1s}(\rho, z) = - \frac{2\beta N e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} + \frac{\beta N \rho^2 e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]^{3/2}}$$

$$+ \frac{\beta^2 N \rho^2 e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]}$$

$$- \frac{\beta N e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} + \frac{\beta N z^2 e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]^{3/2}}$$

$$+ \frac{\beta^2 N z^2 e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]}$$

$$= -3\beta N e^{-\beta\sqrt{\rho^2 + z^2}} + \frac{\beta N (\rho^2 + z^2) e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]^{3/2}}$$

$$+ \frac{\beta^2 N (\rho^2 + z^2) e^{-\beta\sqrt{\rho^2 + z^2}}}{[\rho^2 + z^2]}$$

$$= - \frac{2\beta N e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} + \beta^2 N e^{-\beta\sqrt{\rho^2 + z^2}}$$

C.26

Therefore,

$$\nabla^2 \Psi_{1s}(\rho, z) = - \frac{2\beta N e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

$$+ \beta^2 N e^{-\beta\sqrt{\rho^2 + z^2}}$$

C.26'

Multiplication of Equation G.5' by $-\dfrac{\hbar^2}{2m^*}$ and $\psi_{1s}(\rho,z)$ gives

$$\Psi^*_{1s}(\rho,z)\left(-\frac{h^2}{2m^*}\nabla^2\,\Psi_{1s}(\rho,z)\right)$$

$$= \frac{h^2\beta N^2\, e^{-2\beta\sqrt{\rho^2+z^2}}}{m*\sqrt{\rho^2+z^2}}$$

$$- \frac{h^2\beta^2 N^2\, e^{-2\beta\sqrt{\rho^2+z^2}}}{2m^*}$$

C.27

Integration of the two terms in Equation C.30 gives the expectation value of < T >. The integration proceeds as follows:

$$\langle T \rangle = \int_\tau \Psi^*_{1s}\left(-\frac{h^2\nabla^2\,\Psi_{1s}}{2m^*}\right) d\tau$$

$$= \frac{h^2\beta N^2}{m^*}\int_o^{2\pi} d\theta \int_o^a \rho\, d\rho \int_{-\infty}^{\infty} \frac{dz\; e^{-2\beta\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}}$$

$$- \frac{h^2\beta^2 N^2}{2m^*}\int_o^{2\pi} d\theta \int_o^a \rho\, d\rho \int_{-\infty}^{\infty} dz\; e^{-2\beta\sqrt{\rho^2+z^2}}$$

$$= \frac{4\pi h^2\beta N^2}{m^*}\int_o^a \rho\, K_o(2\beta\rho)\, d\rho$$

$$- \frac{4\pi h^2\beta^2 N^2}{2m^*}\int_o^a \rho^2\, K_1(2\beta\rho)\, d\rho$$

C.28

The evaluation of the expectation value of the potential energy with the static dielectric constant proceeds as follows:

$$< V > = \frac{-e^2}{\epsilon(o)} \int_\tau \Psi^*_{1s}(\rho, z) \frac{1}{[\rho^2 + z^2]^{1/2}} \Psi_{1s}(\rho, z)\, d\tau$$

$$= - \frac{e^2 N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho\, d\rho \int_{-\infty}^{\infty} dz \frac{e^{-2\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

$$= - \frac{4\pi e^2 N^2}{\epsilon(o)} \int_o^a \rho\, K_o(2\beta\rho)\, d\rho$$

C.29

The expectation value of the total energy becomes:

$$< H > = < T > + < V >$$

$$= \frac{h^2 \beta N^2}{m^*} \frac{\int_o^a \rho\, K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2\, K_1(2\beta\rho)\, d\rho} - \frac{h^2\beta^2}{2m^*}$$

$$- \frac{4\pi e^2 N^2}{\epsilon(o)} \int_o^a \rho\, K_o(2\beta\rho)\, d\rho$$

C.30

When the static dielectric constant is replaced by the spatial dielectric function, the expectation value of the potential energy is calculated in the following fashion:

$$< V' > = < V > + \Delta V$$

C.31

$$= - e^2 \int_\tau \Psi^*_{1s} \left(\frac{1}{\epsilon(r)} \right) \Psi_{1s} d\tau$$

$$= - e^2N^2 \int_p^{2\pi} d\theta \int_o^a \rho\, d\rho \int_{-\infty}^{\infty} dz \left[\frac{1}{\epsilon(o)} + \frac{(\epsilon(o) - 1)}{\epsilon(o)} e^{-\frac{\sqrt{\rho^2 + z^2}}{c}} \right]$$

$$x \frac{e^{-2\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

$$= - \frac{2\pi e^2N^2}{\epsilon(o)} \int_o^a \rho\, d\rho \int_{-\infty}^{\infty} dz \frac{e^{-2\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

$$- \frac{2\pi e^2N^2}{\epsilon(o)} (\epsilon(o) - 1) \int_o^a \rho\, d\rho \int_{-\infty}^{\infty} dz \frac{e^{-(2\beta + \frac{1}{c})\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

C.32

The first term becomes

$$- \frac{4\pi e^2N^2}{\epsilon(o)} \int_o^a \rho\, K_o(2\beta\rho)\, d\rho = - \frac{e^2\beta}{\epsilon(o)}$$

and the second term becomes

$$- \frac{4\pi e^2N^2 (\epsilon(o) - 1)}{\epsilon(o)} \int_o^a \rho\, K_o[(2\beta + \frac{1}{c})\rho]\, d\rho$$

and the expression for the expectation value of the potential energy becomes

$$< V' > = - \frac{e^2(\epsilon)o) - 1)}{\epsilon(o)} \frac{\int_o^a \rho\, K_o[(2\beta + \frac{1}{c})\rho]\, d\rho}{\int_o^a \rho^2\, K_1(2\beta\rho)\, d\rho}$$

C.33

$$- \frac{e^2}{\epsilon(o)} \frac{\int_o^a \rho K_o(2\beta\rho)\, d\rho}{\int_o^a \rho^2 K_1(2\beta\rho)\, d\rho}$$

The expression for the expectation value of the total energy now becomes:

$$< H' > = < H > + \Delta V$$

$$< T > - \frac{e^2}{\epsilon o} \frac{\int_o^a \rho \; K_o(2\beta\rho)\,d\rho}{\int_o^a \rho^2 \; K_1(2\beta\rho)\,d\rho} - \frac{e^2(\epsilon(o) - 1)}{\epsilon(o)} \frac{\int_o^a \rho \; K_o[(2\beta + \frac{1}{C})\;\rho]\,d\rho}{\int_o^a \rho^2 K_1(2\beta\rho)\,d\rho} \qquad \text{C.34}$$

With this result, the binding energy becomes:

$$E_b(a,\beta) = \frac{h^2\alpha^2}{2m^*} - < T > + \frac{e^2}{\epsilon(o)} \frac{\int_o^a \rho \; K_o(2\beta\rho)\,d\rho}{\int_o^a \rho^2 \; K_1(2\beta\rho)\,d\rho}$$

$$+ \frac{e^2(\epsilon(o) - 1)}{\epsilon(o)} \qquad \text{C.36}$$

$$x \frac{\int_o^a \rho \; K_o[(2\beta + \frac{1}{C})\,\rho]\,d\rho}{\int_o^a \rho^2 K_1(2\beta\rho)\,d\rho}$$

The final results are obtained using numerical techniques.

D. Calculation of the Binding Energy of an On-Axis Hydrogenic and Non-Hydrogenic Donor in the First Excited (2s) State.

In this appendix are presented the detailed calculations for the binding energy of an on-axis donor in its first excited 2s state.

The trial wave function is chosen as

$$\Phi_{2s}(\rho, z) = NJ_o(\alpha, \rho) \left\{ e^{-\beta\sqrt{\rho^2 + z^2}} + 2K\, e^{-\lambda\sqrt{\rho^2 + z^2}} - \lambda\, K\sqrt{\rho^2 + z^2}\; e^{-\lambda\sqrt{\rho^2 + z^2}} \right\} \qquad \text{D.1}$$

where λ is a variational parameter, β is the variational parameter which was obtained in the calculation of the binding energy of the 1s state of an on-axis hydrogenic donor using the static dielectric constant $\epsilon(o)$. K is the orthogonality constant. This constant appears since $\phi_{2s}(\rho,z)$ is orthogonalized to $\psi_{1s}(\rho,z)$ the ground state trial wave function. The orthogonality requirement is

$$\int_\tau \Psi_{1s}^*(\rho, z)\; \Phi_{2s}(\rho, z)\, d\tau = 0 \qquad \text{D.1'}$$

This can be written as:

$$\int_\tau \left\{ A\, N\, J_o^2(\alpha\rho)\, e^{-2\beta\sqrt{\rho^2 + z^2}} + 2\, K\, A\, N\, J_o^2(\alpha\rho)\, e^{(\beta + \lambda)\sqrt{\rho^2 + z^2}} - \lambda\, K\, A\, N\, J_o^2(\alpha\rho)\sqrt{\rho^2 + z^2}\; e^{-(\beta + \lambda)\sqrt{\rho^2 + z^2}} \right\} d\tau = 0 \qquad \text{D.2}$$

where A is the normalization constant in $\psi_{1s}(\rho,z)$. The quantities A and N cancel out and the remaining integrals can be evaluated from:

$$\int_o^a d\theta \int_o^a \rho\, J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\; e^{-2\beta\sqrt{\rho^2 + z^2}} \qquad \text{D.3}$$

$$2K \int_o^{2\pi} d\theta \int_o^a \rho\, J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\; e^{-(\beta + \lambda)\sqrt{\rho^2 + z^2}} \qquad \text{D.4}$$

$$-\lambda K \int_o^{2\pi} d\theta \int_o^a \rho\, J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\, \sqrt{\rho^2+z^2}\; e^{-(\beta+\lambda)\sqrt{\rho^2+z^2}} \qquad \text{D.5}$$

Integration of the first term of D.3 gives:

$$\int_o^{2\pi} d\theta \int_o^a \rho\, J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\; e^{-2\beta\sqrt{\rho^2 + z^2}} \qquad \text{D.6}$$

$$= 4\pi \int_o^a \rho^2\, J_o^2(\alpha\rho)\, K_1(2\beta\rho)\, d\rho$$

while the second term D.4 becomes:

$$2K \int_o^{2\pi} d\theta \int_o^a \rho\, J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\; e^{-(\beta + \lambda)\sqrt{\rho^2 + z^2}} \qquad \text{D.7}$$

$$= 8\,\pi\, K \int_o^a \rho^2\, J_o^2(\alpha\rho)\, K_1[(\beta + \lambda)\rho]\, d\rho$$

