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# The generalised Brillouin theorem

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**Abstract.** By using the new calculus on complex Banach spaces developed by Sharma and Rebelo, we give a rigorous proof of the simplest and yet the most generalised version of the Brillouin theorem as given by Sharma and SriRankanathan.

## 1. Introduction

Sharma and SriRankanathan (1980) have used ordinary calculus to prove a very powerful generalisation of the Brillouin theorem. However, it is evident that this result is basically one in the calculus of variations, and the appropriate calculus to use for giving a properly rigorous proof of the result is the new calculus on complex Banach spaces introduced by Sharma and Rebelo (1975) and developed further by Fonte (1979) and Pian and Sharma (1980, 1981). The purpose of the present work is to demonstrate the applicability of the new calculus by proving the generalised Brillouin theorem and some related results with greater rigour than has been possible before.

## 2. Formalities

The following definitions and notations will be used throughout this work.

*Notation 2.1.* The rational, the real and the complex fields will be denoted by  $\mathbb{Q}$ ,  $\mathbb{R}$  and  $\mathbb{C}$  respectively.

*Notation 2.2.* The letters  $X$  and  $Y$  will denote Banach spaces over  $\mathbb{C}$ .

*Definition 2.1.* A map  $f: X \rightarrow Y$  is said to be *additive* if and only if

$$f(x_1 + x_2) = f(x_1) + f(x_2) \quad \forall x_1, x_2 \in X.$$

It should be noted that  $f$  is additive implies that  $f(qx) = qf(x) \forall q \in \mathbb{Q}$  and  $f$  is additive and continuous implies that  $f(rx) = rf(x) \forall r \in \mathbb{R}$ .

*Definition 2.2.* A map  $f: X \rightarrow Y$  is said to be *linear* (resp. *semilinear*) if and only if

- (i)  $f$  is additive and
- (ii)  $f(\alpha x) = \alpha f(x)$  (resp.  $= \bar{\alpha} f(x)$ ).

*Notation 2.3.*  $L(X, Y)$  and  $SL(X, Y)$  will denote the Banach spaces of bounded linear and semilinear functions respectively from  $X$  to  $Y$ . When  $Y = \mathbb{C}$ , the abbreviations

$L(X)$  and  $SL(X)$  will be used for  $L(X, \mathbb{C})$  and  $SL(X, \mathbb{C})$  respectively. It should be noted that if  $V$  is a real normed linear space and  $f$  is any additive continuous function from  $V$  to another real normed linear space  $W$ , then  $f$  is bounded and linear.

*Definition 2.3.* A map  $T: X \rightarrow Y$  is said to belong to  $L(X, Y) \oplus SL(X, Y)$  if and only if  $T$  can be written as

$$T = {}^L T + {}^S T$$

with  ${}^L T \in L(X, Y)$  and  ${}^S T \in SL(X, Y)$ . It should be observed that  $T \in L(X, Y) \oplus SL(X, Y)$  implies that  $T$  is additive and bounded.

*Notation 2.4.* The notation  $A(X, Y)$  will be used to denote the Banach space of continuous additive functions from  $X$  to  $Y$ . It is easily verified that

- (i)  $T \in A(X, Y) \Leftrightarrow T$  is additive and bounded and
- (ii)  $T \in A(X, Y) \Rightarrow T(0) = 0$ .

(It should be noted that for the second property continuity is not necessary and additivity is enough.)

*Definition 2.4.* A function  $f$  from a Banach space  $X$  to a Banach space  $Y$  is said to be *semidifferentiable* at a point  $x \in X$ , if there exists a function  $f_x^{(s)} \in L(X, Y) \oplus SL(X, Y)$  such that

$$\lim_{\|u\| \rightarrow 0} \|f(x+u) - f(x) - f_x^{(s)}(u)\|/\|u\| = 0.$$

The function  $f_x^{(s)}$ , if it exists, is called the *semiderivative* of  $f$  at  $x$ . If the function  $f$  is semidifferentiable at each point in  $X$ , it is said to be *semidifferentiable* in  $X$ , and the rule which assigns to each point  $x \in X$  the semiderivative of  $f$  at that point is called the semiderivative of  $f$  in  $X$  and is denoted by  $f^{(s)}$ .

