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A comparison between R-matrix and variational procedures

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Abstract

A class of variational methods that can be used in solving either bound state problems or those that involve scattering by a potential is reviewed with particular regard to the constraints that it is necessary to impose upon the basis functions. The R-matrix method is also reviewed and it is shown that there is a formal similarity between the two methods but that the basis functions of the R-matrix method are excluded as a basis for the variational procedure. As a result, the convergence properties of the two methods differ, the variational procedures converge rapidly but the R-matrix method needs a 'correction' to improve the convergence. The relations between the variational procedures discussed and two other methods, one due to Kohn (1948) and one due to Rudge (1973), are also mentioned.

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1. Introduction

The R-matrix method (Wigner and Eisenbud 1947, Lane and Thomas 1958, Duke and Wigner 1964, Burke and Robb 1975) is a highly successful procedure that is extensively used in atomic physics. One disadvantage of the R-matrix method however lies in its slow convergence, a defect that is normally remedied by using the so-called 'Buttle correction' (Buttle 1967). Variational methods, on the other hand, accounts of which appear in the literature (Nesbet 1980, Abdel-Raouf 1982, 1984, Adikhari 1998), have enjoyed less popularity in part because of the apparent variety of such methods and in part because of perceived convergence problems. In fact the two methods are formally very similar, and the connection between one of the Kohn (1948) variational methods and the R-matrix method has been described by Nesbet (1980).

The purpose of this paper is to reexamine several variational methods and to demonstrate the formal similarity that they have with the R-matrix method and the differences that arise, through the constraints on the basis functions, in the context of potential scattering. In particular, it is shown that the 'R-matrix basis' is not a suitable basis for the variational method which is rapidly convergent and does not require a Buttle correction.

2. Theory

2.1. The eigenvalue problem

Consider the equation

$$[\mathscr{L}_0 + \lambda_j] f_j(r) = 0 \tag{1}$$

where $0 \leqslant r \leqslant a$, subject to the boundary conditions

$$f(0) = 0 : k^{-1} f'(a) \sin\theta + f(a) \cos\theta = 0 \tag{2}$$

where k and θ are parameters and

$$\mathscr{L}_0 = \frac{\mathrm{d}^2}{\mathrm{d}r^2} - 2mV(r). \tag{3}$$

For a two-body problem $V(r)$ is the potential and m is the reduced mass. Using the notation

$$\langle f \rangle \equiv \int_0^a f(r)\,\mathrm{d}r \tag{4}$$

define the functionals

$$L_0(f) = -\langle f'^2 \rangle - 2m\langle fVf \rangle \tag{5}$$

$$N(f) = \langle f^2 \rangle \tag{6}$$

and

$$K_1(f) = 2f(a)f'(a)\cos^2\theta + \sin\theta\cos\theta[k^{-1}f'^2(a) - kf^2(a)] - 2f(0)f'(0). \tag{7}$$

It is seen that

$$\delta(L_0 + K_1 + \lambda N) = 2\langle \delta f(\mathscr{L}_0 + \lambda) f \rangle + 2(f(a)\cos\theta + k^{-1}f'(a)\sin\theta)\delta(f'(a)\cos\theta - kf(a)\sin\theta) - 2f(0)\delta f'(0) \tag{8}$$

and is zero if f is an exact solution of (1) that satisfies (2). Conversely if

$$\delta(L_0 + K_1 + \lambda N) = 0 \tag{9}$$

for arbitrary δf then the solution of (9) satisfies (1) and (2). On choosing a basis $\boldsymbol{t}(r)$ a linear trial function can be written

$$f(r) = \tilde{\mathbf{c}}\boldsymbol{t}(r) \tag{10}$$

where $\mathbf{c}$ is a vector of coefficients and the tilde is used to denote a transpose. A suitable basis should be minimal (cf Mikhlin 1971) which includes the particular choice of a set of orthogonal polynomials.

