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Discrete Least Squares Method for the Solution of the Schrödinger Equation; Application to the Nuclear Three-Body Problem

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ABSTRACT

We discuss the properties of a discrete least squares method for the solution of the Schrödinger equation, including in particular its convergence properties as the number of points in the mesh used and the number of terms in the trial function are each increased. The method provides a possible alternative to the usual Rayleigh–Ritz procedure especially when the matrix elements in this latter scheme have to be evaluated numerically; we therefore compare these two methods in the context of a simple nuclear three-body problem. We conclude that the least squares method forms a useful adjunct to the Rayleigh–Ritz procedure, and provides in particular a useful estimate of its numerical accuracy.

I. INTRODUCTION

A great many variational calculations have been undertaken to give approximate solutions of the Schrödinger equation for few body systems. For trial wavefunctions and potentials of more than the slightest complexity the appropriate integrals must be evaluated numerically. This is so, for instance, in variational calculations on the nuclear three-body problem with realistic local two nucleon potentials (ref. [1]). Moreover for a good eigenvalue estimate, it is well known that the integrals must be computed with high accuracy, especially where linear variational parameters are employed (ref. [2]). It is therefore of interest to investigate alternative numerical methods which offer economy of computation.

In this paper we investigate a least squares method which does not require the evaluation of any integrals. This is a modification of the method used by Frost *et al.* [3] in atomic few body calculations.

In Section II we formulate the equations and discuss the expected convergence properties of the method. In Section III we present numerical examples for the

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case of a simple nuclear three body system with central local potentials with and without hard cores, and compare the results with variational estimates. In both the variational and least squares methods the factors governing the estimates are the number of variable parameters in the trial function, and the number of mesh points used.

We investigate in detail the dependence of the results on these factors.

We conclude with a discussion of the apparent merits of the technique.

II. Formulation

There are a number of different (and non-equivalent) formulations of the least squares method (ref. [3], [4]). We discuss here only one variant which we first derive.

We wish to solve the Schrödinger equation

$$(H - E)\psi = 0 \tag{1}$$

Consider the functional

$$\epsilon = \sum_p w(\mathbf{r}_p)\, |(H - \alpha)\, \psi(\mathbf{r}_p)|^2 \tag{2}$$

where the sum is taken over the discrete point set $\mathbf{r}_p$ in the coordinate space involved, and $w(\mathbf{r}_p)$ is a suitable weighting function to be discussed below. This expression is positive definite, and vanishes only when α, ψ satisfy (1) over the point set.

We take $\psi(\mathbf{r})$ to be a trial function and consider the minimisation of ϵ with respect to α and simultaneously with respect to parameters in ψ. These parameters must be subject to a suitable normalisation condition to keep ψ finite.

In this paper we consider the case of linear parameters:

$$\psi(\mathbf{r}) = \sum_{n=1}^{N} a_n \phi_n(\mathbf{r})$$

and impose the normalisation condition $a_1^2 = 1$.[1] With this trial function (assumed real)

$$\epsilon = \sum_p w_p |(H - \alpha) \sum_i a_i \phi_i|^2 \tag{3}$$

$$= \sum_{ijp} w_p a_i a_j (H - \alpha)\, \phi_i (H - \alpha)\, \phi_j$$

$$= \mathbf{a}^T (H^2 - 2\alpha H + \alpha^2 S)\mathbf{a} \tag{4}$$

[1] The solutions found do not depend, apart from a multiplicative constant, on the normalisation condition chosen provided that in the exact wavefunction $a_1 \neq 0$.

where we have used matrix notation with

$$H_{ij} = \sum_p w_p \tfrac{1}{2}[\phi_i(\mathbf{r}_p)\, H\phi_j(\mathbf{r}_p) + \phi_j(\mathbf{r}_p)\, H\phi_i(\mathbf{r}_p)]$$

$$H^2_{ij} = \sum_p w_p [H\phi_i(\mathbf{r}_p)][H\phi_j(\mathbf{r}_p)]$$

$$S_{ij} = \sum_p w_p \phi_i(\mathbf{r}_p)\, \phi_j(\mathbf{r}_p)$$

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix} \tag{5}$$

The restriction $a_1^2 = 1$ can be written

$$\mathbf{a}^T P \mathbf{a} = 1 \tag{6}$$

where P is the matrix

$$\begin{bmatrix} 1 & 0 & 0 & \ldots \\ 0 & 0 & 0 & \ldots \\ 0 & 0 & 0 & \ldots \\ \vdots & & & \end{bmatrix}$$

We introduce the Lagrange multiplier λ and minimise

$$\epsilon - \lambda(\mathbf{a}^T P \mathbf{a} - 1)$$

Differentiating with respect to α, $\mathbf{a}^T$ yields the equations

$$\alpha = \frac{\mathbf{a}^T H \mathbf{a}}{\mathbf{a}^T S \mathbf{a}} \tag{7}$$

$$(H^2 - 2\alpha H + \alpha^2 S)\mathbf{a} - \lambda P \mathbf{a} = 0 \tag{8}$$

These are a set of simultaneous linear equations in $\mathbf{a}$ coupled to an equation for α, which may be solved iteratively on a computer.