*Definition 2.5.* Let  $T$  be a continuously semidifferentiable function from an open set  $D$  in a Banach space  $X$  into a Banach space  $Y$ , that is,  $T^{(s)}$  is defined on the whole of  $D$  and is continuous. Let  $x_0 \in D$  be such that  $T_{x_0}^{(s)}$  is surjective; then the point  $x_0$  is said to be a *regular point* of the function  $T$ .

*Notation 2.5.* Further,  $H$  will denote a Hilbert space over the complex field,  $A$  will denote a self-adjoint endomorphism on  $H$  whose spectrum  $\text{Sp } A$  is of type H (cf Sharma and SriRanganathan 1975), which for an endomorphism merely implies that the lower part of the spectrum is purely discrete and the first  $N$  points of the spectrum ordered to form an increasing enumeration have all finite multiplicities (here  $N$  is either a positive integer or the cardinality  $\aleph_0$  of the set of positive integers). For a subset  $S$  of a vector space,  $\hat{S}$  is used to denote  $S \setminus \{0\}$ .

Further, we use the following propositions which are proved in Pian and Sharma (1981).

*Proposition 2.1.*  $A(X, Y) = L(X, Y) \oplus SL(X, Y)$ .

*Proposition 2.2.* (The generalised Lagrange multiplier theorem). Let  $X$  be a complex Banach space. Let  $U$  be an open set containing  $x_0 \in X$ . Let  $f$  be a real functional on  $X$  continuously semidifferentiable on  $U$  and let  $H$  be a mapping from  $X$  to another

complex Banach space  $Y$  with the properties that  $f(x)$  restricted to the set  $\{x : H(x) = 0\}$  has an extremum at  $x_0$  and that  $H$  is continuously semidifferentiable on  $U$ . Then there exists an element  $\lambda \in A(Y, \mathbb{C})$  such that the functional

$$f_{x_0}^{(s)} + \lambda \circ H_{x_0}^{(s)} = 0.$$

### 3. Definitions of stationary points of a functional

*Definition 3.1.* Let  $F$  be a real semidifferentiable functional on a complex Banach space  $X$ . A point  $\psi \in X$  is said to be a *stationary point* of  $F$  if  $F_{\psi}^{(s)} = 0$ .

The semiderivative, if it exists, at a point  $\psi \in X$  has the following property:

$${}^L F_{\psi}^{(s)}(\phi) + {}^S F_{\psi}^{(s)}(\phi) = \lim_{t \rightarrow 0} \frac{F(\psi + t\phi) - F(\psi)}{t} \quad \forall \phi \in X.$$

In view of this property and the assumed semidifferentiability of  $F$ , it is easy to see that definition 3.1 is completely equivalent to the following.

*Definition 3.2.* Let  $F$  be a real semidifferentiable functional on a complex Banach space  $X$ . A point  $\psi \in X$  is said to be a *stationary point* of  $F$  if whenever  $\lambda : ]a, b[ \rightarrow X$  is a differentiable curve passing through  $\psi$  (that is,  $\lambda(c) = \psi$ , for some  $c \in ]a, b[$ ), then at  $t = c$

$$d(F \circ \lambda)/dt = 0.$$

Taking the hint from the generalised Lagrange multiplier theorem (Pian and Sharma 1981), we now define the stationary point of a functional constrained to the null set of a function  $G$  from  $X$  to another Banach space  $Y$ .