The third term D.5 yields

$$-\lambda\ K \int_0^{2\pi} d\theta \int_0^a \rho\ J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\ \sqrt{\rho^2 + z^2}\ e^{-(\beta+\lambda)\sqrt{\rho^2+z^2}}$$

$$= -\ 2\pi\ \lambda K \int_0^a \rho\ J_o^2(\alpha\rho)\{\ 2\rho K_o[(\beta+\lambda)\rho]$$

$$+\ \frac{2\rho K_1[(\beta+\lambda)\rho]}{(\beta+\lambda)\rho}\Big\}\ d\rho$$

$$= -4\pi\lambda K \int_0^a \rho^3 J_o^2(\alpha\rho)\, K_o\{\ (\beta+\lambda)\rho\ \}\ d\rho \qquad \text{D.8}$$

$$-\ \frac{4\pi\lambda K}{(\beta+\lambda)} \int_0^a \rho^2 J_o^2(\alpha\rho)\, K_1\{\ (\beta+\lambda)\rho\ \}\ d\rho$$

Adding D.3, D.4 and D.5, one obtains

$$-\ 4\pi\ \lambda K \int_0^a \rho^3\ J_o^2(\alpha\rho)\, K_o[(\beta+\lambda)\rho]\, d\rho$$

$$-\ \frac{4\pi\lambda K}{(\beta+\lambda)} \int_0^a \rho^2\ J_o^2(\alpha\rho)\, K_1[(\beta+\lambda)\rho]\, d\rho$$

$$= 0$$

D.9

Solving for K gives

$$K\left\{ 2\int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1[(\beta+\lambda)\rho]\, d\rho \right.$$

$$- \lambda \int_o^a \rho^3\, J_o^2(\alpha\rho)\, K_o[(\beta+\lambda)\rho]\, d\rho$$

$$\left. - \frac{\lambda}{(\beta+\lambda)} \int_o^a \rho^2\, J_o^2(\alpha\rho)\, K_1[(\beta+\lambda)\rho]\, d\rho \right\} \qquad \text{D.10}$$

$$= - \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\beta\rho)\, d\rho$$

Thus

$$K = - \frac{\int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\beta\rho)\, d\rho}{\left\{\left[2 - \frac{\lambda}{(\beta+\lambda)} \right] \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1[(\beta+\lambda)\rho]\, d\rho - \lambda \int_o^a \rho^3 J_o^2(\alpha\rho)\, K_o[(\beta+\lambda)\rho]\, d\rho \right\}} \qquad \text{D.11}$$

The calculations of the normalization constant N proceeds from

$$\int_\tau \Phi_{2s}^* \, \Phi_{2s}\, d\tau = 1 \qquad \text{D.12}$$

$$\Phi_{2s}^{*}\,\Phi_{2s} = N^2 J_o^2(\alpha\rho)\, e^{-2\beta\sqrt{\rho^2 + z^2}} \qquad \text{D.12.a}$$

$$+\ 4KN^2 J_o^2(\alpha\rho)\, e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}} \qquad \text{D.12.b}$$

$$-\ 2\lambda KN^2 J_o^2(\alpha\rho)\sqrt{\rho^2 + z^2}\ e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}} \qquad \text{D.12.c}$$

$$+\ 4K^2N^2 J_o^2(\alpha\rho)\ e^{-2\lambda\sqrt{\rho^2 + z^2}} \qquad \text{D.12.d}$$

$$-\ 4\lambda K^2N^2 J_o^2(\alpha\rho)\sqrt{\rho^2 + z^2}\ e^{-2\lambda\sqrt{\rho^2 + z^2}} \qquad \text{D.12.e}$$

$$+\ \lambda^2K^2N^2 J_o^2(\alpha\rho)\ \rho^2\ e^{-2\lambda\sqrt{\rho^2 + z^2}} \qquad \text{D.12.f}$$

$$+\ \lambda^2K^2N^2 J_o^2(\alpha\rho)\ z^2\ e^{-2\lambda\sqrt{\rho^2 + z^2}} \qquad \text{D.12.g}$$

In detail, one can write

a.

$$N^2 \int_o^{2\pi} d\theta \int_o^a \rho \; J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz \; e^{-2\beta\sqrt{\rho^2 + z^2}}$$

$$= 4\pi N^2 \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\beta\rho)\, d\rho$$

D.12.1

b.

$$4KN^2 \int_o^{2\pi} d\theta \int_o^a \rho \; J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz \; e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$= 16\pi KN^2 \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1[(\beta+\lambda)\rho]\, d\rho$$

c.

$$- 2\lambda KN^2 \int_o^{2\pi} d\theta \int_o^a \rho J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz \sqrt{\rho^2+z^2} \; e^{-(\beta+\lambda)\sqrt{\rho^2+z^2}}$$

$$= -4\pi\lambda KN^2 \int_o^a d\rho \; \rho J_o^2(\alpha\rho) \Big\{ 2\rho^2 K_o[(\beta+\lambda)\rho]$$

$$+ \frac{2\rho K_1[(\beta+\lambda)\rho]\, d\rho}{(\beta+\lambda)} \Big\}$$

$$= -8\pi \; \lambda \; KN^2 \int_o^a \rho^3 \; J_o^2(\alpha\rho)\, K_o([(\beta+\lambda)\rho]\, d\rho$$

$$- \frac{8\pi\lambda KN^2}{(\beta+\lambda)} \int_o^a \rho^2 \; J_o^2(\alpha\rho)\, K_1[(\beta+\lambda)\rho]\, d\rho$$

d.

$$4K^2N^2 \int_o^{2\pi} d\theta \int_o^{2\pi} \rho J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\ e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$= 16\pi K^2N^2 \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\lambda\rho)\, d\rho$$

e.

$$-4\lambda K^2N^2 \int_o^{2\pi} d\theta \int_o^a \rho\ J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz \sqrt{\rho^2 + z^2}\ e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$= -8\pi\lambda KN^2 \int_o^a d\rho\ \rho\ J_o^2(\alpha\rho) \left\{ 2\rho^2 K_o(2\lambda\rho) + \frac{\rho K_1(2\lambda\rho)}{\lambda} \right\}$$

$$= -\ 16\pi\lambda K^2N^2 \int_o^a \rho^3 J_o^2(\alpha\rho)\, K_o(2\lambda\rho)\, d\rho$$

$$-8\pi K^2N^2 \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\lambda\rho)\, d\rho$$

f.

$$\lambda^2K^2N^2 \int_o^{2\pi} d\theta \int_o^a \rho^3 J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\ e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$= 4\pi\lambda^2K^2N \int_o^a \rho^4 J_o^2(\alpha\rho)\, K_1(2\lambda\rho)\, d\rho$$

g.

$$\lambda^2 K^2 N^2 \int_o^{2\pi} d\theta \int_o^a \rho\, J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz, z^2\, e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$= 2\pi\lambda^2 K^2 N^2 \int_o^a d\rho\, \rho\, J_o^2(\alpha\rho) \left\{ \frac{\rho K_1(2\lambda\rho)}{\lambda^2} + \frac{\rho^2 K_o(2\lambda\rho)}{\lambda} \right\}$$

$$= 2\pi K^2 N^2 \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\lambda\rho)\, d\rho$$

$$+ 2\pi\lambda K^2 N^2 \int_o^a \rho^3 J_o^2(\alpha\rho)\, K_o(2\lambda\rho)\, d\rho$$

The normalization constant N^2 can now be obtained from the sum of D.12.a, b, c, d, e, f, g. The result is

$$+ 16\pi K N^2 \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1[(\beta+\lambda)\rho]\, d\rho$$

$$- 8\pi\lambda K N^2 \int_o^a \rho^3 J_o^2(\alpha\rho)\, K_o[(\beta+\lambda)\rho]\, d\rho$$

$$- \frac{8\pi\lambda K N^2}{(\beta+\lambda)} \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1[(\beta+\lambda)\rho]\, d\rho$$

$$+ 16\pi K^2 N^2 \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\lambda\rho)\, d\rho$$

$$- 16\pi\lambda K^2 N^2 \int_o^a \rho^3 J_o^2(\alpha\rho)\, K_o(2\lambda\rho)\, d\rho$$

$$- 8\pi K^2 N^2 \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho$$

$$+ 4\pi\lambda^2 K^2 N^2 \int_o^a \rho^4 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho$$

$$+ 2\pi K^2 N^2 \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho \qquad \text{D.13}$$

$$+ 2\pi\lambda K^2 N^2 \int_o^a \rho^2 J_o^2(\alpha\rho) K_o(2\lambda\rho)\, d\rho$$

From the above expression the normalization constant is given by

$$-7\lambda K^2 \int_o^a \rho^3 J_o^2(\alpha\rho) K_o(2\lambda\rho)\, d\rho$$

$$+ 2\lambda^2 K^2 \int_o^a \rho^4 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho$$

$$+ 2 \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho$$

$$+8K \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho$$

$$- 4\lambda K \int_o^a \rho^3 J_o^2(\alpha\rho) K_o[(\beta+\lambda)\rho]\, d\rho \qquad \text{D.14}$$

$$- \frac{4\lambda K}{(\beta+\lambda)} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho \;\Big]\Big\}^{-1}$$

The rest of the integration is done numerically.

The calculation of the expectation value of the kinetic energy is now given below.

The Hamiltonian for the kinetic energy in circular cylindrical coordinates is

$$T = -\frac{1}{2m^*}\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\right] + \frac{\partial^2}{\partial z^2}\right\} \qquad \text{D.15}$$

One can then write

$$T\,\Phi_{2s}(\rho,z) = -\frac{1}{2m^*}\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\right] + \frac{\partial^2}{\partial z^2}\right\}\Phi_{2s}(\rho,z) \qquad \text{D.16}$$

Since there are many terms involved in this calculation, it is convenient to do the differentiations term by term

$$\Phi_{2s}(\rho,z) = NJ_o(\alpha\rho)\,e^{-\beta\sqrt{\rho^2+z^2}} \qquad \text{D.17.a}$$

$$+2\,K\,N\,J_o(\alpha\rho)\,e^{-\lambda\sqrt{\rho^2+z^2}} \qquad \text{D.17.b}$$

$$-\lambda\,K\,N\,J_o(\alpha\rho)\sqrt{\rho^2+z^2}\;e^{-\lambda\sqrt{\rho^2+z^2}} \qquad \text{D.17.c}$$