If the basis is chosen to satisfy the essential boundary conditions

$$\boldsymbol{t}(a)\cos\theta + k^{-1}\boldsymbol{t}'(a)\sin\theta = \mathbf{0} \qquad \boldsymbol{t}(0) = \mathbf{0} \tag{11}$$

then the boundary terms in (8) vanish and all the solutions of the variational principle (9) satisfy (2) identically. If not, then it follows from (8) that provided the conditions

$$\boldsymbol{t}'(a)\cos\theta - k\boldsymbol{t}(a)\sin\theta \neq \mathbf{0} \qquad \boldsymbol{t}'(0) \neq \mathbf{0} \tag{12}$$

are satisfied, then the solutions of (9) will converge to the boundary conditions (2). Using (10) in (9) gives the linear equations

$$[\mathbf{L}_0 + \mathbf{K}_1 + \lambda\mathbf{N}]\mathbf{c} = \mathbf{0} \tag{13}$$

where

$$\mathbf{L}_0 = -\langle \boldsymbol{t}'\tilde{\boldsymbol{t}}' \rangle - 2m\langle \boldsymbol{t}V\tilde{\boldsymbol{t}} \rangle \tag{14}$$

$$\mathbf{N} = \langle \boldsymbol{t}\tilde{\boldsymbol{t}} \rangle \tag{15}$$

and

$$\mathbf{K}_1 = \sin\theta\cos\theta[k^{-1}\boldsymbol{t}'(a)\tilde{\boldsymbol{t}}'(a) - k\boldsymbol{t}(a)\tilde{\boldsymbol{t}}(a)] + \cos^2\theta[\boldsymbol{t}(a)\tilde{\boldsymbol{t}}'(a) + \boldsymbol{t}'(a)\tilde{\boldsymbol{t}}(a)] \\ - \boldsymbol{t}(0)\tilde{\boldsymbol{t}}'(0) - \boldsymbol{t}'(0)\tilde{\boldsymbol{t}}(0). \tag{16}$$

If the eigenvalues in (13) are λ_j and the eigenvectors are $\boldsymbol{c}_j$ then the eigenfunctions are

$$w_j(r) = \tilde{\boldsymbol{c}}_j\boldsymbol{t}(r). \tag{17}$$

The eigenfunctions that correspond to smaller λ_j converge to the boundary conditions more rapidly than those that correspond to larger λ_j. If $\theta = 0$ then $w_j(a) \cong 0$ and if $\theta = \pi/2$ then $w_j'(a) \cong 0$.

2.2. *Continuum variational principles*

Consider the equation

$$\mathscr{L}f \equiv [\mathscr{L}_0 + k^2]f(r) = 0 \tag{18}$$

subject to the boundary conditions

$$f(0) = 0 : k^{-1}f'(a)\sin\theta + f(a)\cos\theta = 1. \tag{19}$$

The boundary conditions (19) reflect the fact that in this case $f(a)$, $f'(a)$ or any linear combination of these can be specified beforehand but not the ratio $f'(a)/f(a)$. The particular case of $\theta = 0$ was treated by Rudge (2000). On defining

$$K_2 = 2[kf(a)\sin\theta - f'(a)\cos\theta] \tag{20}$$

it is seen that

$$\delta(L_0 + K_1 + K_2 + k^2N) = 2\langle\delta f\mathscr{L}f\rangle + 2(f(a)\cos\theta \\ + k^{-1}f'(a)\sin\theta - 1)\delta(f'(a)\cos\theta - kf(a)\sin\theta) - 2f(0)\delta f'(0). \tag{21}$$

In this case the variational principle

$$\delta(L_0 + K_1 + K_2 + k^2N) = 0 \tag{22}$$

converges to the boundary conditions at $r = 0$ and $r = a$ provided that the basis satisfies the conditions

$$k\boldsymbol{t}(a)\cos\theta + \boldsymbol{t}'(a)\sin\theta \neq \mathbf{0} \qquad \boldsymbol{t}'(a)\cos\theta - k\boldsymbol{t}(a)\sin\theta \neq \mathbf{0} \qquad \boldsymbol{t}'(0) \neq \mathbf{0}. \tag{23}$$