*Definition 3.3.* Let  $F$  be a real semidifferentiable functional on a complex Banach space  $X$ . Let  $G$  be a continuously semidifferentiable map from  $X$  to another complex Banach space  $Y$ . Let  $S = G^{-1}(\{0\})$ . A point  $\psi \in S$  is said to be a *stationary point* of the restriction of  $F$  to  $S$ , which we denote by  $F|_S$ , if there exists a bounded additive functional  $\lambda$  on  $Y$  such that

$$F_{\psi}^{(s)} = \lambda \circ G_{\psi}^{(s)}.$$

Note that we have shown elsewhere (Pian and Sharma 1981) that  $A(X, Y)$  (the space of additive maps from  $X$  to  $Y$ ) is a direct sum of  $L(X, Y)$  (the space of bounded linear maps from  $X$  to  $Y$ ) and  $SL(X, Y)$  (the space of bounded semilinear maps from  $X$  to  $Y$ ).

Finally, by recasting the definition of Sharma and SriRankanathan (1980), we obtain yet another definition of a stationary point of a functional.

*Definition 3.4.* Let  $F$  be a semidifferentiable functional on a complex Banach space  $X$  and let  $S$  be an arcwise connected subset of  $X$ . A point  $\psi \in S$  is said to be a *stationary point* of  $F|_S$  if whenever  $\lambda : ]-a, a[ \rightarrow S$  is a differentiable curve passing through  $\psi = \lambda(c)$ ,

$$F_{\psi}^{(s)}(\tilde{\psi}) = 0$$

where  $\tilde{\psi}$  is the tangent vector  $(d\lambda/dt|_{t=c})$  of the curve  $\lambda$  at  $\psi$ .

We now prove that if  $S$  in definition 3.4 is the same as the  $S$  in definition 3.3, then a stationary point in the sense of definition 3.3 is so also in the sense of definition 3.4.

*Proposition 3.1.* Let  $S$  of definition 3.4 satisfy  $S = G^{-1}(\{0\})$  where  $G$  is a continuously semidifferentiable map from  $X$  to another Banach space  $Y$ . Then  $\psi$  is a stationary point of  $F|_S$  in the sense of definition 3.3 only if it is stationary in the sense of definition 3.4.

*Proof.* Let  $\psi$  be a stationary point of  $F|_S$  in the sense of definition 3.3. Let  $\lambda$  be a differentiable curve lying in  $S$ . Now there exists a

$$\gamma \in L(Y, \mathbb{C}) \oplus SL(Y, \mathbb{C})$$

such that

$$F_{\psi}^{(s)} = \gamma \circ G_{\psi}^{(s)}.$$

Let

$$\tilde{\psi} = d\lambda/dt|_{t=c}.$$

We show that

$$G_{\psi}^{(s)}(\tilde{\psi}) = 0,$$

implying

$$F_{\psi}^{(s)}(\tilde{\psi}) = 0.$$

Indeed, since

$$G(\psi) = 0$$

we have

$$\begin{aligned} G_{\psi}^{(s)}(\tilde{\psi}) &= \lim_{\varepsilon \rightarrow 0} \frac{G(\psi + \varepsilon \tilde{\psi})}{\varepsilon} \\ &= \lim_{\varepsilon \rightarrow 0} \left( \frac{1}{\varepsilon} \right) G(\psi + \varepsilon) \left( \lim_{t \rightarrow 0} \frac{\lambda(c+t) - \lambda(c)}{t} \right) \\ &= \lim_{\varepsilon \rightarrow 0} \lim_{t \rightarrow 0} \left( \frac{1}{\varepsilon} \right) G\left( \psi + \frac{\varepsilon[\lambda(c+t) - \psi]}{t} \right). \end{aligned}$$

From the uniqueness theorem for semiderivatives (Sharma and Rebelo 1975), we know that the double limit is unique; hence we can choose

$$t = \varepsilon$$

to obtain

$$G_{\psi}^{(s)} = \lim_{\varepsilon \rightarrow 0} (1/\varepsilon) G[\lambda(c + \varepsilon)].$$

But for sufficiently small  $\varepsilon$ ,  $\lambda(c + \varepsilon) \in S$ . Hence

$$G[\lambda(c + \varepsilon)] = 0,$$

implying

$$G_{\psi}^{(s)}(\tilde{\psi}) = 0.$$

The proof of our proposition is now complete.

