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Variable operator technique and the min-max theorem

SAMBHU NATH DATTA
Department of Chemistry, Indian Institute of Technology, Powai, Mumbai 400 076, India
Email: sndatta@ether.chem.iitb.ernet.in

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Abstract. We investigate a variation method where the trial function is generated from the application of a variable operator on a reference function. Two conditions are identified, one for obtaining a maximum and another for a minimum. Although the conditions are easy to understand, the overall formulation is somewhat unusual as each condition gives rise to a two-step variation process. As an example, projection operators are used to form the variable operator, and by this tactics one obtains the *new* interpretation that the pseudopotential formalism is in fact equivalent to a minimax procedure.

The two-step variational process is nevertheless more flexible than the pseudopotential formalism, for it can also be used when the variable operator is *not* manifestly expressed in terms of projectors. This is illustrated by a comparison of the two-step method with the variational solution of Dirac's relativistic electron equation. The same comparison leads to an *alternative proof* that the process of maximizing energy by varying the u–l coupling operator eliminates all negative-energy contributions from a trial spinor. The latter observation is crucial for the derivation of the min-max theorem in relativistic quantum mechanics.

Keywords. Variable operator; pseudopotential; min-max theorem; relativistic.

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1. Introduction

The aim of this work is to present certain general quantum mechanical results when the trial function ψ is generated from the application of a variable operator $\mathbf{Q}$ on a reference function ϕ : $|\psi\rangle = \mathbf{Q}|\phi\rangle$. The definition of the expectation value E as a functional of ψ leads to the relationship

$$\langle\phi|\mathbf{Q}^\dagger(\mathbf{H}-E)\mathbf{Q}|\phi\rangle = 0. \tag{1}$$

The value E changes as $\mathbf{Q}$ or $\mathbf{Q}^\dagger$ is changed. In fact,

$$\delta E = \langle\phi|\mathbf{Q}^\dagger\mathbf{Q}|\phi\rangle^{-1}\langle\phi|[\delta\mathbf{Q}^\dagger(\mathbf{H}-E)\mathbf{Q}+\mathbf{Q}^\dagger(\mathbf{H}-E)\delta\mathbf{Q}]|\phi\rangle,$$

and

$$\delta^2 E = \langle\phi|\mathbf{Q}^\dagger\mathbf{Q}|\phi\rangle^{-1}[\langle\phi|\delta\mathbf{Q}^\dagger(\mathbf{H}-E)\delta\mathbf{Q}|\phi\rangle - \delta E\langle\phi|\delta\mathbf{Q}^\dagger\mathbf{Q}+\mathbf{Q}^\dagger\delta\mathbf{Q}]|\phi\rangle]. \tag{2}$$

The variations $\delta\mathbf{Q}^\dagger$ and $\delta\mathbf{Q}$ are independent of each other. The stationary point curvature is determined from the second-order change subject to the condition $\delta E = 0$. The nature of the stationary point depends upon whether the numerator on the right side of the second equation in eq. (2) is less than or greater than zero for variations $\delta\mathbf{Q}$ and $\delta\mathbf{Q}^\dagger$. Also, if $\delta E = 0$ for *all arbitrary variations* $\delta\mathbf{Q}$ and $\delta\mathbf{Q}^\dagger$, then, to within a constant multiplicative factor, $\mathbf{Q}|\phi\rangle$ becomes identical with one of the eigenfunctions $|\psi_i\rangle$ of $\mathbf{H}$ and E equals E_i, the corresponding eigenvalue.

These general results have been used here to discuss two fundamental topics of quantum chemistry. It is shown in §2 that when $\mathbf{Q}$ is expressed in the general form, two limiting cases can be identified – one for clearly obtaining a maximum, and the other for clearly obtaining a minimum. The operator $\mathbf{Q}$ is restricted to the diagonal representation in §3, and the two limiting forms become very transparent. Nevertheless, what is *new* here is that the possibility of varying both ϕ and $\mathbf{Q}$ gives rise to a two-step variation procedure. The two-step variation is illustrated in two cases. First, the diagonal forms are investigated in the context of valence electron calculations in §4 where we show that the formation of the pseudopotential is equivalent to the maximization of energy for variation of the core orbital contributions. Thus the pseudopotential technique can be interpreted as a minimax procedure. This is a *new* interpretation. Its importance lies in the possibility that it may be exploited in future to generate effective potentials for systems with more than one valence electron. The variable nature of $\mathbf{Q}$ gives the two-step procedure a greater flexibility than what is normally given in a pseudopotential formalism. To illustrate this flexibility, the general form for $\mathbf{Q}$ is next considered in §5, in the context of a variational approach to the solution of Dirac's relativistic electron equation. This comparison provides an *alternative proof* of the fact that the process of maximizing energy by varying the $u - l$ coupling operator eliminates all negative-energy contributions from a trial four-component spinor. The latter observation is crucial for the derivation of the min-max theorem in relativistic quantum mechanics.

