

Finite Element Method for Solving the Two-Dimensional Schroedinger Equation

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Received August 11, 1976; revised April 21, 1977

A finite element package is presented that is able to treat two-dimensional Schroedinger equation problems over a finite region with an arbitrary potential and homogeneous boundary conditions. In order to present the applicability and accuracy of this approach, two cases for which the exact solution is known are solved: (i) a free particle in a spherical box, (ii) a hydrogen atom enclosed in a finite sphere. The results definitely indicate that the finite element method is both accurate and efficient and could serve as a useful tool in various single particle quantum mechanical problems.

INTRODUCTION

During the past few years there was a rapid development of finite element methods replacing the widely used finite differences approach, in various areas of numerical analysis. However, only recently [1] this new method was applied regarding the Schroedinger equation. The case considered was that of one particle in a Coulomb field, reduced, due to spherical symmetry, to a one-dimensional problem.

The purpose of this work is to present a finite element package for solving a certain class of two-dimensional elliptic partial differential equations. This package was modified to enable one to treat two-dimensional Schroedinger equation problems over a finite region with an arbitrary potential and homogeneous boundary conditions. The method is applicable to a variety of problems such as the quantum cell model [2], the compressed hydrogen atom [3-5], low lying π - π^* transitions in

substituted benzenes [6], and for the calculation of the nuclear potential energy by the microscopic method [7].

In order to demonstrate the applicability and accuracy of this approach, two cases for which the exact solution can be found are solved: (i) a free particle in a spherical box; (ii) a hydrogen atom enclosed in a finite sphere. It should be stressed that although these cases are very simple and specific, the results test the method for the general case. They definitely indicate that the finite element method is both accurate and efficient, and could serve as a useful tool in various single particle quantum mechanical problems.

THE NUMERICAL METHOD—MANFEP

(a) Formulation of the General Problem

In order to solve the Schroedinger equation, a two-dimensional finite element package, MANFEP [8], is used. This package can solve either a general second order elliptic partial differential equation of a certain form over a finite region, with Dirichlet, homogeneous Neumann, or mixed boundary conditions, or a general eigenvalue problem related to the same operator.

Let R be a finite region at the x - y plane and let Γ be its boundary. Consider the following elliptic partial differential equation

$$L\psi \equiv \frac{\partial}{\partial x} \left(a \frac{\partial \psi}{\partial x} + b \frac{\partial \psi}{\partial y} \right) + \frac{\partial}{\partial y} \left(b \frac{\partial \psi}{\partial x} + c \frac{\partial \psi}{\partial y} \right) + d\psi = -p, \quad (x, y) \in R, \quad (1)$$

where $a, b, c \in C^1(R)$; $d, p \in C(R)$; and $ac > b^2$. The general boundary value problem for MANFEP would be formulated as follows: Find a function $\psi \in C^2(R)$ that satisfies (1) as well as the boundary conditions

$$\psi = f \quad \text{on } \Gamma_1, \quad (2)$$

$$-D(\psi) \cdot \hat{n} \equiv \begin{pmatrix} \frac{\partial \psi}{\partial x} & \frac{\partial \psi}{\partial y} \end{pmatrix} \begin{pmatrix} a & b \\ b & c \end{pmatrix} \begin{pmatrix} n_x \\ n_y \end{pmatrix} = 0 \quad \text{on } \Gamma_2, \quad (3)$$

$$-D(\psi) \cdot \hat{n} + \sigma\psi = h \quad \text{on } \Gamma_3, \quad (4)$$

where $\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_3$; $f \in C(\Gamma_1)$; $\sigma, h \in C(\Gamma_3)$; $\sigma > 0$, and \hat{n} is the outward normal unit vector at the boundary. The general eigenvalue problem is given as follows Find a real λ and a nontrivial function $\psi \in C^2(R)$ that satisfies

$$L\psi + \lambda e\psi = 0, \quad (x, y) \in R \quad (5)$$

along with homogeneous Dirichlet or Neumann boundary conditions on Γ , i.e.,

$$\psi = 0 \quad \text{on } S_1 \quad (6)$$

and

$$-D(\psi) \cdot \hat{n} = 0 \quad \text{on } S_2, \quad (7)$$

where $\Gamma = S_1 + S_2$.