The ρ-differentiation is performed first; thus the first term D.17.a yields

$$\frac{N}{\rho}\frac{\partial}{\partial\rho}\left\{\rho\frac{\partial}{\partial\rho}J_o(\alpha\rho)\,e^{-\beta\sqrt{\rho^2+z^2}}\right\}$$

$$= \frac{N}{\rho}\frac{\partial}{\partial\rho}\left\{\rho\left[-\alpha J_1(\alpha\rho)\,e^{-\beta\sqrt{\rho^2+z^2}}\right.\right.$$

$$\left.\left.-\frac{\beta\rho J_o(\alpha\rho)}{\sqrt{\rho^2+z^2}}\,e^{-\beta\sqrt{\rho^2+z^2}}\right]\right\}$$

$$= \frac{N}{\rho}\frac{\partial}{\partial\rho}\left\{-\alpha\rho J_1(\alpha\rho)\,e^{-\beta\sqrt{\rho^2+z^2}} - \frac{\beta\rho^2 J_o(\alpha\rho)\;e^{-\beta\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}}\right\}$$

$$= \frac{N}{\rho}\left\{-\alpha J_1(\alpha\rho) - \alpha\rho\left[\alpha J_o(\alpha\rho) - \frac{J_1(\alpha\rho)}{\rho}\right]\right.$$

$$+\frac{\alpha\beta\rho^2 J_1(\alpha\rho)}{\sqrt{\rho^2+z^2}} + \frac{\beta\rho^3 J_o(\alpha\rho)}{[\rho^2+z^2]}$$

$$\left.+\frac{\beta^2\rho^3 J_o(\alpha\rho)}{[\rho^2+z^2]}\right\} x\; e^{-\beta\sqrt{\rho^2+z^2}}$$

$$= \frac{N}{\rho} \left\{ - \alpha J_1(\alpha\rho) - \alpha^2 \rho J_o(\alpha\rho) + \alpha J_1(\alpha\rho) \right.$$

$$+ \frac{\alpha\beta\rho^2 J_1(\alpha\rho)}{\sqrt{\rho^2 + z^2}} - \frac{2\beta\rho J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}}$$

$$\left. + \frac{\alpha\beta\rho^2 J_1(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \frac{\beta\rho^3 J_o(\alpha\rho)}{[\rho^2 + z^2]^{3/2}} + \frac{\beta^2\rho^3 J_o(\alpha\rho)}{[\rho^2 + z^2]} \right\}$$

$$x\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$= \left\{ -\alpha^2 N J_o(\alpha\rho) - \frac{2\beta N J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \frac{2\beta\alpha N J_1(\alpha\rho)\ \rho}{\sqrt{\rho^2 + z^2}} \right.$$

$$\left. + \frac{\beta N J_o(\alpha\rho)\rho^2}{[\rho^2 + z^2]^{3/2}} + \frac{\beta^2 N J_o(\alpha\rho)\ \rho^2}{[\rho^2 + z^2]} \right\}$$

$$x\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

D.17.a

Differentiation of D.17.b leads to

$$\frac{2KN}{\rho}\frac{\partial}{\partial\rho}\left\{\rho\frac{\partial}{\partial\rho}J_o(\alpha\rho)\,e^{-\lambda\sqrt{\rho^2+z^2}}\right\}$$

$$= \frac{2KN}{\rho}\frac{\partial}{\partial\rho}\left\{\rho\left[-\alpha J_1(\alpha\rho)\,e^{-\lambda\sqrt{\rho^2+z^2}} - \frac{\lambda\rho J_o(\alpha\rho)\;e^{-\lambda\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}}\right]\right\}$$

$$= \frac{2KN}{\rho}\frac{\partial}{\partial\rho}\left\{-\alpha\rho J_1(\alpha\rho)\,e^{-\lambda\sqrt{\rho^2+z^2}} - \frac{\lambda\rho^2 J_o(\alpha\rho)\;e^{-\lambda\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}}\right\}$$

$$= \frac{2KN}{\rho}\left\{-\alpha J_1(\alpha\rho) - \alpha\rho\left[\alpha J_o(\alpha\rho) - \frac{J_1(\alpha\rho)}{\rho}\right]\right.$$

$$- \frac{\alpha\rho J_1(\alpha\rho)(-\lambda\rho)}{\sqrt{\rho^2+z^2}} - \frac{2\lambda\rho J_o(\alpha\rho)}{\sqrt{\rho^2+z^2}}$$

$$\left. + \frac{\alpha\lambda\rho^2 J_1(\alpha\rho)}{\sqrt{\rho^2+z^2}} + \frac{\lambda\rho^3 J_o(\alpha\rho)}{[\rho^2+z^2]^{3/2}} + \frac{\lambda^2\rho^3 J_o(\alpha\rho)}{[\rho^2+z^2]}\right\}$$

$$x\;e^{-\lambda\sqrt{\rho^2+z^2}}$$

Differentiation of D.17.b leads to

$$= \frac{2KN}{\rho} \frac{\partial}{\partial\rho} \left\{ - \alpha\rho J_1(\alpha\rho) e^{-\lambda\sqrt{\rho^2 + z^2}} - \frac{\lambda\rho^2 J_o(\alpha\rho)\ e^{-\lambda\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} \right\}$$

$$= \frac{2KN}{\rho} \left\{ - \alpha J_1(\alpha\rho) - \alpha\rho \left[\alpha J_o(\alpha\rho) - \frac{J_1(\alpha\rho)}{\rho} \right] \right.$$

$$- \frac{\alpha\rho J_1(\alpha\rho)(-\lambda\rho)}{\sqrt{\rho^2 + z^2}} - \frac{2\lambda\rho J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}}$$

$$\left. + \frac{\alpha\lambda\rho^2 J_1(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \frac{\lambda\rho^3 J_o(\alpha\rho)}{[\rho^2 + z^2]^{3/2}} + \frac{\lambda^2\rho^3 J_o(\alpha\rho)}{[\rho^2 + z^2]} \right\}$$

$$x\ e^{-\lambda\sqrt{\rho^2 + z^2}}$$

which simplifies to

$$= \left\{ -2\alpha^2 K\, N\, J_o(\alpha\rho) + \frac{4\alpha\lambda K\, N\, J_1(\alpha\rho)\,\rho}{\sqrt{\rho^2 + z^2}} \right.$$

$$- \frac{4\lambda\ K\, N\, J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \frac{2\lambda\ K\, N\, J_o(\alpha\rho)\,\rho^2}{[\rho^2 + z^2]^{3/2}}$$

$$\left. + \frac{2\lambda^2 K\, N\, J_o(\alpha\rho)\,\rho^2}{[\rho^2 + z^2]} \right\} x\ e^{-\lambda\sqrt{\rho^2 + z^2}}$$

D.17.b'

Differentiation of D.17.c gives

$$- \frac{\lambda KN}{\rho} \frac{\partial}{\partial\rho} \left\{ \rho \frac{\partial}{\partial\rho} J_o(\alpha\rho) \sqrt{\rho^2 + z^2}\ e^{-\lambda\sqrt{\rho^2 + z^2}} \right\}$$

$$= - \frac{\lambda KN}{\rho} \frac{\partial}{\partial\rho} \left\{ \rho \left[-\alpha J_1(\alpha\rho) \sqrt{\rho^2 + z^2}\ e^{-\lambda\sqrt{\rho^2 + z^2}} \right.\right.$$

$$\left.\left. + \frac{\rho J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}}\ e^{-\lambda\sqrt{\rho^2 + z^2}} - \frac{\lambda\rho J_o(\alpha\rho) \sqrt{\rho^2 + z^2}}{\sqrt{\rho^2 + z^2}}\ e^{-\lambda\sqrt{\rho^2 + z^2}} \right] \right\}$$

$$= - \frac{\lambda KN}{\rho} \frac{\partial}{\partial\rho} \left\{ -\alpha J_1(\alpha\rho) \sqrt{\rho^2 + z^2}\ e^{-\lambda\sqrt{\rho^2 + z^2}} \right.$$

$$\left. + \frac{\rho^2 J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}}\ e^{-\lambda\sqrt{\rho^2 + z^2}} - \lambda\rho^2 J_o(\alpha\rho)\ e^{-\lambda\sqrt{\rho^2 + z^2}} \right\}$$

$$= \frac{-\lambda KN}{\rho} \left\{ -\alpha J_1(\alpha\rho) \sqrt{\rho^2 + z^2} - \alpha\rho\sqrt{\rho^2 + z^2} \left[\alpha J_o(\alpha\rho) \quad \frac{-J_1(\alpha\rho)}{\rho} \right] \right.$$

$$- \frac{\alpha\rho^2 J_1(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \frac{\alpha\lambda\rho^2 J_1(\alpha\rho) \sqrt{\rho^2 + z^2}}{\sqrt{\rho^2 + z^2}} + \frac{2\rho J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}}$$

$$- \frac{\alpha \rho^2 J_1(\alpha\rho)}{\sqrt{\rho^2 + z^2}} - \frac{\rho^3 J_o(\alpha\rho)}{[\rho^2 + z^2]^{3/2}} - \frac{\lambda \rho^3 J_o(\alpha\rho)}{[\rho^2 + z^2]}$$

$$- 2\lambda\rho J_o(\alpha\rho) + \alpha\lambda\rho^2 J_1(\alpha\rho) + \frac{\lambda^2 \rho^3 J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} \Bigg\}$$

$$x \; e^{-\lambda\sqrt{\rho^2 + z^2}}$$

$$= \Big\{ \alpha^2 \lambda K\, N\, J_o(\alpha\rho) \sqrt{\rho^2 + z^2} + \alpha\lambda K\, N\, J_1(\alpha\rho)\,\rho$$

$$- \alpha\lambda^2 K\, N\, J_1(\alpha\rho)\,\rho - \frac{2\lambda K\, N\, J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}}$$

$$+ \frac{\alpha\lambda K\, N\, J_1(\alpha\rho)\,\rho}{\sqrt{\rho^2 + z^2}} + \frac{\lambda K\, N\, J_o(\alpha\rho)\,\rho^2}{[\rho^2 + z^2]^{3/2}}$$

$$+ \frac{\lambda^2 K\, N\, J_o(\alpha\rho)\,\rho^2}{[\rho^2 + z^2]} + 2\lambda^2 K\, N\, J_o(\alpha\rho)$$

$$- \alpha\lambda^2 K\, N\, J_1(\alpha\rho) - \frac{\lambda^3 K\, N\, J_o(\alpha\rho)\,\rho^2}{\sqrt{\rho^2 + z^2}} \Bigg\}$$

$$x \; e^{-\lambda\sqrt{\rho^2 + z^2}}$$

D.17.c

Differentiation with respect to z of D.1, results in

$$NJ_o(\alpha\rho)\ \frac{\partial^2}{\partial z^2}\ \Big\{ e^{-\beta\sqrt{\rho^2 + z^2}} + 2K\, e^{-\lambda\sqrt{\rho^2 + z^2}}$$

$$- 2K\sqrt{\rho^2 + z^2}\ \Big\}\ x\ e^{-\lambda\sqrt{\rho^2 + z^2}}$$

$$= NJ_o(\alpha\rho)\ \frac{\partial}{\partial z}\ \Bigg\{ - \frac{\beta z e^{-\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} - \frac{2\lambda Kz\ e^{-\lambda\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

$$- \frac{\lambda Kz\ e^{-\lambda\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} - \frac{\lambda K\sqrt{\rho^2 + z^2}}{\sqrt{\rho^2 + z^2}}\ (-\lambda z)\ e^{-\lambda\sqrt{\rho^2 + z^2}} \Bigg\}$$

$$= NJ_o(\alpha\rho)\ \Bigg\{\Bigg[\frac{-\beta}{\sqrt{\rho^2 + z^2}} + \frac{\beta z^2}{[\rho^2 + z^2]^{3/2}} + \frac{\beta^2 z^2}{[\rho^2 + z^2]} \Bigg]\ e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$\Bigg[- \frac{3\lambda K}{\sqrt{\rho^2 + z^2}} + \frac{3\lambda K z^2}{[\rho^2 + z^2]^{3/2}} + \frac{3\lambda^2 K z^2}{[\rho^2 + z^2]}$$

$$+ \lambda^2 K - \frac{\lambda^3 K z^2}{\sqrt{\rho^2 + z^2}} \Bigg]\ x\ e^{-\lambda\sqrt{\rho^2 + z^2}}$$

$$= \left[\frac{-\beta N J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \frac{\beta N J_o(\alpha\rho) z^2}{[\rho^2 + z^2]^{3/2}} + \frac{\beta^2 N J_o(\alpha\rho) z^2}{[\rho^2 + z^2]} \right] x\, e^{-\beta\sqrt{\rho^2 + z^2}}$$

$$+ \left[- \frac{3\lambda K N J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \frac{3\lambda K N J_o(\alpha\rho) z^2}{[\rho^2 + z^2]^{3/2}} + \frac{3\lambda^2 K N J_o(\alpha\rho) z^2}{[\rho^2 + z^2]} \right.$$

$$\left. + \lambda^2 K N J_o(\alpha\rho) - \frac{\lambda^3 K N J_o(\alpha\rho) z^2}{\sqrt{\rho^2 + z^2}} \right] x\, e^{-\lambda\sqrt{\rho^2 + z^2}}$$