2. The general picture

To allow for all possible variations of $\mathbf{Q}$ one must write it in the most general form as

$$\mathbf{Q} = \sum_{i,j} |\psi_i\rangle q_{ij} \langle\psi_j|. \tag{3}$$

One may also require that $\mathbf{Q}$ be hermitean. This would imply $q_{ji} = q_{ij}^*$. The requirement, however, is not always necessary, and henceforth we will assume $\mathbf{Q}$ to be a general (non-hermitean) operator.

When $\delta E = 0$ for the change $q_{ij} \to q_{ij} + \delta q_{ij}$ one obtains

$$\delta q_{ij}(E_i - E)\langle\psi_j|\phi\rangle \sum_k \langle\phi|\psi_k\rangle q_{ik}^* + \text{c.c.} = 0. \tag{4}$$

In general, E can be stationary when (i) $\sum_k \langle\phi|\psi_k\rangle q_{ik}^* = \langle\phi|\mathbf{Q}^\dagger|\psi_i\rangle = 0$, or (ii) the reference function ϕ is orthogonal to ψ_j, or even (iii) $E = E_i$. The second-order change in energy at the stationary point is given by

$$\delta^2 E = \frac{|\delta q_{ij}|^2 |\langle\psi_j|\phi\rangle|^2 (E_i - E)}{\sum_k |\langle\psi_k|\mathbf{Q}|\phi\rangle|^2} \tag{5}$$

which can be non-zero when $\langle\phi|\mathbf{Q}^\dagger|\psi_i\rangle = 0$ but $E \neq E_i$ and $\langle\psi_j|\phi\rangle \neq 0$, that is, when ϕ and E are completely general but $\mathbf{Q}$ has the form

$$Q = \sum_{m(\neq i)} \sum_n |\psi_m\rangle q_{mn} \langle\psi_n|. \tag{6}$$

The nature of the stationary state can be precisely specified for an arbitrary ϕ in two and only two limiting cases. One notes

$$E_i - E = \frac{\sum_p (E_i - E_p) |\langle\psi_p|\mathbf{Q}|\phi\rangle|^2}{\sum_p |\langle\psi_p|\mathbf{Q}|\phi\rangle|^2}. \tag{7}$$

This ensures

$$\text{(i)} \qquad \delta^2 E < 0 \tag{8a}$$

unambiguously when

$$\mathbf{Q} = \sum_{\substack{m \\ (E_m > E_i)}} \sum_n |\psi_m\rangle q_{mn} \langle\psi_n|. \tag{8b}$$

The corresponding stationary value is greater than E_i and is a maximum. Similarly,

$$\text{(ii)} \qquad \delta^2 E > 0 \tag{9a}$$

when

$$\mathbf{Q} = \sum_{\substack{m \\ (E_m < E_i)}} \sum_n |\psi_m\rangle q_{mn} \langle\psi_n|. \tag{9b}$$

The corresponding stationary value is a minimum and it is less than E_i.

The meaning of these two results become clear when we consider the effect of the operation of $\mathbf{Q}$ on the state vector $|\phi\rangle$. The latter task generates a superposition of the states with energy eigenvalues greater than E_i and less than E_i respectively in the two cases. But this must *not* generate the idea that these results are trivial. The reasons are as follows: (i) By the very choice of building ψ from $\mathbf{Q}$ and ϕ, the formulation includes the possibility of carrying out the variation of energy in two steps. Thus one can find the minimum of maxima, or the maximum of minima. (ii) Besides, the operator $\mathbf{Q}$ may not manifestly appear in terms of projection operators. The intention of this work is to show in §4 and §5 that these peculiarities can be exploited to obtain the inside knowledge of a variation treatment.