(b) *The Functional*

Both the boundary value and the eigenvalue problems are solved by minimizing a certain functional that depends upon L , p , or e and the boundary conditions. To solve the boundary value problem one should minimize

$$F_B = \iint_R \left[a \left(\frac{\partial \psi}{\partial x} \right)^2 + 2b \frac{\partial \psi}{\partial x} \frac{\partial \psi}{\partial y} + c \left(\frac{\partial \psi}{\partial y} \right)^2 - d\psi^2 - 2\psi p \right] dx dy + \int_{\Gamma_3} (\sigma\psi^2 - 2h\psi) ds_3 \quad (8)$$

over

$$M_B = \{ \psi \mid \psi \in C^2(R + \Gamma); \psi = f \text{ on } \Gamma_1 \}. \quad (9)$$

The minimum solution ψ_0 would then satisfy (1)–(4). The homogeneous Neumann boundary condition over Γ_2 is automatically fulfilled by ψ_0 and is therefore often mentioned as a “natural” boundary condition.

In order to solve the general eigenvalue problem a similar functional

$$F_E = \iint_R \left[a \left(\frac{\partial \psi}{\partial x} \right)^2 + 2b \frac{\partial \psi}{\partial x} \frac{\partial \psi}{\partial y} + c \left(\frac{\partial \psi}{\partial y} \right)^2 - d\psi^2 - \lambda e\psi^2 \right] dx dy \quad (10)$$

needs to be minimized over

$$M_E = \{ \psi \mid \psi \in C^2(R + \Gamma); \psi = 0 \text{ on } S_1 \}. \quad (11)$$

In the particular case of a Neumann eigenvalue problem, F_E is minimized over

$$M_E^N = \{ \psi \mid \psi \in C^2(R + \Gamma) \}. \quad (12)$$

(c) *The Finite Element Method*

Clearly, one cannot expect to minimize (8) and (10) simply by trial of a large sequence of test functions. A more algorithmic approach is needed. The finite element approach, coupled with the Rayleigh–Ritz method, is the technique used. In particular, MANFEP uses triangular isoparametric elements [9], and is superior to a finite differences approach in treating singular terms and curved boundaries. A detailed comparison is given by Askar [1].

A “triangle” (or “element”), not necessarily with straight sides, is given in “global” coordinates $x - y$ together with M specified points $\{(x_i, y_i)\}_{i=1}^M$ on its boundary and in its interior. We seek a transformation from “local” coordinates $\zeta - \eta$ to global coordinates, so that M fixed points in a “local triangle,” $\{(\zeta_i, \eta_i)\}_{i=1}^M$, will transfer to $\{(x_i, y_i)\}_{i=1}^M$. This is done by introducing “shape” functions $\{\alpha_i(\zeta, \eta)\}_{i=1}^M$ that satisfy

$$\alpha_i(\zeta_j, \eta_j) = \delta_{ij}. \quad (13)$$

The transformation is then

$$x = \sum_{i=1}^M \alpha_i(\zeta, \eta) x_i,$$

$$y = \sum_{i=1}^M \alpha_i(\zeta, \eta) y_i. \quad (14)$$

The shape functions may be of any form provided (13) holds. However, throughout MANFEP, restriction is made to polynomials. Also, the source of any global element at the local plane is always taken as the triangle $(0, 0), (1, 0), (0, 1)$.