A reference to the theory of Lagrange multipliers (Pian and Sharma 1981) will show that the definition of a stationary point in definition 3.3 corresponds to an extremum of  $F$ , while the stationary point in all other definitions can correspond to either an extremum or a saddle point or a point of inflection. This is why the converse of our proposition is not true.

**4. The generalised Brillouin theorem**

We use definition 3.4 in stating and proving the generalised Brillouin theorem.

*Proposition 4.1.* (The generalised Brillouin theorem). Let  $S$  be an arcwise connected subset of  $H$ . Let  $F$  be the Ritz-Rayleigh quotient on  $\hat{H}$  defined by

$$F(x) = \langle x, Ax \rangle / \langle x, x \rangle.$$

Let  $\psi$  be a stationary point of the restriction of  $F$  to  $S$ . Let  $\phi \in \hat{S}$  be such that

- (i)  $\langle \psi, \phi \rangle = 0$ ,
- (ii)  $\text{Span}\{\phi, \psi\} \subset S$ .

Then

$$\langle \psi, A\phi \rangle = 0.$$

(Note that according to notation 2.5  $A$  denotes an endomorphism, that is,  $A$  is bounded.)

*Proof.* An easy computation shows that

$$F_{\psi}^{(s)}(h) = \frac{1}{\langle \psi, \psi \rangle} \left( \left\langle h, A\psi - \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle} \psi \right\rangle + \left\langle A\psi - \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle} \psi, h \right\rangle \right). \tag{4.1}$$

Let  $\lambda_1 : ]-a, a[ \rightarrow S, a > 1$ , be defined by

$$\lambda_1(t) = t\psi + (1-t)\phi.$$

Then

$$\lambda_1(1) = \psi$$

and

$$\lambda_1'(t) = \psi - \phi \quad \forall t \in ]-a, a[.$$

Since  $\psi$  is a stationary point, we must have

$$F_{\psi}^{(s)}(\psi - \phi) = 0.$$

Remembering that

$$\langle \psi, \phi \rangle = 0,$$

it follows from equation (4.1) that

$$\langle \phi, A\psi \rangle + \langle A\psi, \phi \rangle = 0. \tag{4.2}$$

Now let  $\lambda_2: ]-a, a[ \rightarrow \mathbb{S}$ ,  $a > 1$ , be defined by

$$\lambda_2(t) = t\psi + i(1-t)\phi.$$

Then

$$\lambda_2(1) = \psi$$

and

$$\lambda_2'(t) = \psi - i\phi \quad \forall t \in ]-a, a[.$$

Since  $\psi$  is a stationary point, we must also have

$$F_\psi^{(s)}(\psi - i\phi) = 0$$

which with the help of equation (4.1) implies that

$$\langle \phi, A\psi \rangle - \langle A\psi, \phi \rangle = 0. \tag{4.3}$$

From equations (4.2) and (4.3) we can now conclude that

$$\langle \phi, A\psi \rangle = \langle A\psi, \phi \rangle = \langle \psi, A\phi \rangle = \langle A\phi, \psi \rangle = 0.$$

This completes our proof.

We now have an easy corollary which shows that the Hylleraas–Undheim theorem (Hylleraas and Undheim 1930, Sharma and SriRanganathan 1975, 1981) is related to the Brillouin theorem.

*Corollary 4.1.* Let  $S$  in proposition 4.1 be a subspace of  $H$ . Then each stationary point of the Ritz–Rayleigh quotient in  $\hat{S}$  is an eigenvector of  $PAP$ , where  $P$  is the orthogonal projection on  $S$ .