Convergence

The variance ϵ of equation (3) may be made as small as we please by including sufficient terms in the trial function, for a fixed point set $\{r_p\}$, and hence we can always find a solution to the original equation over the point set. But if the net

used is too sparse, we will not expect this solution to be a good approximation to the solution over the whole space $\mathbf{r}$. We are therefore interested in the relationship between convergence in $\{\mathbf{r}_p\}$ and $\{\mathbf{r}\}$; it is difficult to give such a discussion in general, but in Appendix A we analyse in detail the one-dimensional problem. We give there a discussion of the conditions under which the least squares procedure leads to a solution of the Schrödinger equation. The results may be stated as follows.

Suppose the number of terms N in the trial function Ψ is increased. If at the same time the number of points P is increased sufficiently fast, and if convergence is observed in the energy estimates α, then these values will have converged to a solution of the Schrödinger equation.

We have yet to specify "sufficiently fast", and this must be determined by detailed reference to the physical problem under consideration; an explicit criterion is given for one-dimensional problems in Appendix A. Note that if the number of terms N is increased for a fixed number of mesh points P, a situation will arise where we are trying to fit the wavefunction at a number of points with more free parameters than constraints. It is therefore to be expected that the Least Squares (L.S.) estimates will break down as N is increased for given P. Appendix A shows that the onset of this instability occurs earlier for a wavefunction with large second derivatives.

In the numerical examples of this paper, we demonstrate this expected convergence behaviour with respect to both N and P.

Choice of Points and Weights

Within wide limits, Appendix A shows that we may expect convergence for an almost arbitrary choice of weights and points. In this paper we choose these so that the sums approach the integrals over the space as the number of points increases. With this choice of points and weights the L.S. estimate of the energy, eqn. (7), is identical in form to the expression for the variational upper bound given by the Rayleigh–Ritz (R.R.) procedure. However, the equations determining the linear parameters $\mathbf{a}$ differ. If the integrals are evaluated exactly the L.S. estimate therefore provides not only a variational estimate of α, but even a R.R. bound. In general, the integration rule leading to the chosen points and weights will not give exact estimates of the matrices S and H. However, provided the matrix S has nonnegative eigenvalues the R.R. vector $\mathbf{a}$ minimises expression (7) and therefore the R.R. estimate of the energy is lower than the L.S. estimate. One is therefore tempted to conclude that the least squares procedure is actually *inferior* to the R.R. procedure. However, this assumes that the integrals are exact and in practice of course this will not be true, so that the R.R. estimate may fall *below* the exact solution. In the examples which follow we discuss the behaviour of the two estimates as both the number of linear parameters and the number of quadrature points increase.

III. Numerical Examples

In this section we present the results of calculations on the binding energy of a simple triton model with spin and charge independent central forces. Two internucleon potentials are utilized, one containing a hard core, and one not.

For various choices of N and P, the matrices H^2, H and S were computed, and the L.S. and R.R. estimates derived. We demonstrate the convergence of the L.S. estimates, and compare them with the variational estimates.

Potentials

We first specify the interparticle potentials used.

Potential A. Attractive Yukawa well–no hard core

$$V(r) = -V_0 e^{-r/\beta}/(r/\beta)$$

with

$$V_0 = 49.7616 \text{ Mev} \qquad \beta = 1.58\,F \qquad \hbar^2/m = 41.468 \text{ Mev } F^2$$

Potential B (Ref. [5]).

$$\begin{aligned} V(r) &= -V_{os}e^{-\beta_s(r-r_c)} - V_{ot}e^{-\beta_t(r-r_c)} && r > r_c \\ &= \infty && r < r_c \\ V_{os} &= 235.414 \text{ Mev} \qquad \beta_s = 2.03435F^{-1} \\ V_{ot} &= 475.044 \text{ Mev} \qquad \beta_t = 2.5214F^{-1} \qquad r_c = 0.4F \end{aligned}$$

Trial Functions

For each case the set of trial wavefunctions was of the form

$$\phi_i = S\{u_l(r_1)\, u_m(r_2)\, u_n(r_3)\} \tag{9}$$

where S indicates that a sum symmetric in $r_1 r_2 r_3$ is formed from the quantities in parenthesis, and l, m, n, are integers chosen as in Table I. $r_1 r_2 r_3$ are the interparticle distances.

For the potential A the one dimensional function employed was of the form

$$u_l(r) = e^{-\alpha l r} \tag{10}$$

and for the potential B

$$u_l(r) = [1 - e^{-\gamma(r-r_c)}]\, \frac{e^{-\delta r}}{r^{1/2}}\, P_l\{e^{-2\delta(r-r_c)}\} \tag{11}$$

TABLE I

PARAMETERS IN THE TRIAL WAVEFUNCTION OF EQUATION (9)

i	l	m	n
1	1	1	1
2	1	1	2
3	1	2	2
4	1	1	3
5	2	2	2
6	1	2	3
7	2	2	3
8	1	3	3

where $P_i(x)$ is a polynomial of degree $l-1$ in x. This is the form chosen in a recent series of calculations on the triton (ref. [1]).

In each case, the nonlinear parameters α, and γ and δ were optimised by finding the values which minimised the variational estimate of the energy with a single term wavefunction.