On using the linear trial function (10), (22) gives the linear equations

$$[\mathbf{L}_0 + \mathbf{K}_1 + k^2\mathbf{N}]\mathbf{c} = \boldsymbol{t}'(a)\cos\theta - k\boldsymbol{t}(a)\sin\theta. \tag{24}$$

If $V(r) \equiv 0$ for $r \geqslant a$ then, on equating solutions and their first derivatives at $r = a$, phase shifts, η, are defined by

$$\cot(ka + \theta + \eta) = \frac{f'(a)\cos\theta - kf(a)\sin\theta}{f'(a)\sin\theta + kf(a)\cos\theta}. \tag{25}$$

On convergence the denominator has the value k. One procedure is to compute η by replacing f in (25) by the variationally computed function $f_v = \tilde{\mathbf{t}}\mathbf{c}$. The variational solution and its derivative at $r = a$ are then continuous at $r = a$ whether or not convergence has been achieved.

An alternative procedure, that can be used prior to convergence, is to use the function f_v in the numerator of (25) and replace the denominator by its exact value k. This procedure is justified by observing that, on choosing $\boldsymbol{t}(0) = \mathbf{0}$, so that $\delta f(0) = 0$, then (cf Kohn 1948)

$$\langle f_\text{v} \mathscr{L} f_\text{v} \rangle = f_\text{v} \delta f' - f_\text{v}' \delta f|_a + \langle \delta f \mathscr{L} \delta f \rangle. \tag{26}$$

But,

$$\langle f_\text{v} \mathscr{L} f_\text{v} \rangle \equiv \tilde{\mathbf{c}}[\mathbf{L}_0 + k^2 \mathbf{N} + \mathbf{t}\tilde{\mathbf{t}}'|_a]\mathbf{c} \tag{27}$$

and so by virtue of (24) it follows that, with $f(0) = 0$,

$$\langle f_\text{v} \mathscr{L} f_\text{v} \rangle = -(f_\text{v}' \cos\theta - k f_\text{v} \sin\theta)\delta(f \cos\theta + k' f' \sin\theta) \tag{28}$$

where the functions are evaluated at $r = a$. On equating (26) and (28) it follows that the error in the numerator in (25) is of second order and so an improved or 'corrected' value of the phase shift, $\eta_\mathbf{c}$, prior to convergence, is given by

$$k \cot(ka + \theta + \eta_\mathbf{c}) = f_\text{v}' \cos\theta - k f_\text{v} \sin\theta. \tag{29}$$

If $(1 - f_\text{v} \cos\theta - k^{-1} f_\text{v}' \sin\theta) \neq 0$ then the derivative of the solution that contains $\eta_\mathbf{c}$ for $r \geqslant a$ differs from the derivative of the solution for $r \leqslant a$ at their common point. However, if the basis is chosen so that $\boldsymbol{t}(0) = \mathbf{0}$ and

$$\det[\mathbf{L}_0 + k^2 \mathbf{N} + \mathbf{t}\tilde{\mathbf{t}}'|_a] = 0 \tag{30}$$

(cf Rudge 1973, 1975) then a solution of (24) is given by $\mathbf{c} = \mathbf{c}_0$ where

$$[\mathbf{L}_0 + k^2 \mathbf{N} + \mathbf{t}\tilde{\mathbf{t}}'|_a]\mathbf{c}_0 = 0 \qquad \tilde{\mathbf{c}}_0[\boldsymbol{t}(a)\cos\theta + k^{-1}\boldsymbol{t}'(a)\sin\theta] = 1. \tag{31}$$

In this case $(1 - f_\text{v} \cos\theta - k^{-1} f_\text{v}' \sin\theta) = 0$, there is a zero 'correction' and the solution and its first derivative are continuous at $r = a$. It can be seen that all three methods give the same values if the basis $\mathbf{t}$ is replaced by any linear combination of itself.