*Proof.* Since  $S$  is a subspace, for every  $\phi \in S$ ,  $(t\psi + (1-t)\phi) \in S$ ,  $\forall t \in \mathbb{R}$ . Hence, for every  $\phi \in S$ , there is a curve  $\lambda_\phi$  lying entirely in  $S$  and passing through  $\psi$  whose tangent at each point is  $\psi - \phi$ . Since  $\psi$  is a stationary point, we must have

$$\begin{aligned} F_\psi^{(s)}(\psi - \phi) &= 0 \quad \forall \phi \in S \\ \Rightarrow \left\langle \phi, A\psi - \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle} \psi \right\rangle + \left\langle A\psi - \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle} \psi, \phi \right\rangle &= 0 \quad \forall \phi \in S \\ \Rightarrow A\psi - \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle} \psi &\in S^\perp \\ \Rightarrow A\psi &= k\psi + v \text{ with } v \in S^\perp \text{ and } k = \langle \psi, A\psi \rangle / \langle \psi, \psi \rangle \\ \Rightarrow PAP\psi &= k\psi \end{aligned}$$

because  $\psi \in S$  and therefore  $P\psi = \psi$  and  $v \in S^\perp$  and therefore

$$Pv = 0.$$

The proof of our corollary is complete.

As a consequence of proposition 3.1, stationary points corresponding to extrema as given by definition 3.3 necessarily satisfy the Brillouin theorem. However, it is instructive to examine what kind of function  $G$  (cf definition 3.3) can be in a real

problem. There is no requirement for  $G$  to be linear or even additive. The range of  $G$  is another Banach space over  $\mathbb{C}$ ; the simplest such space is  $\mathbb{C}$  itself, and in that case  $G$  becomes a functional. In view of proposition 3.1, the real point of our next proposition is that the null set of functionals (which are not necessarily linear or additive) can be used to constrain the optimisation to the orthogonal complement of only a one-dimensional subspace. The proof also indicates how both proposition 4.1 and corollary 4.1 can be proved directly from definition 3.3.

*Proposition 4.2.* Let  $F$  be the Ritz–Rayleigh quotient on  $H \setminus \{0\}$  defined by

$$F(x) = \langle x, Ax \rangle / \langle x, x \rangle.$$

Let  $S$  be the null set of a semidifferentiable functional  $G$  such that  $G$  is regular at the stationary point  $\psi$  of  $F|_S$ . Then

- (i)  $[\text{Ker}(F_\psi^{(s)})]^\perp$  is one-dimensional and
- (ii)  $\psi$  is an eigenvector of  $PAP$  where  $P$  is the orthogonal projection on  $(\text{Ker } F_\psi^{(s)})^{\perp\perp} \supset \text{Ker } F_\psi^{(s)}$ .

*Proof.* It follows from the Lagrange multiplier theorem (see Pian and Sharma 1981) that there exists a bounded functional  $\lambda$  on  $\mathbb{C}$  such that

$$F_\psi^{(s)} = \lambda \circ G_\psi^{(s)}.$$

We know from the Riesz representation theorem that there exist vectors  $g_1$  and  $g_2$  in  $H$  such that

$$G_\psi^{(s)}(h) = \langle h, g_1 \rangle + \langle g_2, h \rangle.$$

Since  $\lambda \in L(\mathbb{C}, \mathbb{C}) \oplus SL(\mathbb{C}, \mathbb{C})$ , we can write  $\lambda$  as

$$\lambda = \lambda^1 + \lambda^2$$

where  $\lambda^1$  and  $\lambda^2$  are functions from  $\mathbb{C}$  to  $\mathbb{C}$  defined by

$$\lambda^1(c) = \lambda_1 c$$

and

$$\lambda^2(c) = \lambda_2 \bar{c}$$

where  $\lambda_1$  and  $\lambda_2$  are complex constants. We therefore have

$$\begin{aligned} F_\psi^{(s)}(h) &= \frac{1}{\langle \psi, \psi \rangle} \left( \left\langle h, A\psi - \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle} \psi \right\rangle + \left\langle A\psi - \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle} \psi, h \right\rangle \right) \\ &= (\lambda^1 + \lambda^2)(\langle h, g_1 \rangle + \langle g_2, h \rangle) \\ &= \langle h, \bar{\lambda}_1 g_1 + \bar{\lambda}_2 g_2 \rangle + \langle \lambda_2 g_1 + \lambda_1 g_2, h \rangle. \end{aligned}$$