In the hard core case, the coefficients of the polynomials $P_i(x)$ were chosen so as to make some of the set of trial functions orthogonal (by analytic evaluation of the appropriate integrals). This will tend to reduce the effects of roundoff errors in the R.R. estimates (see ref. [2]) in individual cases, although for trial functions containing those terms which exhaust the triplet lmn satisfying

$$l + m + n < \text{some positive integer}$$

the energy given by both the R.R. and L.S. procedure is independent of this orthogonalisation procedure.

Integration Rules

It is convenient to transform the three-body configuration space into a sum of regions defined by independent coordinates in which the integrand is well behaved.

For the potential with no hard core the space is defined by

$$r_1 \leqslant r_2 + r_3$$
$$r_2 \leqslant r_3 + r_1$$
$$r_3 \leqslant r_1 + r_2$$

Here we utilize the perimetric coordinates uvw defined by

$$\begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix}$$

so that

$$\iiint dr_1\, dr_2\, dr_3 = \frac{1}{4}\int_0^\infty \int_0^\infty \int_0^\infty du\, dv\, dw$$

In the case of a potential with hard core the space is specified by

$$r_c \leqslant r_1 \leqslant r_2 + r_3$$
$$r_c \leqslant r_2 \leqslant r_3 + r_1$$
$$r_c \leqslant r_3 \leqslant r_1 + r_2$$

We have used the transformation

$$\iiint dr_1\, dr_2\, dr_3 = \frac{1}{4}\int_0^\infty du' \int_0^\infty dv' \int_0^\infty dw' + 3\int_0^\infty dr_3' \int_0^\infty dr_2' \int_0^\infty dw$$

where

$$u' = u - r_c \qquad w = -r_1 + r_2 + r_3$$
$$v' = v - r_c \qquad r_3' = r_3 - r_c$$
$$w' = w - r_c \qquad r_2' = r_2 - r_c$$

which holds for an integrand symmetric in the labels 1, 2, 3. The integration in the transformed spaces are carried out by Gauss Laguerre or Gauss Legendre rules, using P points in each dimension together with any symmetry reduction possible. We refer to the resulting rule as containing P^3 points nominally.

For each case, Table II gives the relationship of the number of points actually used in the integration meshes to this nominal value.

TABLE II

RELATIONSHIP OF THE ACTUAL NUMBERS OF QUADRATURE POINTS EMPLOYED TO THE NOMINAL VALUES QUOTED ELSEWHERE

NOMINAL		2^3	4^3	6^3	8^3	10^3	12^3	14^3
ACTUAL	No Hard Core	4	20	56	120	220	364	560
	Hard Core	10	60	182	408	770	1300	2030

Table III and IV indicate the accuracy of the integration procedures and show the convergence of the matrix elements as more mesh points are employed.

TABLE III

SAMPLE MATRIX ELEMENTS FOR POTENTIAL A,
ILLUSTRATING THE ACCURACY OF THE INTEGRATION PROCEDURE

Matrix Element	NUMBER OF MESH POINTS			
	2^3	5^3	8^3	10^3
$H^2_{1,1}$	0.4161609454,5	0.4232086508,5	0.4275129195,5	0.4291690052,5
$H_{1,1}$	−0.7809840578,3	−0.7744992250,3	−0.7744992101,3	−0.7744992100,3
$S_{1,1}$	0.1538085937,2	0.1538085937,2	0.1538085936,2	0.1538085936,2
$H^2_{20,20}$	0.3344575157,3	0.5605989821,4	0.1285896207,5	0.1426778729,5
$H_{20,20}$	−0.2894197868,1	0.3544301567,1	0.7889143271,1	0.7836155643,1
$S_{20,20}$	0.3410537961,1	0.4016431921, −2	0.2367236821, −1	0.2371377327, −1

TABLE IV

SAMPLE MATRIX ELEMENTS FOR POTENTIAL B,
ILLUSTRATING THE ACCURACY OF THE INTEGRATION PROCEDURE

Matrix Element	Number of Mesh Points		
	6^3	10^3	14^3
$H^2_{1,1}$	0.3247381821,7	0.3439260924,7	0.3458315374,7
$H_{1,1}$	−0.5480665939,4	−0.6537618829,4	−0.6663862495,4
$S_{1,1}$	0.9970352568,3	0.1155165390,4	0.1171820400,4
$H^2_{20,20}$	0.5537564930,8	0.5569957979,8	0.5708896360,8
$H_{20,20}$	0.8691674939,4	0.8787405116,4	0.9108835830,4
$S_{20,20}$	0.3628785539,1	0.4086498322,1	0.4879227064,1

Results and Discussion

Tables V and VII present the L.S. energy estimates in the two cases considered, for several integration mesh sizes and for various numbers of terms in the trial function.

TABLE V

LEAST SQUARES ESTIMATES OF THE THREE BODY BINDING ENERGY USING POTENTIAL A. P DENOTES THE NUMBER OF QUADRATURE POINTS AND N THE NUMBER OF LINEAR PARAMETERS.

N \ P	2^3	4^3	6^3	8^3	10^3	12^3	14^3
1	50.776	50.355	50.355	50.355	50.355	50.355	50.355
4	49.842	50.788	50.801	50.800	50.800	50.800	50.800
8		50.894	50.836	50.831	50.830	50.830	50.830
12			50.823	50.848	50.848	50.848	50.848
16			51.123	50.868	50.854	50.853	50.853
20			50.879	50.841	50.852	50.851	50.853

TABLE VI

RAYLEIGH–RITZ ESTIMATES OF THE THREE BODY BINDING ENERGY USING POTENTIAL A.