D.18

Addition of all the terms in Equation D.18 yields $\nabla^2_z \Phi_{2s}$. This quantity can be expressed by

$$\nabla^2\Phi_{2s} = \left\{ \frac{-\beta N J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} + \frac{\beta N J_o(\alpha\rho) z^2}{[\rho^2 + z^2]^{3/2}} \right.$$

$$\left. + \frac{\beta^2 N J_o(\alpha\rho) z^2}{[\rho^2 + z^2]} \right\} e^{-\beta\sqrt{\rho^2 + z^2}} + \left\{ - \frac{3\lambda K N J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} \right.$$

$$+ \frac{3\lambda K N J_o(\alpha\rho) z^2}{[\rho^2 + z^2]^{3/2}} + \frac{3\lambda^2 K N J_o(\alpha\rho) z^2}{[\rho^2 + z^2]}$$

$$\left. + \lambda^2 K N J_o(\alpha\rho) - \frac{\lambda^3 K N J_o(\alpha\rho) z^2}{\sqrt{\rho^2 + z^2}} \right\} e^{-\lambda\sqrt{\rho^2 + z^2}}$$

$$+ \left\{ - \alpha^2 N J_o(\alpha\rho) - \frac{2\beta N J_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} \right.$$

$$+ \frac{2\alpha\beta N J_1(\alpha\rho)\rho}{\sqrt{\rho^2 + z^2}} + \frac{\beta N J_o(\alpha\rho)\rho^2}{[\rho^2 + z^2]^{3/2}}$$

$$\left. + \frac{\beta^2 N J_o(\alpha\rho)\rho^2}{[\rho^2 + z^2]} \right\} x\, e^{-\beta\sqrt{\rho^2 + z^2}} + \left\{ - 2\alpha^2 K N J_o(\alpha\rho) \right.$$

$$+ \frac{4\alpha\lambda KNJ_1(\alpha\rho)}{\sqrt{\rho^2 + z^2}} - \frac{4\lambda KNJ_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}}$$

$$+ \frac{2\lambda KNJ_o(\alpha\rho)\rho^2}{[\rho^2 + z^2]^{3/2}} + 2\lambda^2 KNJ_o(\alpha\rho)\rho^2$$

$$+ \alpha^2\lambda KNJ_o(\alpha\rho)\sqrt{\rho^2 + z^2}$$

$$+ \frac{\alpha\lambda KNJ_1(\alpha\rho)\rho}{\sqrt{\rho^2 + z^2}} - \alpha\lambda^2 KNJ_1(\alpha\rho)\rho$$

$$\left. - \frac{2\lambda KNJ_o(\alpha\rho)}{\sqrt{\rho^2 + z^2}} \right\} x\, e^{-\lambda\sqrt{\rho^2 + z^2}}$$

$$\left\{ + \frac{\alpha\lambda KNJ_1(\alpha\rho)\rho}{\sqrt{\rho^2 + z^2}} + \frac{\lambda KNJ_o(\alpha\rho)\rho^2}{[\rho^2 + z^2]^{3/2}} \right.$$

$$+ \frac{\lambda^2 KNJ_o(\alpha\rho)\rho^2}{[\rho^2 + z^2]} + 2\lambda^2 KNJ_o(\alpha\rho)$$

$$\left. - \alpha\lambda^2 KNJ_1(\alpha\rho)\rho - \frac{\lambda^3 KNJ_o(\alpha\rho)\rho^2}{\sqrt{\rho^2 + z^2}} \right\} e^{-\lambda\sqrt{\rho^2 + z^2}}$$

D.19

Multiplying the terms in Equation D.20.a to D.20.j by Φ^*_{2s} and $(-\frac{\hbar^2}{2m^*})$ results in:

$$\Phi^*_{2s}\ (-\frac{\hbar^2}{2m^*}\quad D.20.a)$$

$$= 3h^2\lambda KN^2 J_o^2(\alpha\rho)\, e^{-(b+\lambda)\sqrt{\rho^2+z^2}}$$

$$+ \frac{6h^2\lambda K^2N^2J_o^2(\alpha\rho)}{m^*\sqrt{\rho^2+z^2}}\ e^{-2\lambda\sqrt{\rho^2+z^2}}$$

$$- \frac{3h^2\lambda^2K^2N^2J_o^2(\alpha\rho)}{m^*}\ e^{-2\lambda\sqrt{\rho^2+z^2}}$$

which, upon integration, becomes

$$\int_\tau \Phi^*_{2s}\left(\frac{-h^2}{2m^*}\ D.20.a\right)$$

$$= \frac{3h^2\lambda KN^2}{m^*}\int_o^{2\pi} d\theta \int_o^a \rho\ J_o^2(\alpha\rho)\ d\rho \int_{-\infty}^{\infty} \frac{dz\ e^{-(\beta+\lambda)\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}]}$$

$$+ \frac{6h^2\lambda K^2N^2}{m^*}\int_o^{2\pi} d\theta \int_o^a \rho\ J_o^2(\alpha\rho)\ d\rho \int_{-\infty}^{\infty} \frac{dz\ e^{-(\beta+\lambda)\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}}$$

$$- \frac{3h^2\lambda^2K^2N^2}{m^*}\int_o^{2\pi} d\theta \int_o^a \rho\ J_o^2(\alpha\rho)\ d\rho \int_{-\infty}^{\infty} dz\ e^{-2\lambda\sqrt{\rho^2+z^2}}$$

$$= \frac{12\pi h^2 \lambda K N^2}{m^*} \int_o^a \rho\ J_o^2(\alpha\rho)\ K_o[(\beta + \lambda)\rho]\, d\rho$$

$$+ \frac{2\ 4\pi h^2 \lambda K^2 N^2}{m^*} \int_o^a \rho\ J_o^2(\alpha\rho)\ K_o(2\lambda\rho)\, d\rho$$

$$- \frac{12\pi h^2 \lambda^2 K^2 N^2}{m^*} \int_o^a \rho^2\ J_o^2(\alpha\rho)\ K_1(2\lambda\rho)\, d\rho \qquad \text{D.20.a}$$

The second terms yields

$$\Phi_{2s}^* \left(\frac{-h^2}{2m^*}\ D.20.b \right)$$

$$= \frac{h^2 \beta N^2 J_o^2(\alpha\rho)}{m^* \sqrt{\rho^2 + z^2}}\ e^{-2\beta\sqrt{\rho^2 + z^2}}$$

$$+ \frac{2h^2 \beta K N^2 J_o^2(\alpha\rho)}{m^* \sqrt{\rho^2 + z^2}}\ e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$- \frac{h^2 \beta \lambda K N^2 J_o^2(\alpha\rho)}{m^*}\ e^{-(\beta + \lambda)\sqrt{\rho^2 + z^2}} \qquad \text{D.20.b}$$

When the integrations in D.20.b' are carried out, the following expression results

$$\int_\tau \Phi_{2s}^* \left(-\frac{h^2}{2m^*}\ D.20.b \right)$$

$$= \frac{h^2 \beta N^2}{m^*} \int_o^{2\pi} d\theta \int_o^a \rho\ J_o^2(\alpha\rho)\ d\rho \int_{-\infty}^{\infty} \frac{dz\ e^{-2\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

$$+ \frac{2h^2\beta KN^2}{m^*}\int_0^{2\pi} d\theta \int_0^a \rho\ J_o^2(\alpha\rho)\ d\rho \int_{-\infty}^{\infty} \frac{dz\ e^{-(\beta+\lambda)\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}}$$

$$- \frac{h^2\beta\lambda KN^2}{m^*}\int_0^{2\pi} d\theta \int_0^a \rho\ J_o^2(\alpha\rho)\ d\rho \int_{-\infty}^{\infty} dz\ e^{-(\beta+\lambda)\sqrt{\rho^2+z^2}}$$

$$= \frac{4\pi h^2\beta N^2}{m^*}\int_0^a \rho\ J_o^2(\alpha\rho)\ K_o(2\beta\rho)\,d\rho$$

$$+ \frac{8\pi h^2\beta KN^2}{m^*}\int_0^a \rho\ J_o^2(\alpha\rho)\,K_o[(\beta+\lambda)\rho]\,d\rho$$

$$- \frac{4\pi h^2\beta\lambda KN^2}{m^*}\int_0^a \rho^2\ J_o^2(\alpha\rho)\,K_1[(\beta+\lambda)\rho]\,d\rho \qquad \text{D.20.b}$$

D.20.c yields

$$\Phi_{2s}^*\left(-\frac{h^2}{2m^*}\ D.20.c\right)$$

$$= 3h^2KN^2J_o^2(\alpha\rho)\ e^{-(\beta+\lambda)\sqrt{\rho^2+z^2}}$$

$$- \frac{6h^2\lambda^2K^2N^2}{m^*}\ J_o^2(\alpha\rho)\ e^{-2\lambda\sqrt{\rho^2+z^2}}$$

$$+ 3h^2\lambda^3K^2N^2J_o^2(\alpha\rho)\sqrt{\rho^2+z^2}\ e^{-2\lambda\sqrt{\rho^2+z^2}}$$