The shape functions are used to approximate a given function $\psi(x, y)$ within a global element. First, using the Rayleigh-Ritz procedure, ψ is represented by an N th order polynomial

$$\psi(x, y) = \sum_{i+j \leq N} c_{ij} x^i y^j. \quad (15)$$

The number of the unknown coefficients is

$$M = (N + 1)(N + 2)/2. \quad (16)$$

However, they can be replaced by an equivalent set of M variables, the "node potentials" $\{\psi_i = \psi(x_i, y_i), i = 1, \dots, M\}$, thus getting

$$\psi(x, y) = \sum_{i=1}^M \alpha_i(\zeta, \eta) \psi_i. \quad (17)$$

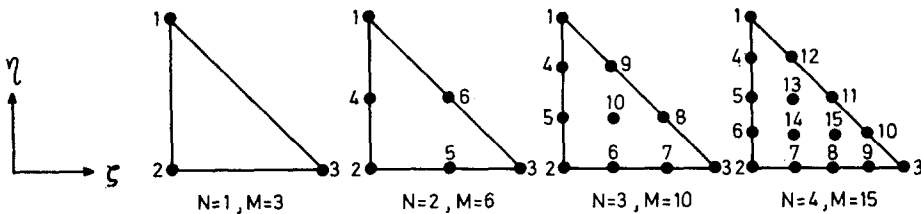


FIG. 1. Nodes assigned to the fixed local element.

The values that N takes are 1, 2, 3, 4. Accordingly, M is given by 3, 6, 10, 15, respectively. The nodes assigned to the fixed local element are shown in Fig. 1. The points in the global element to which the local nodes are transferred are chosen so that all proportions are kept. The original nodes in the local element are created by a homogeneous cartesian grid. The shape functions for the different choices of N are given in [8, p. 14].

To apply the finite element technique, R is divided into elements, and (17) is applied for each of them and substituted into either F_B or F_E . All integrations need to be performed in the global plane, but are practically done over the local element using

Gaussian quadrature formulas. In order to calculate $\partial\alpha_i/\partial x$, $\partial\alpha_i/\partial y$ one should use the relation

$$\begin{pmatrix} \frac{\partial\alpha_i}{\partial x} \\ \frac{\partial\alpha_i}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial\zeta} & \frac{\partial y}{\partial\zeta} \\ \frac{\partial x}{\partial\eta} & \frac{\partial y}{\partial\eta} \end{pmatrix}^{-1} \begin{pmatrix} \frac{\partial\alpha_i}{\partial\zeta} \\ \frac{\partial\alpha_i}{\partial\eta} \end{pmatrix}. \quad (18)$$

The computation of F_B , F_E is given in detail in [8, p. 15–16]. Their final forms are quadratic in $\{\psi_i\}_{i=1}^k$, and to minimize it, one solves a set of linear equations

$$\partial F/\partial\psi_i = 0, \quad i = 1, \dots, k. \quad (19)$$

In the case of a boundary value problem one gets to solve

$$S\vec{\psi} = B, \quad (20)$$

where S , B are the “finite matrices” of size $k \times k$, $k \times 1$, respectively, S is banded and symmetric, and $\vec{\psi}$ is the solution vector of node potentials, i.e., the finite element approximated solution of (1)–(4). Once S is created, the Dirichlet boundary values are imposed, and S is reduced by deleting rows and columns, respectively.

For an eigenvalue problem one finally needs to solve a matrix eigenvalue equation

$$(S + \lambda T)\vec{\psi} = 0, \quad (21)$$

where S , T are both symmetric of size $k \times k$.

(d) *Schroedinger Equation with Homogeneous Dirichlet Boundary Conditions*

Two, rather simple, Schroedinger problems which contain, however, all the ingredients needed for demonstrating and testing the method presented above are dealt with.

Consider the motion of an electron of mass m_0 and charge e in a spherically symmetric, infinitely deep potential well, assuming it to be confined to a sphere of radius r_0 , i.e.,

$$V(r) = \infty, \quad r > r_0, \quad (22)$$

where $V(r)$ is the potential field. The motion inside the spherical “box” is “free” in case (i), i.e.,

$$V(r) = 0, \quad r \leq r_0 \quad (23)$$

and is ruled by Coulomb potential law

$$V(r) = -e^2/r, \quad r \leq r_0 \quad (24)$$

in case (ii).