N \ P	2^3	4^3	6^3	8^3	10^3	12^3	14^3
1	50.776	50.354	50.355	50.355	50.355	50.355	50.355
4	7.291	50.802	50.809	50.810	50.810	50.810	50.810
8		51.946	50.843	50.838	50.838	50.838	50.838
12		3.920	51.053	50.850	50.850	50.852	50.851
16			47.174	51.165	50.856	50.855	50.855
20			41.934	49.626	50.208	50.656	50.859

In each case we observe that for a given number of linear parameters N the estimates converge with increasing number of quadrature points P, i.e. as the integration procedures become more accurate. For fixed P, the estimates at first converge with N and then become unreliable as the number of points becomes of the same order as N. This is indicated also by the failure of the L.S. iteration scheme to converge. As expected, the onset of this breakdown is delayed as P is increased.

With both potentials we see that the estimates converge as N and P simultaneously increase i.e. diagonally down the tables.

Thus in practice the L.S. estimates converge in the expected manner. Examining Tables VI and VIII which show the R.R. estimates for the two potentials we notice the same pattern of convergence. As P is increased for fixed N the estimates converge due to the improved accuracy in the matrix elements, while for fixed P the estimates at first converge and then begin to oscillate as the effect of roundoff errors accumulates.

TABLE VII

LEAST SQUARES ESTIMATES OF THE THREE BODY BINDING ENERGY USING POTENTIAL B. *P* DENOTES THE NUMBER OF QUADRATURE POINTS AND *N* THE NUMBER OF LINEAR PARAMETERS.

N \ P	4^3	6^3	8^3	10^3	12^3	14^3
1	5.254	5.497	5.607	5.659	5.680	5.687
4	8.170	7.355	7.502	7.606	7.649	7.664
8	9.842	7.470	7.541	7.625	7.662	7.676
12	2.756	7.936	7.542	7.532	7.553	7.566
16	2.807	9.470	7.793	7.646	7.644	7.651
20	2.894	7.690	7.565	7.694	7.729	7.743
24				7.814	7.778	7.778
28				7.745	7.779	7.779

TABLE VIII

RAYLEIGH-RITZ ESTIMATES OF THE THREE BODY BINDING ENERGY USING POTENTIAL B.

P	4^3	6^3	8^3	10^3	12^3	14^3
1	5.254	5.497	5.607	5.659	5.680	5.687
4	14.758	7.624	7.631	7.708	7.740	7.750
8		9.684	7.774	7.750	7.771	7.781
12		20.377	8.005	7.772	7.781	7.790
16			8.739	7.831	7.802	7.806
20			11.078	7.864	7.804	7.810
24				8.012	7.817	7.814
28				8.287	7.823	7.814

For each potential the R.R. and L.S. estimates converge to the same value i.e. provided there are sufficient terms in the trial wavefunction and the integration mesh is sufficiently fine, the two approaches provide identical estimates.

In a practical calculation, however, we are interested in using as few terms and quadrature points as possible. Figs. 1 and 2 enable us to compare the R.R. and L.S. estimates for various mesh sizes.

These show clearly the breakdown in the variational estimates as the truncation errors in the matrix elements become larger. Taking the variational estimates on their own, it is easy to be misled into thinking that a lowering in the energy achieved by employing further terms in the wavefunction is an improvement, when in fact it is due to the commencement of this breakdown.

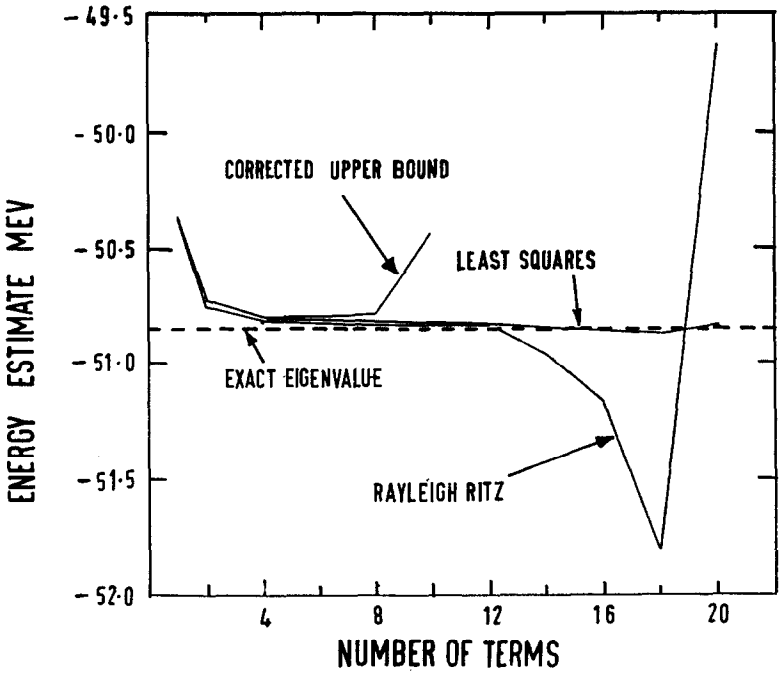

FIG. 1. The dependence of various binding energy estimates on the number of terms in the trial function for potential A using an integration mesh of 8^3 points.