On integration, these terms yield:

$$\int_{\tau} \Phi_{2s}^{*} \left(- \frac{h^2}{2m^*} \; D.20.c \right)$$

$$= - \frac{12\pi h^2\lambda^2 KN^2}{m^*} \int_{o}^{a} \rho^2 \; J_o^2(\alpha\rho) \, K_1[(\beta+\lambda)\rho] \, d\rho$$

$$- \frac{24\pi h^2\lambda^2 K^2N^2}{m^*} \int_{o}^{a} \rho^2 \; J_o^2(\alpha\rho) \, K_1(2\lambda\rho) \, d\rho$$

$$+ \frac{12\pi h^2\lambda^3 K^2N^2}{m^*} \int_{o}^{a} \rho^3 \; J_o^2(\alpha\rho) \, K_o(2\lambda\rho) \, d\rho$$

$$+ \frac{6\pi h^2\lambda^2 K^2N^2}{m^*} \int_{o}^{a} \rho^2 \; J_o^2(\alpha\rho) \, K_1(2\lambda\rho) \, d\rho$$

$$\int_{\tau} \Phi_{2s}^{*} \left(- \frac{h^2}{2m^*} \; D.20.c \right)$$

$$= - \frac{3h^2\lambda^2 KN^2}{m^*} \int_{o}^{2\pi} d\theta \int_{o}^{a} \rho \; J_o^2(\alpha\rho) \, d\rho \int_{-\infty}^{\infty} dz \; e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$- \frac{6h^2\lambda^2 K^2N^2}{m^*} \int_{o}^{2\pi} d\theta \int_{o}^{a} \rho \; J_o^2(\alpha\rho) \, d\rho \int_{-\infty}^{\infty} dz \; e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$+ \frac{3h^2\lambda^3 K^2N^2}{m^*} \int_{o}^{2\pi} d\theta \int_{o}^{a} \rho \; J_o^2(\alpha\rho) \, d\rho \int_{-\infty}^{\infty} dz \; e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$= - \frac{12\pi h^2\lambda^2 KN^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho$$

$$- \frac{24\pi h^2\lambda^2 K^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho$$

$$+ \frac{12\pi h^2\lambda^3 K^2 N^2}{m^*} \int_o^a \rho^3 J_o^2(\alpha\rho) K_o(2\lambda\rho)\, d\rho$$

$$+ \frac{6\pi h^2\lambda^2 K^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho$$

D.20.c'

while D.20.d becomes:

$$\Phi_{2s}^* \left(- \frac{h^2}{2m^*} D.20.d \right)$$

$$= - \frac{h^2\beta^2 N^2 J_o^2(\alpha\rho)}{2m^*} e^{-2\beta\sqrt{\rho^2 + z^2}}$$

$$- \frac{h^2\beta^2 KN^2 J_o^2(\alpha\rho)}{m^*} e^{(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$+ \frac{h^2\beta^2\lambda KN^2 J_o^2(\alpha\rho)\sqrt{\rho^2 + z^2}}{2m^*} e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$= - \frac{h^2\beta^2 N^2 J_o^2(\alpha\rho)}{2m^*} e^{-2\beta\sqrt{\rho^2 + z^2}}$$

$$- \frac{h^2\beta^2 KN^2 J_o^2(\alpha\rho)}{m^*} e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

D.20.d'

$$+ h^2\beta^2\lambda KN^2 J_o^2(\alpha\rho)\sqrt{\rho^2 + z^2}\, e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

Integration of D.20.d' yields

$$\int_\tau \Phi_{2s}^* \left(- \frac{h^2}{2m^*} D.20.d \right)$$

$$= - \frac{2\pi h^2 \beta^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

$$- \frac{4\pi h^2 \beta^2 K N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho$$

$$+ \frac{4\pi h^2 \beta^2 \lambda K N^2}{m^*} \int_o^a \rho^3\, J_o^2(\alpha\rho) K_o[(\beta+\lambda)\rho]\, d\rho$$

$$+ \frac{4\pi h^2 \beta^2 \lambda K N^2}{m^*(\beta+\lambda)} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho \qquad \text{D.20.d''}$$

$$\Phi_{2s}^* \left(- \frac{h^2}{2m^*} D.20.e \right)$$

$$= \frac{h^2 \lambda^3 K N^2 J_o^2(\alpha\rho) \sqrt{\rho^2 + z^2}}{2m^*} e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$+ h^2 \lambda^3 K^2 N^2 J_o^2(\alpha\rho) \sqrt{\rho^2 + z^2}\; e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$- h^2 \lambda^4 K^2 N^2 J_o^2(\alpha\rho) \rho^2\; e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$- \frac{h^2 \lambda^4 K^2 N^2 J_o^2(\alpha\rho) z^2}{2m^*} e^{-2\lambda\sqrt{\rho^2 + z^2}} \qquad \text{D.20.e'}$$

On integration with respect to ρ and z, D.20.e' becomes

$$\int_\tau \Phi^*_{2s}\left(- \frac{h^2}{2m^*}\, D.20.e \right)$$

$$= \frac{2\pi h^2\lambda^3 KN^2}{m^*} \int_o^a \rho^3 J_o^2(\alpha\rho) K_o[(\beta+\lambda)\rho]\, d\rho$$

$$+ \frac{2\pi h^2\lambda^3 KN^2}{m^*(\beta+\lambda)} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho$$

$$+ \frac{4\pi h^2\lambda^3 K^2N^2}{m^*} \int_o^a \rho^3 J_o^2(\alpha\rho) K_o(2\lambda\rho)\, d\rho$$

$$+ \frac{2\pi h^2\lambda^2 K^2N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho$$

$$- \frac{2\pi h^2\lambda^4 K^2N^2}{m^*} \int_o^a \rho^4 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho$$

$$- \frac{\pi h^2\lambda^2 K^2N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho$$

$$- \frac{\pi h^2\lambda^3 K^2N^2}{m^*} \int_o^a \rho^3 J_o^2(\alpha\rho) K_o(2\lambda\rho)\, d\rho \quad ,$$

D.20.e

$$\Phi^*_{2s}\left(- \frac{h^2}{2m^*}\, D.20.f \right)$$

$$= \frac{h^2\alpha\lambda^2 KN^2 J_o(\alpha\rho) J_1(\alpha\rho)\rho}{m^*} e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$+ \frac{2h^2\alpha\lambda^2 K^2N^2 J_o(\alpha\rho) J_1(\alpha\rho)\rho}{m^*} e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$- \frac{h^2\alpha\lambda^3 K^2N^2 J_o(\alpha\rho) J_1(\alpha\rho)\sqrt{\rho^2 + z^2}}{m^*} e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

D.20.f

On integration these terms in D.20.f yield

$$\int_{\tau} \Phi_{2s}^{*} \left(- \frac{h^2}{2m^*} D.20.f \right) d\tau$$

$$= \frac{4\pi h^2 \alpha \lambda^2 K N^2}{m^*} \int_o^a \rho^3 J_o(\alpha\rho) J_1(\alpha\rho) K_1[(\beta+\lambda)\rho] d\rho$$

$$+ \frac{8\pi h^2 \alpha \lambda^2 K N^2}{m^*} \int_o^a \rho^3 J_o(\alpha\rho) J_1(\alpha\rho) K_1(2\lambda\rho) d\rho$$

$$- \frac{4\pi h^2 \alpha \lambda^3 K^2 N^2}{m^*} \int_o^a \rho^4 J_o(\alpha\rho) J_1(\alpha\rho) K_o(2\lambda\rho) d\rho$$

$$- \frac{2\pi h^2 \alpha \lambda^2 K^2 N^2}{m^*} \int_o^a \rho^3 J_o(\alpha\rho) J_1(\alpha\rho) K_1(2\lambda\rho) d\rho \ , \qquad \text{D.20.f}$$

$$\Phi_{2s}^{*} \left(- \frac{h^2}{2m^*} D.20.g \right)$$

$$= - \frac{3h^2 \alpha \lambda K N^2 J_o(\alpha\rho) J_1(\alpha\rho) \rho}{m^* \sqrt{\rho^2 \ z^2}} e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$- \frac{6h^2 \alpha \lambda K^2 N^2 J_o(\alpha\rho) J_1(\alpha\rho) \rho}{m^* \sqrt{\rho^2 + z^2}} e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$+ \frac{3h^2 \alpha \lambda^2 K^2 N^2 J_o(\alpha\rho) J_1(\alpha\rho) \rho}{m^*} e^{-2\lambda\sqrt{\rho^2 + z^2}} \qquad \text{D.20.f}$$

n integration become:

$$\int_\tau \Phi^*_{2s}\left(- \frac{h^2}{2m^*} \; D.20.f \right) d\tau$$

$$= - \frac{12\pi h^2\alpha\lambda KN^2}{m^*} \int_o^a \rho^2 J_o(\alpha\rho) J_1(\alpha\rho) K_o[(\beta+\lambda)\rho] \, d\rho$$

$$+ \frac{2 \;\; 4\pi h^2\lambda^2 K^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho) \, d\rho$$

$$- \frac{2 \;\; 4\pi h^2\lambda K^2 N^2}{m^*} \int_o^a \rho \; J_o^2(\alpha\rho) K_o(2\lambda\rho) \, d\rho$$

$$+ \frac{12\pi h^2\alpha\lambda^2 K^2 N^2}{m^*} \int_o^a \rho^3 J_o(\alpha\rho) J_1(\alpha\rho) K_1(2\lambda\rho) \, d\rho \qquad \text{D.20.f}$$

$$\Phi^*_{2s}\left(- \frac{h^2}{2m^*} \; D.20.g \right)$$

$$= \frac{h^2\alpha^2 N^2 J_o^2(\alpha\rho)}{2m^*} \; e^{-2\beta\sqrt{\rho^2 + z^2}}$$

$$+ \frac{h^2\alpha^2 KN^2 J_o^2(\alpha\rho)}{m^*} \; e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$- \frac{h^2\alpha^2\lambda KN^2 J_o^2(\alpha\rho)\sqrt{\rho^2 + z^2}}{2m^*} \; e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}} \qquad \text{D.20.g}$$

Integration of the three terms in D.20.g gives the following result:

$$\int_\tau \Phi^*_{2s} \left(- \frac{h^2}{2m^*} \; D.20.g \right) d\tau$$

$$= \frac{2\pi h^2 \alpha^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho$$

$$+ \frac{4\pi h^2 \alpha^2 K N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho$$

$$- \frac{2\pi h^2 \alpha^2 \lambda K N^2}{m^*} \int_o^a \rho^3 \; J_o^2(\alpha\rho) K_o[(\beta+\lambda)\rho]\, d\rho$$

$$- \frac{2\pi h^{2^2} \alpha \lambda K N^2}{m^*(\beta+\lambda)} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho \qquad \text{D.20.g'}$$

$$\Phi^*_{2s} \left(- \frac{h^2}{2m^*} \; D.20.h \right)$$

$$= - \frac{h^2 \alpha \beta N^2 J_o(\alpha\rho) J_1(\alpha\rho)}{m^* \sqrt{\rho^2 + z^2}} \; e^{-2\beta \sqrt{\rho^2 + z^2}}$$

$$- \frac{2h^2 \alpha \beta K N^2 J_o(\alpha\rho) J_1(\alpha\rho) \rho}{m^* \sqrt{\rho^2 + z^2}} \; e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$+ \frac{h^2 \alpha \beta \lambda K N^2 J_o(\alpha\rho) J_1(\alpha\rho) \rho}{m^*} \; e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}} \qquad \text{D.20.h}$$