2.3. Solution of the linear equations

The solution of (24) can be performed using Gauss elimination but this is unstable if the matrix is nearly singular. The solutions can be obtained in a numerically stable way, and for all values of k^2 (provided that the basis is independent of k^2), using a well-known technique (cf Courant and Hilbert 1953). Let the matrix of eigenvectors $\mathbf{c}_j$ in (13) be

$$\mathbf{C} = [\mathbf{c}_1 \cdots \mathbf{c}_n] \tag{32}$$

normalized so that $\tilde{\mathbf{C}}\mathbf{N}\mathbf{C} = \mathbf{I}$. Then

$$\tilde{\mathbf{C}}[\mathbf{L}_0 + \mathbf{K}_1]\mathbf{C} = -\text{diag}(\lambda_j). \tag{33}$$

and the solution of (24) can now be written as

$$\mathbf{c} = \mathbf{C}[\text{diag}(k^2 - \lambda_j)^{-1}]\tilde{\mathbf{C}}[\boldsymbol{t}'(a)\cos\theta - k\boldsymbol{t}(a)\sin\theta]. \tag{34}$$

In terms of the eigenfunctions $\mathbf{w} = \tilde{\mathbf{C}}\mathbf{t}$, the variational solution of (18) and (19) is therefore

$$f_\text{v}(r) = \cos\theta \sum_j \frac{w_j(r) w_j'(a)}{k^2 - \lambda_j} - k \sin\theta \sum_j \frac{w_j(r) w_j(a)}{k^2 - \lambda_j} \tag{35}$$

and on using (29)

$$k \cot(ka + \theta + \eta_\text{c}) = \cos^2\theta \sum_j \frac{w_j'(a) w_j'(a)}{k^2 - \lambda_j} - k \sin 2\theta \sum_j \frac{w_j'(a) w_j(a)}{k^2 - \lambda_j} + (k \sin\theta)^2 \sum_j \frac{w_j(a) w_j(a)}{k^2 - \lambda_j}. \tag{36}$$

It is important to observe that the $w_j(r)$ are the *variational* solutions of the eigenvalue problem

$$[\mathscr{L}_0 + \lambda_j]w_j(r) = 0 \qquad w_j(0) = 0 \qquad k^{-1}w_j'(a)\sin\theta + w_j(a)\cos\theta = 0. \tag{37}$$

In particular the conditions (23) on the choice of basis are incompatible with the choice (11) for which the solutions satisfy the boundary conditions exactly.

2.4. *The R-matrix method*

The R-matrix method (cf Lane and Thomas 1958, Burke and Robb 1975) is based on the solutions of the eigenvalue problem

$$\mathscr{L}_0 u_n = -k_n^2 u_n \tag{38}$$

subject to the boundary conditions

$$u_n(0) = 0 \qquad a u_n'(a) - b u_n(a) = 0. \tag{39}$$

The eigenvalues k_n^2 can be positive or negative. The eigenfunctions $u_n(r)$ are orthogonal and can be normalized so that

$$\langle u_m u_n \rangle = \delta_{mn}. \tag{40}$$

It can be seen that

$$\langle u_n \mathscr{L} f \rangle = [u_n f' - u_n' f]_0^a + \langle f \mathscr{L} u_n \rangle = u_n(a)[f' - bf/a] + \left(k^2 - k_n^2\right)\langle u_n f \rangle$$

so that

$$\langle u_n f \rangle = u_n(a)[-f' + bf/a] \Big/ \left(k^2 - k_n^2\right). \tag{41}$$

Assuming that the Fourier series

$$f(r) = \sum_n \langle f u_n \rangle u_n(r) \tag{42}$$

converges to $f(a)$ at $r = a$, it is seen that

$$\frac{f(a)}{af'(a) - bf(a)} = \mathscr{R} \tag{43}$$

where

$$\mathscr{R} = a^{-1} \sum_n \frac{u_n(a)u_n(a)}{k_n^2 - k^2} \tag{44}$$

is the R-matrix. If $V(r) = 0$ for $r > a$ then, on choosing $b = 0$, the phase shift is given by

$$(ka)^{-1}\tan(ka + \eta) = \mathscr{R}. \tag{45}$$

The convergence of (44) may be slow but the R-matrix method can be improved (cf Burke and Robb 1975) using a device due to Buttle (1967).