Before the oscillation in the R.R. values occurs, the two estimates are in good agreement and we see that a large difference between them is indicative of excessive errors in the matrix elements. However, long after the R.R. estimate has become unreliable, the L.S. value not only remains reliable but continues to improve.

In Fig. 1 a plot is also made of a corrected upper bound to the energy described in ref. [2] which takes explicit account of the errors in the matrix elements. This bound is pessimistic in that it overestimates the effect of roundoff errors. However, where it differs greatly from the uncorrected bound it also warns of excessive buildup of the errors. We may further compare the reliability of the two estimates by a consideration of the variance

$$\epsilon = \sum_p w_p |(H - \alpha)\phi|^2 \simeq \int d\tau |(H - \alpha)\phi|^2$$

This quantity provides a kind of antithesis to the energy, since it is guaranteed to be lower for the L.S. wavefunction than for the R.R. function. However, we are interested in the dependence of ϵ on N.

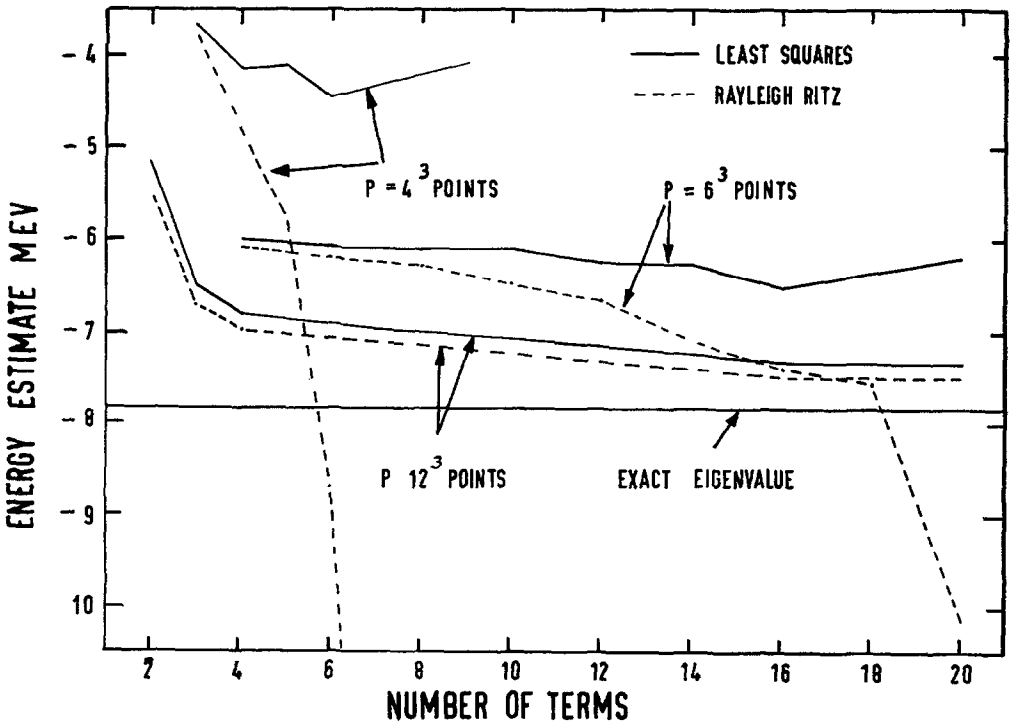

FIG. 2. The dependence of various binding energy estimates on the number of terms in the trial function for several mesh sizes using the potential B.

In Fig. 3 plots of the variance derived from the R.R and L.S. estimates are shown. We see that the region where the R.R. procedure breaks down is evidenced also by an erratic behaviour in ϵ as a function of the number of terms

Convergence of R.R. *and* L.S. *vectors*

For sufficiently large N and P we have seen that the R.R. and L.S. energies both converge to the exact eigenvalue. Presumably then the corresponding eigenvectors should also converge to the same vector. Fig. 4 demonstrates that the linear parameters **a** derived from the L.S. and R.R. approaches appear to be converging to the same values with simultaneous increase in N and P.

IV. CONCLUSION

A R.R. calculation only gives a rigorous upper bound to the energy when the matrix elements of H and S are known exactly. With the approximate numerical