Integrating D.20.h, one obtains

$$\int_\tau \Phi_{2s} \left(- \frac{h^2}{2m^*} \; D.20.h \right) d\tau$$

$$= - \frac{4\pi h^2 \beta N^2}{m^*} \int_o^a \rho \; J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho$$

$$+ \frac{4\pi h^2 \beta^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\beta\rho)\, d\rho$$

$$- \frac{8\pi h^2 \beta K N^2}{m^*} \int_o^a \rho \; J_o^2(\alpha\rho) K_o[(\beta+\lambda)\rho]\, d\rho$$

$$+ \frac{4\pi h^2 \beta^2 K N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho$$

$$+ \frac{4\pi h^2 \beta \lambda K N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho$$

$$+ \frac{4\pi h^2 \alpha \beta \lambda K N^2}{m^*} \int_o^a \rho^3 J_o(\alpha\rho) J_1(\alpha\rho) K_1[(\beta+\lambda)\rho]\, d\rho \quad \text{D.20.h}$$

$$\Phi_{2s}^* \left(- \frac{h^2}{2m^*} \; D.20.i \right)$$

$$= \frac{h^2 \alpha^2 K N^2 J_o^2(\alpha\rho)}{m^*} \; e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$+ \frac{2h^2 \alpha^2 K^2 N^2 J_o^2(\alpha\rho)}{m^*} \; e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$- \frac{h^2 \alpha^2 \lambda K^2 N^2}{m^*} \; J_o^2(\alpha\rho) \; \sqrt{\rho^2 + z^2} \; e^{-2\lambda\sqrt{\rho^2 + z^2}} \quad \text{D.20.i}$$

D.20.i on integration, becomes:

$$\int_\tau \Phi_{2s}^* \left(- \frac{h^2}{2m^*} D.20.i \right) d\tau$$

$$= \frac{4\pi h^2 \alpha^2 K N^2}{m^*} \int_o^a \rho^2 \; J_o^2(\alpha\rho)\, K_1[(\beta+\lambda)\rho]\, d\rho$$

$$+ \frac{8\pi h^2 \alpha^2 K^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\lambda\rho)\, d\rho$$

$$- \frac{4\pi h^2 \alpha^2 \lambda K^2 N^2}{m^*} \int_o^a \rho^3 \; J_o^2(\alpha\rho)\, K_o(2\lambda\rho)\, d\rho$$

$$- \frac{2\pi h^2 \alpha^2 K^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\lambda\rho)\, d\rho \qquad \text{D.20.i"}$$

Finally, the last term D.20.j yields

$$\Phi_{2s}^* \left(- \frac{h^2}{2m^*} D.20.j \right)$$

$$= - \frac{h^2 \alpha^2 \lambda K N^2}{2m^*} J_o^2(\alpha\rho) \sqrt{\rho^2 + z^2} \; e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}}$$

$$- \frac{h^2 \alpha^2 \lambda K^2 N^2}{m^*} J_o^2(\alpha\rho) \sqrt{\rho^2 + z^2} \; e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$+ \frac{h^2 \alpha^2 \lambda^2 K^2 N^2}{2m^*} J_o^2(\alpha\rho)\, \rho^2 \; e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$+ \frac{h^2 \alpha^2 \lambda^2 K^2 N^2}{2m^*} J_o^2(\alpha\rho) \; z^2 \; e^{-2\lambda\sqrt{\rho^2 + z^2}} \qquad \text{D.20.j}$$

On integrating D.20.j one obtains

$$\int_{\tau} \Phi^{*}_{2s} \left(- \frac{h^2}{2m^*} \; D.20.j \right) d\tau$$

$$= - \frac{2\pi h^2 \alpha^2 \lambda K N^2}{m^*} \int_o^a \rho^3 J_o^2(\alpha\rho) K_o[(\beta+\lambda)\rho] \, d\rho$$

$$- \frac{2\pi h^2 \alpha^2 \lambda K N^2}{m^*(\beta+\lambda)} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho] \, d\rho$$

$$- \frac{4\pi h^2 \alpha^2 \lambda K^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_o(2\lambda\rho) \, d\rho$$

$$- \frac{2\pi h^2 \alpha^2 K^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho) \, d\rho$$

$$+ \frac{2\pi h^2 \alpha^2 \lambda^2 K^2 N^2}{m^*} \int_o^a \rho^4 J_o^2(\alpha\rho) K_1(2\lambda\rho) \, d\rho$$

$$+ \frac{\pi h^2 \alpha^2 K^2 N^2}{m^*} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho) \, d\rho$$

$$+ \frac{\pi h^2 \alpha^2 \lambda K^2 N^2}{m^*} \int_o^a \rho^3 J_o^2(\alpha\rho) K_o(2\lambda\rho) \, d\rho \qquad \text{D.20.j''}$$

Now, the kinetic energy terms, comprising D.20.a to D.20.j, can be added together and simplified by making use of the following notations:

$$R1 = \int_o^a \rho^2 \, J_o^2(\alpha\rho) K_1(2\beta\rho) \, d\rho \qquad \text{E.1}$$

$$R2 = \int_o^a \rho^2 \, J_o^2(\alpha\rho) K_1(2\lambda\rho) \, d\rho \qquad \text{E.2}$$

$$R3 = \int_o^a \rho^4 \, J_o^2(\alpha\rho) K_1(2\lambda\rho) \, d\rho \qquad \text{E.3}$$

$$R4 = \int_o^a \rho^3 \, J_o^2(\alpha\rho) K_o(2\lambda\rho) \, d\rho \qquad \text{E.4}$$

$$R5 = \int_o^a \rho^3 \, J_o^2(\alpha\rho) K_o[(\beta+\lambda)\rho] \, d\rho \qquad \text{E.5}$$

$$R6 = \int_o^a \rho^2 \, J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho] \, d\rho \qquad \text{E.6}$$

$$R7 = \int_o^a \rho^3 \, J_o^2(\alpha\rho) K_1[(\beta+\lambda)\rho] \, d\rho \qquad \text{E.7}$$

$$R8 = \int_o^a \rho^3 \, J_o^2(\alpha\rho) K_1(2\lambda\rho) \, d\rho \qquad \text{E.8}$$

$$R9 = \int_o^a \rho^3 \, J_o^2(\alpha\rho) K_o(2\beta\rho) \, d\rho \qquad \text{E.9}$$

$$R10 = \int_o^a \rho \, J_o^2(\alpha\rho) K_o[(\beta+\lambda)\rho] \, d\rho \qquad \text{E.10}$$

$$R11 = \int_o^a \rho \, J_o^2(\alpha\rho) K_o(2\lambda\rho) \, d\rho \qquad \text{E.11}$$

In the integrations above, use was made of the relation [44]:

$$\int_o^a \rho^2 J_o(\alpha\rho) J_1(\alpha\rho) K_o(2\lambda\rho)\, d\rho$$

$$= -\frac{1}{2\alpha} \int_o^a \left[\frac{d}{d\rho} J_o^2(\alpha\rho) \right] K_o(2\lambda\rho)\, \rho^2 d\rho$$

$$+ \frac{1}{2\alpha} \int_o^a J_o^2(\alpha\rho) \left\{ 2\rho K_o(2\lambda\rho) - 2\lambda\rho^2 K_1(2\lambda\rho) \right\} d\rho$$

$$= \frac{\rho^2}{2\alpha} J_o^2(\alpha\rho)\, K_o(2\lambda\rho) \Big|_o^a$$

$$+ \frac{1}{\alpha} \int_o^a \rho J_o^2(\alpha\rho) K_o(2\lambda\rho)\, d\rho$$

$$- \frac{\lambda}{\alpha} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho \qquad \text{E.12}$$

The integrated part of E.12 vanishes at the boundaries and the result is

$$\int_o^a \rho^2 J_o(\alpha\rho) J_1(\alpha\rho) K_o(2\lambda\rho)\, d\rho \qquad \text{E.13}$$

$$= \frac{1}{\alpha} \int_o^a \rho J_o^2(\alpha\rho) K_o(2\lambda\rho)\, d\rho - \frac{\lambda}{\alpha} \int_o^a \rho^2 J_o^2(\alpha\rho) K_1(2\lambda\rho)\, d\rho$$

The final expression for the expectation value of the kinetic energy becomes:

$$\langle T \rangle = \frac{13\pi h^2\lambda^2K^2N^2}{m^*} R8 + \frac{10\pi h^2\beta\lambda KN^2}{m^*} R7$$

$$- \frac{2\pi h^2\lambda^2KN^2}{m^*} R6 - \frac{11\pi h^2\lambda^3K^2N^2}{m^*} R4$$

$$+ \frac{2\pi h^2\beta^2N^2}{m^*} R1 + \frac{2\pi h^2\beta^2\lambda KN^2}{m^*} R5$$

$$+ \frac{4\pi h^2\beta^2\lambda KN^2}{m^*(\beta+\lambda)} R6 + \frac{4\pi h^2\lambda^3KN^2}{m^*(\beta+\lambda)} R6$$

$$+ \frac{2\pi h^2\lambda^4K^2N^2}{m^*} R3 - \frac{2\pi h^2\beta\lambda^2KN^2}{m^*} R5$$

$$- \frac{7\pi h^2\alpha^2\lambda K^2N^2}{m^*} R4 + \frac{5\pi h^2\alpha^2K^2N^2}{m^*} R2$$

$$+ \frac{2\pi h^2\alpha^2\lambda^2K^2N^2}{m^*} R3 - \frac{2\pi h^2\beta\lambda^2KN^2}{m^*} R5$$

$$- \frac{2\pi h^2\alpha^2N^2}{m^*} R1 \qquad \text{E.14}$$

The expectation value of the potential energy with the static dielectric constant $\epsilon(o)$ is determined as follows:

$$\langle V \rangle = - \frac{e^2}{\epsilon(o)} \langle \Phi_{2s} \mid \frac{1}{r} \mid \Phi_{2s} \rangle \qquad \text{F.1}$$

$$= - \frac{e^2}{\epsilon(o)} \int_\tau \Phi^*_{2s} \left([\, \rho^2 + z^2 \,]^{-1/2} \, \Phi_{2s} \right) d\tau$$

Now

$$\Phi^{*}_{2s} [\rho^2 + z^2]^{-1/2} \Phi_{2s}$$

$$= - \frac{e^2 N^2 J_o^2(\alpha\rho)}{\epsilon(o) \sqrt{\rho^2 + z^2}} e^{-2\beta\sqrt{\rho^2 + z^2}} \qquad \text{F.2}$$

$$- \frac{4 e^2 K N^2 J_o^2(\alpha\rho)}{\epsilon(o) \sqrt{\rho^2 + z^2}} e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}} \qquad \text{F.3}$$

$$+ \frac{2 e^2 \lambda K N^2 J_o^2(\alpha\rho)}{\epsilon(o)} e^{-(\beta+\lambda)\sqrt{\rho^2 + z^2}} \qquad \text{F.4}$$

$$= - \frac{4 e^2 K^2 N^2 J_o^2(\alpha\rho)}{\epsilon(o) \sqrt{\rho^2 + z^2}} e^{-2\lambda\sqrt{\rho^2 + z^2}} \qquad \text{F.5}$$

$$+ \frac{4 e^2 \lambda K^2 N^2 J_o^2(\alpha\rho)}{\epsilon(o)} e^{-2\lambda\sqrt{\rho^2 + z^2}} \qquad \text{F.6}$$

$$- \frac{e^2 \lambda^2 K^2 N^2 J_o^2(\alpha\rho) \sqrt{\rho^2 + z^2}}{\epsilon(o)} e^{-2\lambda\sqrt{\rho^2 + z^2}} \qquad \text{F.7}$$