Suppose that

$$\mathscr{M}_0 = \frac{\mathrm{d}^2}{\mathrm{d}r^2} - 2mV_0(r)$$

and that the solutions of

$$(\mathscr{M}_0 + k^2)\varphi(r) = 0 \tag{46}$$

and the eigenfunctions v_n that satisfy

$$M_0 v_n = -k_n'^2 v_n \tag{47}$$

are known.

Table 1. The relative errors in the phase shift $\varepsilon = 1 - \eta/\eta_{\text{exact}}$ as a function of the number of terms, N, where ε_{R} refers to (44), ε_{B} to (48) and ε_{v} to the variational method.

N	ε_{R}	ε_{B}	ε_{v}
4	8.90, −2	9.19, −5	2.0, −7
8	4.46, −2	1.17, −5	1.2, −8
12	2.97, −2	3.48, −6	
16	2.23, −2	1.47, −6	
20	1.78, −2	7.53, −7	
24	1.49, −2	4.36, −7	

The Buttle corrected R-matrix is then

$$\mathscr{R}_{\text{B}} = \left[\frac{a\varphi'}{\varphi} - b\right]^{-1} + a^{-1}\sum_{n=1}^{N}\frac{u_n(a)u_n(a)}{k_n^2 - k^2} - a^{-1}\sum_{n=1}^{N}\frac{v_n(a)v_n(a)}{k_n'^2 - k^2}. \tag{48}$$

Essentially the terms for $n > N$ in (44), which would be neglected in a truncated expansion, are replaced by the corresponding terms for the potential V_0.

On choosing $\theta = \pi/2$ there is a clear similarity between (45) and (36). The difference lies in the fact that in the R-matrix method the $u_n(r)$ are *exact* solutions of (38) and (39) while the functions $w_j(r)$ in (36) are the *variational* solutions of (37) and in particular *do not* satisfy the boundary conditions exactly. This apparent slight difference makes a large difference to the relative convergence of the methods as can be seen from the trivial example of the square well potential

$$2mV(r) = \begin{cases} -1 & \text{for} \quad r \leqslant 1 \\ 0 & \text{for} \quad r > 1. \end{cases}$$

In this case (18) becomes

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + K^2\right] f(r) = 0 \tag{49}$$

where $K^2 = 1 + k^2$. The R-matrix basis functions for $b = 0$ in this case are

$$u_n(r) = \sqrt{2}\,\sin k_n r \qquad k_n = (n - 1/2)\pi \qquad n \geqslant 1. \tag{50}$$

For this case, wherein $a = 1$, the R-matrix method (45) therefore gives

$$k^{-1}\tan(k + \eta) = 2\sum_{n=1}^{N}\frac{1}{[(n - 1/2)\pi]^2 - K^2}. \tag{51}$$

The right-hand side (cf Duke and Wigner 1964, Lane and Thomas 1958, Knopp 1947) is recognized as the truncated partial fraction, or Mittag–Leffler expansion of $K^{-1}\tan K$.

A possible, rather good choice of V_0, from which a Buttle correction can be computed is

$$2mV(r) = \begin{cases} -1/2 & r \leqslant 1 \\ 0 & r > 1. \end{cases}$$

A variational calculation was conducted by taking the value $\theta = 0$ and choosing, in harmony with (23), the basis

$$t_n(r) = rT_{n-1}(r) \qquad n \geqslant 1$$

where $T_n(r)$ is a Chebyshev polynomial (Abramowitz and Stegun 1970). The relative errors of the three methods are displayed in table 1.

The convergence of (44) is clearly slow though much improved by the Buttle correction: this contrasts strongly with the variational method in which different basis functions are used and much faster convergence is achieved.