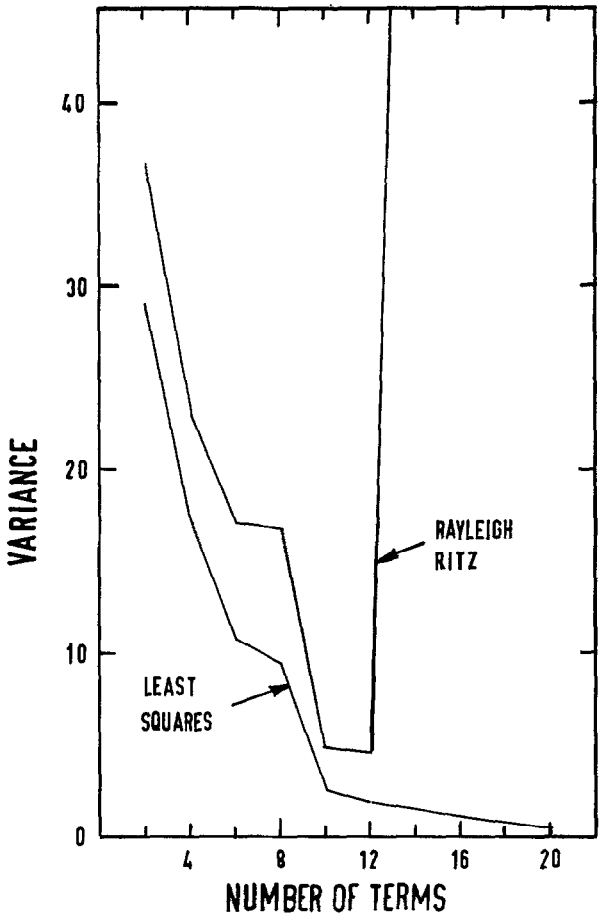

FIG. 3. The variance as a function of the number of terms in the trial function for potential A with 7^3 points.

evaluation of these matrix elements the R.R. eigenvalue estimates may misleadingly drop below the exact value. The calculation of the L.S. estimate in addition to the R.R. value provides a means of assessing when the effects of truncation errors is appreciable and moreover where the effects *are* important the L.S. estimate will continue to provide a good estimate. We pay for this relative insensitivity to the integration mesh by having to provide the matrix H^2 where the R.R. method requires only H and S. However, this matrix is in this context rather cheap to provide, since it is constructed from a knowledge of $H\psi$ at the points in the mesh,

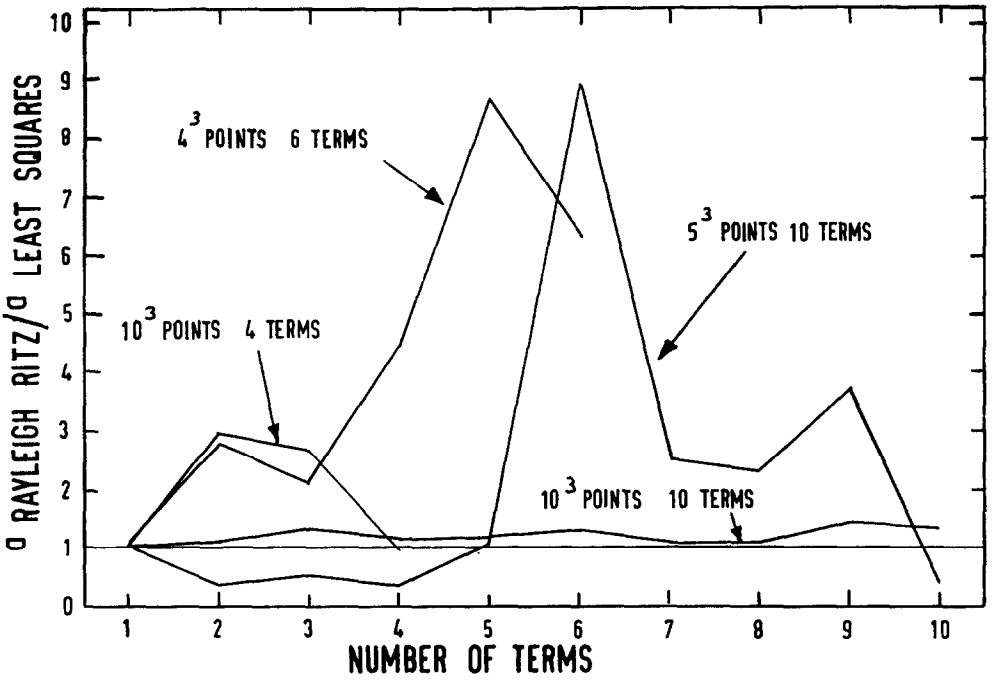

FIG. 4. Ratio of the linear parameters provided by the Rayleigh–Ritz approach to those given by the least squares procedure shown for various numbers of mesh points and linear parameters for potential A.

and this function serves also to evaluate the matrix of H. Moreover, if we intend to carry out also lower bound calculations, we must anyway provide H^2 for these [ref. 1].

The results we obtain suggest strongly that the L.S. method forms at least a useful adjunct to the R.R. method whenever the matrices are computed numerically, and can give an apparently reliable guide to the numerical accuracy of the energy estimates. A similar conclusion is reached also in application of the method to atomic calculations (ref. [6]).

APPENDIX A

ON THE CONVERGENCE PROPERTIES OF THE DISCRETE LEAST SQUARES METHOD

In the body of this paper we demonstrate that the discrete least squares method converges sufficiently well in the examples considered to be of some practical use. The same conclusion is reached in the field of atomic problems in ref. [6]. These calculations use a specific choice of points, and of weights; in this appendix we investigate a simple one-dimensional case of the least squares method, and show that convergence can be expected for a wide range of points and weights. We also study the way in which convergence is achieved as both n the number of terms in the trial function, and N the number of points in the mesh, are increased.

The Schrödinger equation for a Hamiltonian H defined on a space R is

$$(H - E)\psi = 0 \qquad \psi \in R \tag{A(1)}$$

The continuous least squares procedure consists in minimising the functional

$$f(\phi) = (\phi, w\phi) \geqslant 0 \tag{A(2)}$$

where w is an Hermitian positive definite operator over R and ϕ is the vector

$$\phi = (H - \alpha)\,\psi_T \tag{A(3)}$$

In A(3) α, ψ_T are the trial energy and eigenvector. Equality in A(2) implies that ϕ is the null vector, and hence that ψ_T is an eigenvector of H for the eigenvalue α. However, this form has the well known disadvantage that the inner products which it involves are difficult to evaluate.