Since this is true for all  $h$  we must have

$$A\psi - \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle} \psi = \bar{\lambda}_1 g_1 + \bar{\lambda}_2 g_2 = \lambda_2 g_1 + \lambda_1 g_2.$$

Therefore either  $g_1$  and  $g_2$  are linearly dependent or

$$\lambda_1 = \bar{\lambda}_2.$$

In either case  $(\text{Ker } F_\psi^{(s)})^\perp$  is clearly one-dimensional, which proves (i).



Let  $g$  be a basis for  $(\text{Ker } F_\psi^{(s)})^\perp$ . Now

$$\begin{aligned} F_\psi^{(s)}(\psi) &= \frac{1}{\langle \psi, \psi \rangle} \left( \left\langle \psi, A\psi - \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle} \psi \right\rangle + \left\langle A\psi - \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle} \psi, \psi \right\rangle \right) \\ &= 0 \\ \Rightarrow \psi &\in \text{Ker } F_\psi^{(s)} \subset [\text{Ker } F_\psi^{(s)}]^\perp. \end{aligned}$$

Let  $\phi \in [\text{Ker } F_\psi^{(s)}]^\perp$ ; then  $\phi$  is perpendicular to  $g$ . Hence

$$\begin{aligned} G_\psi^{(s)}(\phi) &= 0 \\ \Rightarrow F_\psi^{(s)}(\phi) &= 0. \end{aligned}$$

Now let  $\phi \in [\text{Ker } F_\psi^{(s)}]^\perp$  be such that

$$\langle \phi, \psi \rangle = 0;$$

then

$$\begin{aligned} F_\psi^{(s)}(\phi) &= 0 \\ \Rightarrow \langle A\psi, \phi \rangle &= 0. \end{aligned}$$

Since this is true for each such  $\phi$ , we must have  $A\psi \in \text{Span}\{\psi\} \oplus [\text{Ker } F_\psi^{(s)}]^\perp$ . In other words

$$A\psi = a\psi + bg.$$

Hence

$$PAP\psi = PA\psi = a\psi,$$

which proves (ii), completing the proof of our proposition.

We remark that both proposition 4.1 and corollary 4.1 can be proved directly from definition 3.3 by arguments similar to the one used in the preceding proof.

When  $S$  is a subspace of  $H$ , as in the situation relevant to the Hylleraas–Undheim problem, then the constraining function  $G$  can be taken to be  $(I - P)$  where  $I$  is the identity on  $H$  and  $P$  is the orthogonal projection on the subspace  $S$ . The Banach space  $Y$  (the range of  $G$ ) in this case is simply  $S^\perp$ . It is easy to verify that at the stationary points of  $F$ ,  $G$  is regular. The most common use of the Brillouin theorem is related to the Hartree–Fock problem and there  $S$  is not a subspace. However, we do not need a constraining function for the Brillouin theorem, which we have already proved. The work of one of us (J Pian, unpublished) shows how one can use the Lagrange multiplier theorem for deducing the Hartree–Fock equations by using our calculus.

The main advantage of using the new calculus in preference to more conventional methods in deducing the Hartree–Fock equations, the Brillouin theorem and other variational results involving a complex Banach space lies in the fact that our method makes it unnecessary to use the very fruitful but mathematically meaningless rule which allows one to vary a function and its complex conjugate (or a state vector in a Hilbert space and its dual (through the Riesz representation theorem)) independently of each other.

## 5. Concluding remarks

We have assumed that  $A$  is bounded, whereas the Hamiltonians of quantum mechanics are not. All the principal results extend to semibounded operators by using the technique described in Pian and Sharma (1980) or by using a concept which we call weak semidifferentiability. The work on developing the theory of weak semidifferentiability is in progress and will be reported in due course. We shall illustrate the application of weak semidifferentiability by showing how it extends the present results to unbounded operators.