Case (i) is a well-known textbook problem, while case (ii) is the problem of the “compressed hydrogen atom” and can be treated semianalytically [3].

The stationary Schroedinger equation for a single particle of mass m_0 , moving in the potential field $V(\mathbf{r})$ is

$$-(\hbar^2/2m_0) \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r}) \psi(\mathbf{r}) = E \psi(\mathbf{r}), \quad (25)$$

where $\mathbf{r} \equiv (x, y, z)$, E is a possible energy level for the electron, and \hbar is the Planck constant h divided by 2π .

Assume $V(\mathbf{r})$ to be axially symmetric, z being the axis of symmetry. Then the z component of the angular momentum, L_z , is classically conserved, and the corresponding operator \hat{L}_z commutes with the Hamiltonian so that the azimuthal quantum number m is a good quantum number. In spherical coordinates one can separate

$$\psi(r, \theta, \phi) = u(r, \theta) e^{im\phi} \quad (26)$$

and thus replace (25) by

$$\nabla_{r,\theta}^2 u(r, \theta) - \frac{2m_0}{\hbar^2} [V_{\text{eff}}(r, \theta; m) - E] u(r, \theta) = 0 \quad (27)$$

where

$$\nabla_{r,\theta}^2 \equiv \frac{1}{r^2} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \quad (28)$$

and

$$V_{\text{eff}}(r, \theta; m) = V(r, \theta) + \frac{\hbar^2}{2m_0} \frac{m^2}{r^2 \sin^2 \theta}. \quad (29)$$

If, further, $V(\mathbf{r})$ is spherically symmetric, then by substituting

$$u(r, \theta) = f(r) p_l^m(\theta), \quad (30)$$

$p_l^m(\theta)$ being the associated Legendre function, one can reduce (27) to a one-dimensional "radial" equation. Here, however, this last separation is deliberately not done, and the problem's two-dimensional characteristics are thus retained, since it is a relatively easy matter to check the solution's θ dependence.

For a spherically symmetric potential it is also known that the energy levels do not depend on m , and this work therefore confines itself to the simplest case, namely, $m = 0$.

One should now define the reduced units

$$\rho = \alpha^{-1} r, \quad \epsilon = \beta^{-1} E, \quad (31)$$

where

$$\alpha = \hbar^2/m_0 e^2, \quad \beta = \hbar^2/2m_0 \alpha^2, \quad (32)$$

which are the standard atomic units. The Schroedinger equation will then take the forms

$$\text{case (i): } \nabla_{\rho,\theta}^2 u(\rho, \theta) + \epsilon u(\rho, \theta) = 0; \quad (33)$$

$$\text{case (ii): } \nabla_{\rho,\theta}^2 u(\rho, \theta) + [(2/\rho) + \epsilon] u(\rho, \theta) = 0; \quad (34)$$

both with homogeneous Dirichlet boundary conditions

$$u(\rho_0, \theta) = 0, \quad 0 \leq \theta \leq 2\pi \quad (35)$$

where $\rho_0 = \alpha^{-1}r_0$.

In order to solve (33)–(34), these equations should be transformed to the form (1). This can be done by using cartesian coordinates. By substituting $x = \rho \cos \theta$, $y = \rho \sin \theta$ one gets

$$\text{case (i): } y \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + \frac{\partial u}{\partial y} + y\epsilon u = 0; \quad (36)$$

$$\text{case (ii): } y \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + \frac{\partial u}{\partial y} + y \left(\frac{2}{\rho} + \epsilon \right) u = 0. \quad (37)$$