It is possible to simplify the inner products as much as we please by defining the functional, not over R but over some simpler subspace S in which the inner products are more conveniently evaluated. In particular, if we choose S to be a discrete point set $\{P\}$ we generate the *discrete least* squares method

$$\epsilon_P{}^2 = \min \sum_P W(\mathbf{r}_P)|(H - \alpha)\,\phi_T(\mathbf{r}_P)|^2 \tag{A(4)}$$

subject to suitable normalizing conditions on ϕ_T to keep it finite. This is the method studied in this paper. Equation A(4) is also the form taken by A(2) if the integrals are carried out numerically, as is done by Conroy [4]. The solutions of A(4) satisfy

$$\epsilon_P{}^2 = 0 \qquad (H - \alpha)\,\phi_T(\mathbf{r}_P) = 0 \qquad \mathbf{r}_P \in \{P\} \tag{A(5)}$$

and we would hope that, in the limit as the point set $\{P\}$ was extended in a suitable way, A(5) would imply A(1).

In this appendix we consider the simplest case of A(1). We take R to be a finite one-dimensional region, the trial function ϕ_T to be a linear function with n para-

meters, and limit the range of the parameter α to a small enough region that the minimum A(4) is unique. Under these conditions we give two convergence theorems. The first states that, for fixed n, the solution of A(4) tends to A(2), as the number of points N increases without limit. The second considers the case that n and N increase together, and gives conditions under which convergence in $\{P\}$ implies convergence in R. These theorems are given precise form in the next section.

2. Convergence Theorems for Fixed n

We consider the space R of integrable functions of one variable defined on a finite interval which we take to be $0 \leqslant x \leqslant 1$; and the trial function

$$\phi_T(x) = \sum_{i=0}^{n} a_i g_i(x) \qquad \text{A(6)}$$

The functions g_i are assumed linearly independent, and continuous on [0, 1].

Equation A(2) leads to the L_2 deviation ϵ_2 :

$$\epsilon_2^2 = \int_0^1 W(x)|(H - \alpha)\,\phi_T(x)|^2\,dx \qquad \text{A(7)}$$

where $W(x)$ is a positive definite function on R. We shall assume without essential loss of generality that H and ϕ_T are real, and hence the a_i can be chosen real.

We also define point sets P_m containing m points as follows. Let

$$P = \{x_i \mid i = 1, 2,...\} \qquad \text{A(8)}$$

be dense in [0, 1], and take

$$P_m = \{x_i \mid x_i \in P;\ i = 1,..., m\} \qquad \text{A(9)}$$

For each x_i in P_m we define the positive number $\delta_m(x_i)$

$$\delta_m(x_i) = \min_{x_j < x_i} |\, x_i - x_j \,| \qquad \text{A(10)}$$

which is the distance from x_i to its immediate left neighbour. For each set P_m, equation A(4) defines a least squares error relative to the weight function $W(x)\,\delta_m(x)$:

$$\epsilon_m^2 = \sum_{i=1}^{m} W(x_i)\,\delta_m(x_i)|(H - \alpha)\,\phi_T(x_i)|^2 \qquad \text{A(11)}$$

The reason for this choice of weight function will become clear below. Now, the the weighted $L_2(P_m)$ approximation to ϕ_T consists in minimizing $\epsilon_2^2(\epsilon_m^2)$ with

respect to the parameters a_i, α. The minima depend on the domain of a_i, α over which the minimum is sought. We do not restrict the a_i, but make the following restriction on α:

> The range of α is finite and is such that one and only one minimum exists for ϵ_2^2 and all ϵ_m^2. A(12)

This restriction is only a weak one in practice; it implies that we take the minimum m considered to be large enough that a single eigenvalue can be localized within the finite range of variation of α. We now define the best trial functions

$$\phi_T(A_m),\ \phi_T(A^*), \qquad A = \{a_1, \ldots, a_n, \alpha\} \qquad a_0 = 1$$

which minimize ϵ_m^2, ϵ_2^2 subject to the normalizing condition $a_0 = 1$. In accordance with A(12) these minima are unique. We then have

THEOREM 1. *If*

$$\lim_{m\to\infty} \max_{x\in P_m} \delta_m(x) = 0.$$

Then

$$\lim_{m\to\infty} \phi_T(A_m) = \phi_T(A^*)$$

Proof. This theorem is only a slight modification of a theorem concerning the point set approximation of a given function $f(x)$ by a linear approximating function, see e.g., ref [8]. If we define

$$L(A, x) = \sum_{i=1}^{n} a_i(\alpha - H)\, g_i(x) + \alpha g_0(x)$$
$$A = \{a_1, \ldots, a_n\} \qquad \text{A(13)}$$

then for α fixed the problem reduces to that considered by Rice, who proves the following essential steps (for all m)

(i) the minimum is unique

(ii) the parameters $\{a_i\}$ are uniformly bounded in m.

Condition A(12) ensures that (i) and (ii) remain true also when α is varied and hence the theorem follows.