3. The diagonal representation

One may choose to restrict the variable operator $\mathbf{Q}$ to the diagonal form by writing $q_{ij} = d_i \delta_{ij}$ such that

$$\mathbf{Q}_d = \sum_i d_i \mathbf{P}_i, \tag{10}$$

where $\mathbf{P}_i$ is the projection operator $|\psi_i\rangle\langle\psi_i|$. The coefficients d_i's are the parameters of variation. To determine the stationary values, one only needs to consider $\delta E = 0$ in eq. (2) for any arbitrary change δd_j. This procedure yields the results which are quite obvious:

(i) $$\delta^2 E < 0 \tag{11a}$$

for

$$\mathbf{Q}_d = \sum_{\substack{n \\ (E_n > E_j)}} d_n \mathbf{P}_n, \tag{11b}$$

and

(ii) $$\delta^2 E > 0 \tag{12a}$$

when

$$\mathbf{Q}_d = \sum_{\substack{n \\ (E_n < E_j)}} d_n \mathbf{P}_n. \tag{12b}$$

The nature of the stationary point (maximum and greater than E_j, and minimum and less than E_j) is also manifest from the form of $\mathbf{Q}_d$ in the two cases. These results have important applications in the non-relativistic valence electron treatment, as shown in the next section.

4. Valence electron treatment

A reference function *approximately* representing a valence orbital can be written as

$$|\phi\rangle = \sum_i c_i |\psi_i\rangle, \tag{13}$$

where the summation is carried out over all the orbitals, core as well as valence, but the valence orbital coefficients c_vs are much larger than the core orbital coefficients c_cs in the reference function. Actually the vectors $|\psi_i\rangle$s can be the eigenvectors of some other energy operator $\mathbf{F}$ that approximates the concerned Hamiltonian [1,2], but in this work we take these vectors as the eigenvectors of $\mathbf{H}$. The trial function $|\psi\rangle$ can be prepared by the application of $\mathbf{Q}_d$ on this $|\phi\rangle$ with the result

$$|\psi\rangle = \sum_i c_i d_i |\psi_i\rangle. \tag{14}$$

Furthermore, the operator $\mathbf{Q}_d$ can be partitioned as

$$\mathbf{Q}_d = \mathbf{Q}_c + \mathbf{Q}_v, \tag{15}$$

where

$$\mathbf{Q}_c = \mathbf{P}\mathbf{Q}_d \equiv \sum_c \mathbf{P}_c \mathbf{Q}_d,$$

and

$$\mathbf{Q}_v = (1 - \mathbf{P})\mathbf{Q}_d. \tag{16}$$

One must treat the core orbitals coefficients $c_c d_c$s as well as the valence orbital coefficients $c_v d_v$s in the trial function ψ as variables. In fact, one has the option to change either the reference orbital coefficients cs while the ds are kept fixed, or the operator coefficients ds while the cs are kept intact. The latter observation suggests a two-step variation procedure. The first step involves the variation of the core projector coefficients d_cs. In the second step one varies the valence orbital coefficients c_vs in the reference function. Proceeding along these lines, we come across a remarkable observation that is given below in the form of a proposition.

PROPOSITION 4.1

The use of the operator $\mathbf{Q}_v$ corresponds to the generation of the maximum value of E.

Proof. Equation (11a) shows that for any change δd_c, the stationary point curvature $\delta^2 E$ is always negative if $d_{c'} = 0$ for every c'. Hence the Proposition.

Remark. Thus, the first step of the variation, that is, the variation of the d_cs, is replaced by the use of $\mathbf{Q}_v$ which results in the maximum value E. This maximum is given by

$$E = \max_{\mathbf{Q}_c} E = \frac{\langle (1 - \mathbf{P})\mathbf{Q}\phi | H | (1 - \mathbf{P})\mathbf{Q}\phi \rangle}{\langle (1 - \mathbf{P})\mathbf{Q}\phi | (1 - \mathbf{P})\mathbf{Q}\phi \rangle}. \tag{17}$$