These eigenvalue equations need to be solved over $R = \{(x, y) \mid x^2 + y^2 < \rho_0^2\}$ with boundary conditions

$$u(x, y) = 0, \quad x^2 + y^2 = \rho_0^2. \quad (38)$$

Let $u_0(x, y)$ be an eigenvector of either (36) or (37). One can easily show that $u_1(x, y)$ defined as

$$\begin{aligned} U_1(x, y) &= u_0(x, y), & y \geq 0 \\ &= u_0(x, -y), & y < 0 \end{aligned} \quad (39)$$

solves the same equation as well. Thus by using uniqueness one immediately deduces that

$$u_0(x, y) = u_0(x, -y), \quad y < 0. \quad (40)$$

Thus, Eqs. (36)–(37) need to be solved only over the upper half of the circle, $R_1 = \{(x, y) \mid x^2 + y^2 < \rho_0^2, y > 0\}$, with homogeneous Neumann boundary conditions (substitute $y = 0$ in (36)–(37)) along the diameter, i.e.,

$$\partial u / \partial n(x, 0) = 0, \quad |x| \leq \rho_0. \quad (41)$$

Furthermore, instead of solving (36)–(37) over R_1 , one may equivalently consider in each case two different problems, both over the first quadrant

$$R_2 = \{(x, y) \mid x^2 + y^2 < \rho_0^2, x > 0, y > 0\}. \quad (42)$$

The first problem is presented by the boundary conditions

$$\begin{aligned} u(x, y) &= 0, & x^2 + y^2 = \rho_0^2, \\ \partial u / \partial n(x, 0) &= 0, & 0 \leq x \leq \rho_0, \\ \partial u / \partial n(0, y) &= 0, & 0 \leq y \leq \rho_0, \end{aligned} \quad (43)$$

and is considered as a “Neumann problem.” The second set of boundary conditions is

$$\begin{aligned} u(x, y) &= 0, & x^2 + y^2 = \rho_0^2, \\ \partial u / \partial n(x, 0) &= 0, & 0 \leq x \leq \rho_0, \\ u(0, y) &= 0, & 0 \leq y \leq \rho_0, \end{aligned} \quad (44)$$

and presents a “Dirichlet problem.”

Both problems are solved for various values of ρ_0 with and without the singular term $2y/\rho$. This term, although bounded, produces discontinuity at the origin $(0, 0)$. This causes discomfort regarding the numerical integration that has to be performed. For the one-dimensional case [1], it is avoided by using analytic integration. Here one can treat it by properly dividing R_2 into the triangular elements T_1, \dots, T_n . These are chosen to be radial (Fig. 2), thus softening the discontinuity of $2y/\rho$ by having to integrate it separately over different elements that within each of them, can be considered continuous (for integration purposes).

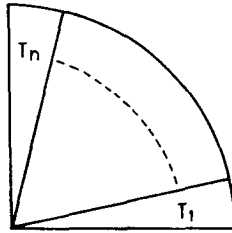


FIG. 2. The division into radial triangular elements.

This approach leads to accurate results and is used throughout the numerical work. Generally, six radial elements and fourth-order polynomial approximations are enough to provide sufficient accuracy in calculating both eigenvalues and eigenvectors for a long range of ρ_0 . The number of node potentials was $k = 36$ (40) for a Dirichlet (Neumann) problem. Upon taking the same number of elements, with only one or two touching at the origin, the accuracy drops significantly as expected.

NUMERICAL RESULTS

This section presents the first 15 energy levels for the case (i)–(ii). In the second case the levels are calculated for various values of ρ_0 . Comparison of the θ dependence of the eigenvalues with $p_l^0(\cos \theta)$ enables one to determine the angular momentum quantum number l , associated with the corresponding energy level.

Case (i)

The results are summarized in Table I. The exact energy levels are given by $\epsilon = j_{l,s}/2\rho_0^2$, where $\{j_{l,s}\}$ are the zeros of Bessel functions of half integer order, i.e., $J_{l+(1/2)}(j_{l,s}) = 0$. One finds that the θ dependence of the finite element solution is sufficiently accurate to determine l . The lower eigenvalues produced by MANFEP are very accurate, and although the accuracy slowly drops as one moves to higher energy levels, it is still satisfactory for a relatively large number of them. The computer time needed for completely solving one problem is approximately 3 min on a CDC-3600 computer.