The integration of the terms F.2 to F.7 yield the following results for the potential energy:

$$\int_\tau (F.2)\, d\tau = \frac{-e^2}{\epsilon(o)} N^2 \int_o^{2\pi} d\theta \int_o^a \rho\, J_o^2(\alpha\rho)\, d\rho \ x$$

$$\int_{-\infty}^{\infty} \frac{dz\ e^{-2\beta\sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}} \qquad \text{F.2}$$

$$= - \frac{4\pi e^2 N^2}{\epsilon(o)} \int_o^a \rho\ J_o^2(\alpha\rho) K_o(2\beta\rho)\, d\rho$$

$\int_\tau (F.3)$

$$= -\frac{4e^2KN^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho\ J_o^2(\alpha\rho)\,d\rho \int_{-\infty}^{\infty} \frac{dz\ e^{-(\beta+\lambda)\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}} \qquad \text{F.3}$$

$$= -\frac{16\pi e^2KN^2}{\epsilon(o)} \int_o^a \rho\ J_o^2(\alpha\rho)\,K_o[(\beta+\lambda)\rho]\,d\rho$$

$\int_\tau (F.4)\,d\tau$

$$= \frac{2\lambda e^2KN^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho\ J_o^2(\alpha\rho)\,d\rho \int_{-\infty}^{\infty} dz\ e^{-(\beta+\lambda)\sqrt{\rho^2+z^2}} \qquad \text{F.4}$$

$$= \frac{8\pi\lambda e^2KN^2}{\epsilon(o)} \int_o^a \rho^2\ J_o^2(\alpha\rho)\,K_1[(\beta+\lambda)\rho]\,d\rho$$

$\int_\tau (F.5)\,d\tau$

$$= -\frac{4e^2K^2N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho\ J_o^2(\alpha\rho)\,d\rho \int_{-\infty}^{\infty} \frac{dz\ e^{-2\lambda\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}} \qquad \text{F.5}$$

$$= -\frac{16\pi e^2K^2N^2}{\epsilon(o)} \int_o^a \rho\ J_o^2(\alpha\rho)\,K_o(2\lambda\rho)\,d\rho$$

$$\int_\tau (F.6)\, d\tau$$

$$= \frac{4\lambda e^2 K^2 N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho\, J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\, e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$= \frac{16\pi\lambda e^2 K^2 N^2}{\epsilon(o)} \int_o^a \rho^2\, J_o^2(\alpha\rho)\, K_1(2\lambda\rho)\, d\rho \qquad \text{F.6}$$

$$\int_\tau (F.7)\, d\tau$$

$$= -\frac{e^2\lambda^2 K^2 N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho\, J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\, \sqrt{\rho^2 \; z^2}\; e^{-2\lambda\sqrt{\rho^2 + z^2}}$$

$$= -\frac{4\pi e^2\lambda^2 K^2 N^2}{\epsilon(o)} \int_o^a \rho^3\, J_o^2(\alpha\rho)\, K_o(2\lambda\rho)\, d\rho$$

$$- \frac{2\pi e^2\lambda K^2 N^2}{\epsilon(o)} \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1(2\lambda\rho)\, d\rho \qquad \text{F.7}$$

Adding all the terms F.2 to F.7, and using the notations of Equations E.1 to E.11, the expectation value of the potential energy, with the static dielectric constant $\epsilon(o)$ becomes:

$$\langle V \rangle = -\frac{4\pi e^2 N^2}{\epsilon(o)} R9 - \frac{16\pi e^2 K N^2}{\epsilon(o)} R10$$

$$+ \frac{8\pi\lambda e^2 K N^2}{\epsilon(o)} R6 - \frac{16\pi e^2 K^2 N^2}{\epsilon(o)} R11$$

$$+ \frac{16\pi\lambda e^2 K^2 N^2}{\epsilon(o)} R2 - \frac{4\pi\lambda^2 e^2 K^2 N^2}{\epsilon(o)} R4$$

$$- \frac{2\pi\lambda e^2 K^2 N^2}{\epsilon(o)} R^2 \qquad \text{F.8}$$

When the static dielectric constant is replaced by the spatial dielectric function, there are additional terms in the expectation value of the potential energy. These additional terms are determined as follows:

$$\Delta V = -e^2 \int_\tau \Phi_{2s}^* \left[\frac{\epsilon(o) - 1}{\epsilon(o)} e^{-\frac{\sqrt{\rho^2 + z^2}}{c}} \right] \Phi_{2s} \, d\tau \qquad \text{F.9}$$

$$= -\frac{e^2 [\epsilon(o) - 1] N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho \, J_o^2(\alpha\rho) \, d\rho \; x$$

$$\int_{-\infty}^{\infty} \frac{dz}{\sqrt{\rho^2 + z^2}} \Big[e^{-\left(2\beta + \frac{1}{c}\right)\sqrt{\rho^2 + z^2}} + 4Ke^{-\left(\beta + \lambda + \frac{1}{c}\right)\sqrt{\rho^2 + z^2}}$$

$$- 2\lambda K \sqrt{\rho^2 + z^2} \, e^{-\left(\beta + \lambda + \frac{1}{c}\right)\sqrt{\rho^2 + z^2}}$$

$$+ 4 K^2 e^{-\left(2\lambda + \frac{1}{c}\right)\sqrt{\rho^2 + c^2}}$$

$$- 4\lambda K \sqrt{\rho^2 + z^2} \, e^{-\left(2\lambda + \frac{1}{c}\right)\sqrt{\rho^2 + z^2}}$$

$$+ \lambda^2 K^2 (\rho^2 + z^2) \, e^{-\left(2\lambda + \frac{1}{c}\right)\sqrt{\rho^2 + z^2}} \Big]$$

Integrating the terms one by one yields:

$$\Delta V = - \frac{e^2 [\epsilon(o) - 1] N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho \, J_o^2(\alpha\rho) \, d\rho$$

$$x \int_{-\infty}^{\infty} dz \, e^{-\left(2\beta + \frac{1}{c} \right) \sqrt{\rho^2 + z^2}}$$

$$- \frac{4Ke^2 [\epsilon(o) - 1] N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho \, J_o^2(\alpha\rho) \, d\rho$$

$$x \int_{-\infty}^{\infty} \frac{dz \, e^{-\left(\beta + \lambda + \frac{1}{c} \right) \sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

$$+ \frac{2\lambda Ke^2 [\epsilon(o) - 1] N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho \, J_o^2(\alpha\rho) \, d\rho$$

$$x \int_{-\infty}^{\infty} dz \, e^{-\left(\beta + \lambda + \frac{1}{c} \right) \sqrt{\rho^2 + z^2}}$$

$$- \frac{4K^2e^2 [\epsilon(o) - 1] N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho \, J_o^2(\alpha\rho) \, d\rho$$

$$x \int_{-\infty}^{\infty} \frac{dz \, e^{-\left(2\lambda + \frac{1}{c} \right) \sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}$$

$$+ \frac{4\lambda K e^2 [\,\epsilon(o)-1\,]\, N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\; e^{-\left(2\lambda + \frac{1}{c}\right)\sqrt{\rho^2+z^2}}$$

$$- \frac{\lambda^2 K^2 e^2 [\epsilon(o)-1] N^2}{\epsilon(o)} \int_o^{2\pi} d\theta \int_o^a \rho J_o^2(\alpha\rho)\, d\rho \int_{-\infty}^{\infty} dz\; \sqrt{\rho^2+z^2}\, e^{-\left(2\lambda + \frac{1}{c}\right)\sqrt{\rho^2+z^2}}$$

$$= - \frac{4\pi e^2 [\,\epsilon(o)\; -1\,]\, N^2}{\epsilon(o)} \int_o^a \rho J_o^2(\alpha\rho)\, K_o \left[\left(2\beta + \frac{1}{c} \right) \rho \right] d\rho$$

$$- \frac{16\pi K e^2 [\,\epsilon(o)\; -1\,]\, N^2}{\epsilon(o)} \int_o^a \rho J_o^2(\alpha\rho)\, K_o \left[\left(\beta + \lambda + \frac{1}{c} \right) \rho \right] d\rho$$

$$+ \frac{8\pi\lambda K e^2 [\,\epsilon(o)\; -\; 1\,]\, N^2}{\epsilon(o)} \int_o^a \rho^2 J_o^2(\alpha\rho)\, K_1 \left[\left(\beta + \lambda + \frac{1}{c} \right) \rho \right] d\rho$$

$$- \frac{16\pi K^2 e^2 [\,\epsilon(o)\; -\; 1\,]}{\epsilon(o)} \int_o^a \rho\; J_o^2(\alpha\rho)\, K_1 \left[\left(\beta\; 2\lambda + \frac{1}{c} \right) \rho \right] d\rho$$

$$+ \frac{16\pi K e^2 [\,\epsilon(o)\; -\; 1\,]\, N^2}{\epsilon(o)} \int_o^a \rho^2\; J_o^2(\alpha\rho)\, K_1 \left[\left(2\lambda + \frac{1}{c} \right) \rho \right] d\rho$$

$$- \frac{4\pi\lambda^2 K^2 e^2 [\,\epsilon(o)\; -\; 1\,]\, N^2}{\epsilon(o)} \int_o^a \rho^3\; J_o^2(\alpha\rho)\, K_o \left[\left(2\lambda + \frac{1}{c} \right) \rho \right] d\rho$$

$$- \frac{4\pi\lambda^2 K^2 e^2 [\,\epsilon(o)\; -\; 1\,]\, N^2}{\epsilon(o) \left(2\lambda + \frac{1}{c} \right)} \int_o^a \rho^2\; J_o^2(\alpha\rho)\, K_1 \left[\left(2\lambda + \frac{1}{c} \right) \rho \right] d\rho$$

E. Calculation of the Free Particle Energy

In this appendix, the details of the calculation of the free particle energy are presented.

The Hamiltonian for a free particle in cylindrical coordinates is given by

$$H = -\frac{h^2}{2m^*}\left\{\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\rho^2} + \frac{\partial^2}{\partial z^2}\right\}$$

H.1

The wave function for the free particle Hamiltonian[1] is:

$$\psi_{nlm}(\rho, z, \phi) = R_{nl}(\rho)\,\Phi_l(\phi)\,Z_m(z)$$

$$= A_{nl}J_{nl}\left(\lambda_{nl}\frac{\rho}{a}\right)e^{il\phi}\,e^{ikz}$$

H.2

where

$$k = \frac{j\pi}{L}$$

and L is Length of the cylinder.