Discussion

This theorem, apart from guaranteeing a sensible answer as the number of points is increased for a fixed length of trial function, also makes precise the observation that one can weight a given region of space heavily in either of two ways: by clustering the points closely, or by increasing the weight function $W(x)$ in the region.

To illustrate this, let us choose the spacing in a regular way:

$$\delta_m(x_i) = \sigma(x_i)\,\delta_m \tag{A14}$$

where $\sigma(x)$ is independent of m and $\delta_m \to 0$ as $m \to \infty$. Further, let us write

$$\sigma(x)\,W(x) = Q(x). \tag{A15}$$

Then A(7) and A(11) become

$$\epsilon_2^2 = \int_0^1 W(x)|(H - \alpha)\,\phi_T\,|^2\,dx \tag{A16a}$$

$$\epsilon_m^2 = \delta_m \sum_{i=1}^{m} Q(x_i)|(H - \alpha)\,\phi_T\,|^2 \tag{A16b}$$

and we have shown that, for large m, the solution of A(16b) tends to that of A(16a).

The theorem remains valid for trial functions containing nonlinear parameters, provided that we *assume* the essential requirements: the minimum with respect to all parameters of ϵ_m^2 is unique for any m, and the parameters at the minimum form a bounded sequence in m.

3. Convergence as $n \to \infty$

The conditions of Theorem 1 do not correspond to those used in a practical calculation. The calculator is usually more interested in increasing the number of terms n in the trial function as far as he can, keeping as few points m as he dare to make the resulting estimate α "representative" of the trial function, in some sense. Specifically, we would like to know how to vary m with n so that convergence to the exact solution over R is assured. The following theorem assumes that convergence over P to some accuracy is attained, and relates this to convergence over R.

Definition. With the trial function (A6) we define:

$$h_i(\alpha) = (H - \alpha)\,g_i(x) \tag{A17a}$$

$$l_i(\alpha) = \frac{d}{dx}\,h_i(\alpha) \tag{A17b}$$

$$\delta = \max_{x \in P_m} \delta_m(x) \tag{A17c}$$

$$C_i = \max_{x \in R} l_i(x) \tag{A17d}$$

$$\epsilon_m^2 = \sum_{i=0}^{m} W(x_i)|(H - \alpha)\,\psi_T\,|^2 \tag{A17e}$$

$$v = \min_{x \in P_m} [W(x_i)]^{1/2} \tag{A17f}$$

In equation A(17c), $\delta_m(x_i)$ is the spacing at point x_i defined by A(10).

We then use the mean value theorem to obtain the following estimate of $(H - \alpha)\,\psi_T(x)$ at a point x not in P_m :

$$\begin{aligned} |(H-\alpha)\,\psi_T(x)| &= |(H-\alpha)\,\psi_T(x_i) + (x_i - x_{i+1})\,\frac{d}{dx}\,[(H-\alpha)\,\psi_T(\xi_i)| \\ & \qquad x_i \leqslant \xi_i \leqslant x_{i+1} \\ &\leqslant |(H-\alpha)\,\psi_T(x_i)| + \delta \sum_{i=0}^{m} |\,a_i\,|\,C_i \\ &\leqslant \epsilon_m/v + \delta \sum_{i=0}^{m} |\,a_i\,|\,C_i\,. \end{aligned} \tag{A18}$$

This estimate then leads to the following simple theorems.

THEOREM 2. *If there exist constants D, N such that for sufficiently large n*

$$|\,a_n\,|\,C_m < DN^{-n} \qquad N > 1 \tag{A19}$$

$$\text{and if } \delta \to 0 \quad \text{as} \quad m \to \infty$$

then convergence in P implies convergence in R.

Proof. For then the series in A(18) converges, and the second term tends to zero.

THEOREM 3. *If the point set $\{P\}$ is chosen sufficiently large for each n so that*

$$\max_{i=0}^{n} \delta |\,a_i\,|\,C_i < E\,n^{-(1+\epsilon)} \qquad \text{where } E \text{ is finite and } \epsilon > 0 \tag{A20}$$

then convergence in P implies convergence in R.

Proof. For then we have

$$\delta \sum_{i=0}^{n} |\,a_i\,|\,C_i < E\,n^{-\epsilon} \to 0 \text{ as } n \to \infty.$$

Discussion

Usually Theorem 2 will not apply; the C_i will rise sufficiently rapidly that $|\,a_i\,|\,C_i$ is unbounded, and the maximum in A(20) is attained at the last term $i = m$. Equation A(20) then gives a simple relation for the minimum number of points as a function of m required to ensure convergence. This relation, and that of Theorem 2, involves the expansion parameters a_i which are not known before the calculation starts. The a priori estimation of a_n for large n has been considered by Schwartz

[7], and in another context by Lighthill [8]; they are always available afterwards to check the convergence of an apparently successful calculation.

Theorems 2 and 3 can also be used to check convergence in any subset R' of R; we merely replace R by R' in the statement of the theorems, and in the definition A(17d) of the C_i. In this way we can avoid regions of R where one or more of the h_i or l_i becomes singular, and isolate these singularities to treat separately their contribution to the L_2 error ϵ_2^2. If the singularities are weak enough, ϵ_2^2 will still exist and tend to zero even though the estimate A(18) taken over the whole space R diverges.

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