TABLE I
Energy Levels of a Free Electron in a Spherical Box of Radius $0.1a_0$ ($a_0 = \text{Bohr radius}$)^a

Angular momentum l	Energy		
	Exact	MANFEP ^b	MANFEP ^c
0	493.48	493.49	
1	1009.54	1009.71	1009.60
2	1660.87	1661.70	
0	1973.92	1975.09	
3	2441.56	2460.76	2442.28
1	2983.98	3079.09	2986.82
4	3347.72	3406.29	
2	4135.96	4598.79	
5	4376.56	4472.64	4391.35
0	4441.32	5078.45	
3	5425.82	5976.32	5450.95
6	5525.98	5644.09	
1	5944.99	6925.99	5990.48
7	6794.32	7043.91	6882.40
4	6850.25	7419.64	

^a The energy is expressed in atomic units (i.e., e^2/a_0).

^b With six radial elements.

^c With seven nonradial elements.

TABLE II
The Energy Levels, ϵ , of the Hydrogen Atom Enclosed in a Spherical Box of Radius ρ_0 as Calculated by MANFEP

$\rho_0 = 0.3$	$\rho_0 = 0.5$	$\rho_0 = 0.81$	$\rho_0 = 2$	$\rho_0 = 2.528$	$\rho_0 = 2.67$	$\rho_0 = 5.02$	$\rho_0 = 5.086$
46.593 (0)	14.748 (0)	4.392 (0)	-0.1249 (0)	-0.3734 (0)		-0.4945 (0)	
106.001 (1)	36.666 (1)	13.084 (1)	1.5764 (1)		0.8247 (1)		0.00026 (1)
179.164 (2)	63.184 (2)	23.297 (2)	3.3280 (2)	1.5589 (0)		0.1381 (0)	
208.992 (0)	72.707 (0)	26.199 (0)	3.3310 (0)	1.7102 (2)		0.3255 (2)	
268.290 (3)	95.352 (3)	35.605 (3)	5.3737 (3)		3.2388 (3)		0.6454 (3)
333.438 (1)	117.951 (1)	43.710 (1)	6.3911 (1)		3.7840 (1)		0.6781 (1)
373.604 (4)	133.327 (4)	50.111 (4)	7.7827 (4)	4.2285 (4)		1.0581 (4)	
492.299 (5)	176.108 (5)	66.443 (5)	10.3750 (0)	5.3726 (0)		1.0894 (0)	
503.933 (2)	179.720 (2)	67.475 (2)	10.4300 (2)	5.6465 (2)		1.3897 (2)	
549.369 (0)	194.148 (0)	71.811 (0)	10.4811 (5)		6.4441 (5)		1 4526 (5)
622.620 (6)	223.062 (6)	84.357 (6)	13.4341 (6)	7.4105 (6)		1.9697 (6)	
658.049 (3)	235.460 (3)	88.869 (3)	14.0402 (3)		8.6383 (3)		1.9542 (3)
765.158 (1)	274.401 (7)	103.994 (7)	16.4742 (1)		10.1294 (1)		2.2926 (1)
774.892 (7)	277.120 (1)	104.513 (1)	16.5550 (7)		10.3152 (7)		2.4176 (7)
818.606 (4)	293.307 (4)	110.940 (4)	17.6795 (4)	9.7565 (4)		2.5980 (4)	

^a ρ_0 , ϵ are expressed in atomic units, a_0 and e^2/a_0 , respectively. The angular momentum quantum number, l , is given in parentheses.

Since the singular term $2y/\rho$ does not appear in case (i), one should expect that for a given number of elements, the radial-type division would not necessarily provide an optimal choice.