For the cylindrical case with $\ell = 0$, and $(\rho/a) = 1$ $J_{n\ell}(\lambda_{n\ell}) = 0$, the first node of the ordinary Bessel function. Then one has:

$$\psi_{nl} = A_{no}J_{no}\left(\lambda_{no}\frac{\rho}{a}\right)e^{ikz}$$

H.3

The normalization constant A_{no} is obtained from

$$1 = \int_{\tau} \Psi_{nml}\Psi_{nml}\, d\tau$$

$$= \int A^{*}_{no}\, J_{no}\left(\lambda_{no}\, \frac{\rho}{a} \right) e^{-ikz}\, A_{no}\, J_{no}\left(\lambda_{no}\, \frac{\rho}{a} \right) e^{ikz}\, d\tau$$

$$= A^{2}_{no} \int_{o}^{2\pi} d\theta \int_{o}^{a} \rho\, J^{2}_{no}\left(\lambda_{no}\, \frac{\rho}{a} \right) d\rho$$

$$x \int_{-\infty}^{\infty} dz\; e^{i(k-k)z}$$

H.4

Therefore,

$$A^{2}_{no} = \frac{1}{2\pi \int_{o}^{a} \rho\, J^{2}_{no}\left(\lambda_{no}\, \frac{\rho}{a} \right) d\rho \int_{-\infty}^{\infty} dz\; e^{i(k-k)z}}$$

$$= \left[2\pi \int_{o}^{a} \rho\, J^{2}_{no}\left(\lambda_{no}\, \frac{\rho}{a} \right) d\rho \int_{-\infty}^{\infty} dz\; e^{i(k-k)z} \right]^{-1}$$

H.5

The kinetic energy is determined as

$$\frac{\partial^2}{\partial \rho^2} J_{no}\left(\lambda_{no}\frac{\rho}{a}\right) = -\frac{\lambda_{no}}{a}\frac{\partial}{\partial \rho} J_1\left(\lambda_{no}\frac{\rho}{a}\right)$$

$$= -\frac{\lambda_{no}}{a}\left\{\frac{\lambda_{no}}{a} J_{no}\left(\lambda_{no}\frac{\rho}{a}\right) - \frac{J_1\left(\lambda_{no}\frac{\rho}{a}\right)}{\rho}\right\}$$

$$= -\frac{\lambda_{no}^2}{a^2} J_{no}\left(\lambda_{no}\frac{\rho}{a}\right) + \frac{\lambda_{no} J_1\left(\lambda_{no}\frac{\rho}{a}\right)}{a\rho}$$

$$\frac{1}{\rho}\frac{\partial}{\partial \rho} J_o\left(\lambda_{no}\frac{\rho}{a}\right) = \frac{1}{\rho}\left\{-\frac{\lambda_{no}}{a} J_1\left(\lambda_{no}\frac{\rho}{a}\right)\right\}$$

$$= -\frac{\lambda_{no}}{a\rho} J_1\left(\lambda_{no}\frac{\rho}{a}\right)$$

The differentiated ρ-part becomes

$$\left\{ \frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho} \frac{\partial}{\partial\rho} \right\} J_o\left(\lambda_{no} \frac{\rho}{a} \right)$$

$$= - \frac{\lambda^2_{no}}{a^2} J_o\left(\lambda_{no} \frac{\rho}{a} \right)$$

$$+ \frac{\lambda_{no} J_1\left(\lambda_{no} \frac{\rho}{a} \right)}{a\rho}$$

$$- \frac{\lambda_{no} J_1\left(\lambda_{no} \frac{\rho}{a} \right)}{a\rho}$$

$$= - \frac{\lambda^2_{no}}{a^2} J_o\left(\lambda_{no} \frac{\rho}{a} \right)$$

H.8

Therefore,

$$\nabla^2 \rho \psi_{no}(\rho, z) = - \frac{\lambda^2_{no}}{a^2} J_o\left(\lambda_{no} \frac{\rho}{a} \right) e^{ikz}$$

H.8'

The z-differentiation yields

$$\frac{\partial^2}{\partial z^2}\psi_{no}(\rho, z) = J_o\left(\lambda_{no}\frac{\rho}{a}\right)\frac{\partial}{\partial z}\left\{\frac{\partial}{\partial z}e^{ikz}\right\}$$

$$= J_o\left(\lambda_{no}\frac{\rho}{a}\right)\frac{\partial}{\partial z}\{ike^{ikz}\}$$

$$= J_o\left(\lambda_{no}\frac{\rho}{a}\right)[-k^2e^{ikz}]$$

$$= -k^2J_o\left(\lambda_{no}\frac{\rho}{a}\right)e^{ikz}$$

H.9

After multiplication by $\frac{\hbar^2}{2m^*}$, the $\nabla^2\ \psi_{no}(\rho,z)$ becomes,

$$-\frac{h^2}{2m^*}\nabla^2\psi_{no}(\rho, z)$$

$$= \left\{\frac{h^2\lambda_{no}^2}{2m^*a^2} + \frac{h^2k^2}{2m^*}\right\}J_o\left(\lambda_{no}\frac{\rho}{a}\right)e^{ikz}$$

H.10

Multiplying H.10 by $\psi^*_{no}(\rho,z)$ and integration of the free particle kinetic energy yields

$$\int_\tau \psi^*_{no}(\rho,z)\left[-\frac{h^2}{2m*}\nabla^2\psi_{no}(\rho,z)\right]d\tau$$

$$= A^2_{no}\left\{\frac{h^2\lambda no^2}{2m^*a^2}+\frac{h^2k^2}{2m^*}\right\}\int_o^{2\pi}d\theta\int_o^a \rho J_o\left(\lambda_{no}\frac{\rho}{a}\right)d\rho$$

$$x\int_{-\infty} dz\, e^{i(k-k)z}$$

$$= A^2_{no}\left\{\frac{h^2\lambda^2_{no}}{2m*a^2}+\frac{h^2k^2}{2m*}\right\}\int_o^{2\pi}d\theta\int_o^a \rho J_o\left(\lambda_{no}\frac{\rho}{a}\right)d\rho$$

$$= \frac{h^2\lambda^2_{no}}{2m^*a^2}+\frac{h^2k^2}{2m^*}$$

$$= \frac{h^2\alpha^2}{2m^*}+\frac{h^2k^2}{2m^*}$$

H.11

where

$$\alpha^2 = \frac{\lambda_{no}^2}{a^2}$$

For the ground state j=0, hence k^2

energy becomes

$$< T >_{free} = \frac{\hbar^2 \alpha^2}{2m^*}$$

For the first node n = 1 and λ_{no} =

and α becomes

$$\alpha = \frac{2.4048}{a}$$

= 0 and the free particle

H.12

λ_{1o} = 2.4048 [45]

H.13

F. Numerical Integration Techniques

The algorithm used is the Q DAGS [47] which is a general purpose integrator. It uses a globally adoptive scheme to reduce the absolute error. It subdivides the interval [A,B] and uses a 21-point Gaussian-Kronrod rule to estimate the integral over each subinterval. The error for each subinterval is estimated by comparison with the 10-point Gauss quadrature rule. This subroutine is designed to handle functions with end point singularities. However, it performs as well on functions which are well-behaved at the end points.

G. Units Used in This Work.

The QWW radii are given in atomic units, where 1 atomic unit is twice the bohr, a_o, and the bohr is given by

$$a_o = 5.29 \times 10^{-9} \text{cm}$$

The units of energy are in meV. From quantum mechanics one has $(e^2/a_o) = 27.2$ eV. Since the energies involved in this work are much less than this, it is necessary to use meV, where 1 eV = 1000 meV. For example, the binding energy of a hydrogenic donor in bulk semiconductors is given by

$$E_d = \frac{e^4 m^*}{2\, \epsilon(o)^2\, h^2}$$

If one substitutes $m^* = 0.067\ m_e$

$$\epsilon(o) = 12.56$$

one multiplies by 1000 and 27.2 eV one obtains $E_d = 5.78$ meV which is the bulk value for GaAs.

Sample Program

```
      PARAMETER (NSTEP=1000,BETA0=0.006,BETA1=.05E-3)
      EXTERNAL F1, F2, F3
      REAL*8 MASS, EPSILON, ESQU,B,BETA,BETA2,N2,V,H,E
      REAL*8 RESULT(NSTEP), A(19)
      REAL*8 INC, LOW, UP, ERRREL, ERRABS, ERREST,ALPHA,ALPHA2
      REAL*8 R1, R2, R3
      INTEGER I, J, INDX
      COMMON BETA,BETA2,ALPHA,ALPHA2
      CALL ERRSET(208,280,-1,1)
      INC = (BETA0-BETA1)/NSTEP
      LOW=0.0
      ERRABS = 0.00001
      ERRREL = 0.5e-6
      ESQU = 1.0
      EPSILON = 12.56
      UP = 1000.0
      ALPHA = 2.4048/UP
      ALPHA2 = ALPHA**2
      MASS = 0.067
      PI = 3.14159
      WRITE (6,*)'a= ',UP
      WRITE(6,*)' E-VALUE                          BETA
      BETA =BETA0 +INC
C NOW LOOP THROUGH THE BETAS FROM BETA0 TO BETA1 IN NSTEP STEPS.
C CALCULATE <E> FOR EACH BETA AND STORE IN ARRAY RESULT.
       DO 2 J=1,NSTEP
         BETA =BETA -INC
         BETA2 =BETA**2
C CALCULATE  N2,V,H
        CALL DQDAGA(F1,LOW,UP,ERRABS,ERRREL,R1,ERREST)
        CALL DQDAGS(F2,LOW,UP,ERRABS,ERRREL,R2,ERREST)
        CALL DQDAGA(F2,LOW,UP,ERRABS,ERRREL,R3,ERREST)
        N2=1/(R1)
        V= -N2*R2/12.56-N2*(11.56/12.56)*R3
        H = 0.5*BETA2/MASS
C CALCULATE E AND STORE IN RESULT ARRAY
          RESULT(J)= (H+V)*27200.0
          WRITE (6,*) RESULT(J),BETA
2        CONTINUE
       STOP
       END
C DEFINE THE FUNCTIONS F1...F3 FOR THE INTEGRALS
      DOUBLE PRECISION FUNCTION F1(R)
      REAL*8 R,BETA
      COMMON BETA
      F1 = (R**2)*DBSK1(2.0*BETA*R)
      RETURN
      END
      DOUBLE PRECISION FUNCTION F2(R)
      REAL*8 R,BETA
      COMMON BETA
      F2 = (R)*DBSKO(2.0*BETA*R)
      RETURN
      END
```

```
DOUBLE PRECISION FUNCTION F3(R)
COMMON BETA
F3 = (R)*DBSKO((2.0*BETA+1.375)*R)
RETURN
END
```

BIOGRAPHY

Hannington Odhiambo Oyoko was born in Kisii Town, South Nyanza District, Kenya on 22nd April, 1948. He received his high school education at Maseno National High School in Nyanza.

He entered University of Nairobi in 1971 and obtained his Bachelor of Science degree in 1974. He taught high school physics and mathematics for one and a half years before joining the Kenya Air Force, from which he retired in 1983 in the rank of Major.

In September 1985, he was enrolled for graduate study in Physics at Fairleigh Dickinson University in New Jersey from which he received his Master of Science Degree in February, 1987.

In April 1987, he joined the teaching staff in the Department of Physics at the University of Nairobi.

In September 1988 he was given study leave by the University of Nairobi and in the same month he was enrolled for Ph.D. program in Physics at the University of Maine and served as a Teaching Assistant in the Department of Physics. He is a candidate for the Doctor of Philosophy degree in Physics from the University of Maine, Orono, in May 1991.