2.5. Kohn's variational principles

Kohn (1948) presented two variational methods. The second of these has been widely used but has unsatisfactory features (cf Nesbet 1980, Rudge 1973). In particular the results are not independent of the trivial transformation in which the basis is replaced by a linear combination of itself. The first method has been relatively little used, but gives, as noted by Nesbet (1980) a value of $f(a)/f'(a)$, or R-matrix.

Kohn observed that if $f(r)$ is a solution of (18) then the identity

$$L_0(f) + k^2 N(f) + \mu f^2(a) = 0 \tag{52}$$

holds where $\mu = f'(a)/f(a)$. He inferred from this that the variational principle (9), that is normally used to give eigenvalues λ for fixed μ, could equally well be used to determine μ for a fixed $\lambda = k^2$. Assuming that $f(0) = 0$,

$$\delta[L_0 + k^2 N + \mu f^2(a)] = 2\langle \delta f \mathscr{L} f\rangle - 2\delta f(a)[f'(a) - \mu f(a)] \tag{53}$$

and it would appear that the variational principle $\delta(L_0 + K_1 + k^2 N) = 0$ implies that $\mathscr{L} f = 0$ only if the essential boundary condition $f'(a) = \mu f(a)$ is satisfied. However, assuming that $\delta(L_0 + K_1 + k^2 N) = 0$ *is* valid and that the basis $\boldsymbol{t}(r)$ satisfies $\boldsymbol{t}(0) = \mathbf{0}$, a linear trial function gives the equations:

$$[\mathbf{L}_0 + k^2 \mathbf{N} + \mu \boldsymbol{t}(a)\tilde{\boldsymbol{t}}(a)]\mathbf{c} = \mathbf{0} \tag{54}$$

and a value of μ can be sought that gives a non-trivial $\mathbf{c}$. Kohn observed that, since $\boldsymbol{t}(a)\tilde{\boldsymbol{t}}(a)$ is of unit rank, (54) is a linear equation for μ.

It is observed that on choosing $\theta = \pi/2$ in (24) the equation becomes

$$[\mathbf{L}_0 + k^2 \mathbf{N}]\mathbf{c}_0 = -k\boldsymbol{t}(a). \tag{55}$$

It follows that $\mathbf{c} = \mathbf{c}_0$ is a solution of (54) and that the corresponding value of μ is

$$\mu = k/[\tilde{\mathbf{c}}\boldsymbol{t}(a)] = k/f_{\mathrm{v}}(a). \tag{56}$$

Therefore the results of the apparently different procedures (24) and (54) are in fact the same. The phase shift can again be computed in two ways, firstly, as in (25), $k\cot(ka + \eta) = f'(a)/f(a)$ and secondly as in (29) as $\cot(ka + \eta_{\mathrm{c}}) = 1/f_{\mathrm{v}}(a)$ or

$$k\cot(ka + \eta_{\mathrm{c}}) = \mu. \tag{57}$$

3. Concluding remarks

A class of variational procedures has been reviewed, one member of which, for $\theta = 0$, was presented by Rudge (2000). The linear equations that arise from the variational method can be solved, whatever choice of basis is made, in a manner that gives a result similar in form to an R-matrix expansion. The difference lies in the fact that a valid R-matrix basis, that satisfies a mixed boundary condition exactly at $r = a$, is excluded as an appropriate basis for the variational principles. On using any suitable basis, comprising for example orthogonal polynomials, the variational method converges more rapidly than the R-matrix method and does not require the device of a Buttle correction. One of the Kohn variational methods, that appears formally different, has been shown to be equivalent to one of the methods discussed here. The 'consistent procedure', advocated by Rudge (1973, 1975), is also equivalent to these methods if the further constraint (30) is placed on the basis. It can be seen that if the R-matrix basis is sought variationally, as discussed in section 2.1, but in such a way that (11) is *not* satisfied, then the R-matrix and variational procedures become equivalent.

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