TABLE III

The Effect of Taking an Increased Number of Radial Elements upon the Lowest Eigenvalues Produced by MANFEP for the Compressed Hydrogen Atom

Level	No. of radial elements	$\rho_0 = 0.81$	$\rho_0 = 2$	$\rho_0 = 5.02$
"1S"	2	4.3934	-0.1242	
	4		-0.1248	-0.4941
	6	4.3917	-0.1249	-0.4945
"2S"	2	26.224	3.3339	
	4		3.3302	0.1369
	6	26.199	3.3310	0.1381

TABLE IV

Comparison between the Results of MANFEP and the Exact Energy Levels for the Compressed Hydrogen Atom

Level	ρ_0	ϵ (MANFEP)	ϵ (exact)
"1S"	0.81	4.39	4.39
"2S"	0.81	26.20	26.2
"2S"	0.5	72.70	72.7
"3S"	0.5	194.15	171.5
"2S"	1.76	4.56	4.56
"3S"	1.76	13.77	12.3

Case (ii)

The results, summarized in Table II, are obtained by using six identical radial triangulars. The effect of taking an increased number of radial elements upon the lower eigenvalues is presented in Table III. In Table IV we compare some of the MANFEP results with the exact semianalytical solution in terms of the confluent hypergeometric function. The accuracy of the eigenfunctions produced by MANFEP is demonstrated in Fig. 3 where we plot the radial probability density of a free electron in a spherical box for the "1s" and "3d" states. The effect of adding the Coulomb potential (which is rather a small perturbation for small boxes) can be seen in Fig. 4.

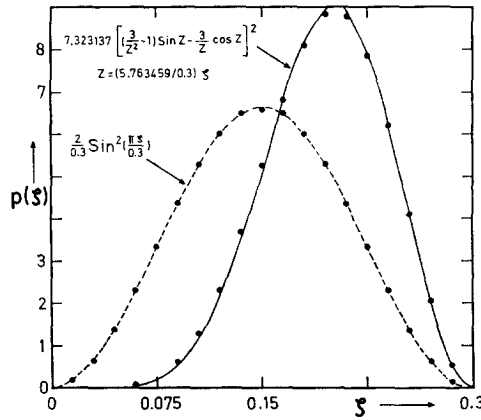


FIG. 3. Radial probability density, $p(\rho)$, of a free electron in a spherical box of radius $\rho_0 = 0.3$ in the states "1s" and "3d." The radius ρ is in units of the Bohr radius, a_0 . The dots represent the results by MANFEP. The curves are the exact analytical solutions.

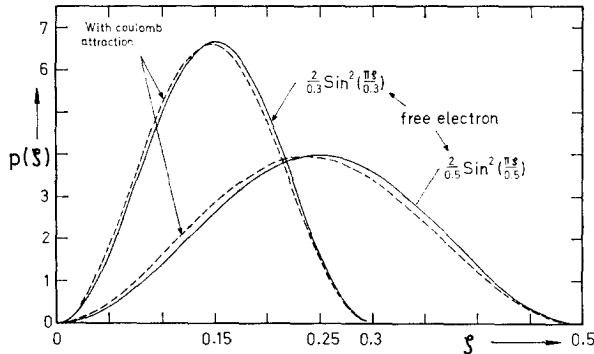


FIG. 4. Radial probability density, $p(\rho)$, of an electron in the ground state of the compressed hydrogen atom (box radii $\rho_0 = 0.3$ and $\rho_0 = 0.5$). To see the effect of the Coulomb potential we plot also $p(\rho)$ for the ground state of the free electron in a box. The energy levels are:

ρ_0	E_0	
Radius of box	Free electron	With Coulomb attraction
0.3	54.831	46.593
0.5	19.739	14.748

CONCLUSION

We presented a finite element package that is able to treat a two-dimensional Schroedinger equation over a finite region with an arbitrary potential and homogeneous boundary conditions. The results for the simple, exactly solvable problems

of the particle in a box and the compressed hydrogen atom definitely indicate the applicability of the method in various single particle quantum mechanical problems. With this tool at hand the road is open for treating more complex physical problems.

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