Though it is possible to extend the results of this paper rigorously to unbounded operators by using either of the techniques mentioned in the preceding paragraph, for practical applications it is, in most cases, enough to have these results for bounded operators. There are two ways of seeing that there is no loss of rigour in treating  $A$  as bounded in applications. All the physical results mentioned in this work—the Ritz–Rayleigh principle, the Hylleraas–Undheim theorem and the Brillouin theorem—are used for finding variational approximations to the energies and eigenfunctions of the ground states and low-lying excited states of atoms and molecules. How good an approximation one gets depends on the wisdom in making the choice of the space of trial functions. It stands to reason that any vector having a significant component in a subspace of  $H$  which corresponds to very high energies of the system cannot be of much use in approximating a low-lying stationary state. Hence, for any reasonable choice of the space of trial functions,  $A$  can be approximated to any desired degree of accuracy by  $A'$ , which is the operator obtained by truncating the spectral integral for  $A$  at an appropriate energy depending on the trial space and how good an approximation one wants. It is common knowledge that in atomic calculations, atomic integrals to infinity are truncated, without loss of desired accuracy, at finite values. Similarly, on the rangefinder of a photographic camera infinity is almost always very finite. Truncating the spectral representation of  $A$  at a finite energy is very similar and gives a bounded approximation to  $A$ . The proof of the assertion that the approximation can be made to any desired degree of accuracy for a finite-dimensional trial space is much more trivial than anything in this paper and is therefore omitted. Furthermore, there is another way of seeing that the result for bounded operators is enough. In these variational calculations one is restricted to a finite-dimensional subspace, say  $M$ , spanned by the trial wavefunctions (with giant computers now available, the dimension of this subspace can be very large, say tens of thousands, but it is nevertheless finite). One is using the trial space to find approximations to a finite number of bound states. Let  $E$  be the subspace spanned by the eigenfunctions of these bound states. Let

$$N = \overline{M + E}$$

where the bar over  $M + E$  denotes that we are taking the closure of this sum. Let  $P$  be the orthogonal projection on  $N$ . We are not concerned with the values of the Ritz–Rayleigh quotient outside  $N$ , and inside  $N$  the Ritz–Rayleigh quotient of  $A$  is the same as that of  $PAP$ , and  $PAP$  can be effectively regarded as an operator on the finite-dimensional space  $N$  and an operator on a finite-dimensional subspace is necessarily bounded. Hence it is enough for our purposes to have the theorems for bounded operators only. This indeed explains why atomic and molecular physicists can disregard the lack of boundedness of  $A$  with impunity. The two explanations are in fact complementary. The method of truncation of the spectral integral, combined with the results of this paper, will yield a rigorous proof of the Ritz–Rayleigh principle for the

ground state. Further, the method of replacing  $A$  by  $PAP$ , combined with our results, will give us rigorous proofs of the orthogonality which is achieved between approximate eigenfunctions of two states by using the Hylleraas–Undheim theorem and of the vanishing of certain matrix elements of  $A$  through the application of the Brillouin theorem in calculations involving the method of configuration interaction. Nevertheless, it is important to have the results for unbounded operators. This is because when one deduces something like the Hartree–Fock equations for atoms, one is doing a theoretical variation in an infinite-dimensional trial space, and neither of the methods described in this paragraph will justify the use of bounded operators for such calculations.

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### References

- Fonte G 1979 *Nuovo Cimento* **49B** 200–19  
Hylleraas E A and Undheim B 1930 *Z. Phys.* **65** 759–72  
Pian J and Sharma C S 1980 *Phys. Lett.* **76A** 365–6  
— 1981 Submitted for publication  
Sharma C S and Rebelo I 1975 *Int. J. Theor. Phys.* **13** 323–36  
Sharma C S and SriRanganathan S 1975 *J. Phys. A: Math. Gen.* **8** 1853–62  
— 1980 *Mol. Phys.* **40** 1021–3  
— 1981 Submitted for publication