The right hand side of eq. (17) can be rearranged to write

$$E = \frac{\langle \mathbf{Q}\phi | H + V^{\mathrm{GPP}} | \mathbf{Q}\phi \rangle}{\langle \mathbf{Q}\phi | \mathbf{Q}\phi \rangle}, \tag{18}$$

where $V^{\mathrm{GPP}} = -\mathbf{HP} - \mathbf{PH} + \mathbf{PHP} + E\mathbf{P}$, which is the generalized pseudopotential (V_R^{GPK}) defined by Weeks and Rice [3] and Weeks *et al* [4]. Actually, a comparison of the minimum of the constrained functional with that of the unconstrained functional led the authors of refs [3] and [4] to identify V_R^{GPK} as a repulsive potential. Here, instead, Proposition 4.1 identifies E as the maximum for variation of $\mathbf{Q}_c$.

With our choice of the eigenfunctions ψ_is, $\mathbf{H}$ commutes with $\mathbf{P}$ and V^{GPP} reduces to the simple form $V^{\mathrm{PP}} = (E - \mathbf{H})\mathbf{P}$. The last operator immediately reduces to the pseudopotential defined by Phillips and Kleinman [5], $V^{\mathrm{PK}} = \sum_c (E - E_c)\mathbf{P}_c$, as discussed in [2].

Next, one varies ϕ, that is, varies the c_cs as well as the c_vs. In this context one finds

COROLLARY 4.2

The variation of E by varying ϕ amounts to the variation of E with respect to only the c_vs.

Proof. Equation (17) shows that E depends only on $\mathbf{Q}_v\phi$, that is, only on the c_vs.

Remark. The use of the pseudopotential means that the energy remains maximized, and the change of the core orbital coefficients in ϕ has no effect on E, the maximum value. When E is made stationary for all changes $\delta(\mathbf{Q}_v\phi)$, one obtains one of the valence eigenvalues. In particular, one can obtain the least value E_{v0} among the valence eigenvalues, by keeping $\mathbf{Q}_v$ fixed with $d_{v0} \neq 0$ but varying ϕ arbitrarily:

$$\min_{\phi} E = E_{V0}. \tag{19}$$

This leads to the following conclusion that constitutes a completely new viewpoint.

COROLLARY 4.3

The pseudopotential formalism is equivalent to a minimax procedure guided by the theorem

$$\min_{\phi} \max_{\mathbf{Q}_c} \langle \mathbf{H} \rangle = E_{V0} \tag{20}$$

and it generates an upper bound to the least valence eigenvalue.

Although in the above we have come across the well-known pseudopotentials, the method described here is somewhat more general. This can be understood by checking the optimized form of the operator $\mathbf{Q}$. In fact, the optimized operator is given by $\mathbf{Q}_v \equiv \sum_v d_v \mathbf{P}_v$. Conventional pseudopotential methods are exclusively based on the choice $d_v = 1$ for every v. So, the present method is more flexible, but its merit can be realized only when one uses for $\mathbf{Q}$ an analytical function or any operator that is not explicitly written down in the form of a projection operator. This point will be made clear in the general representation which we discuss in the next section, and in §6.

A minimization that starts from the variation of $\mathbf{Q}_v$ will correspond to the removal of valence orbital contributions from ϕ, and the newly optimized operator will then be given by

$$\mathbf{Q}_c = \sum_c d_c \mathbf{P}_c. \tag{21}$$

A careful manoeuvre can lead to the max-min theorem for the highest core orbital energy, but this will be of little interest as the procedure requires the knowledge of all the valence orbitals. To acquire the knowledge of the core orbitals is a relatively simple and manageable task.

5. The Dirac problem

The one-electron Dirac Hamiltonian

$$\mathbf{H}_D = c\alpha \cdot \mathbf{p} + \beta c^2 + V \tag{22}$$

has both positive-energy $(+)$ and negative-energy $(-)$ eigenvalues: $E_+ > c^2$ and $E_- < -c^2$ for the continuum states, and $c^2 \geq E_+ \geq 0$ corresponding to the bound state eigenfunctions. The Dirac α and β matrices are written as

$$\alpha = \begin{pmatrix} \mathbf{0} & \sigma \\ \sigma & \mathbf{0} \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}, \tag{23}$$

where **0** is the null matrix, **1** is the unit matrix, and σ is the Pauli spin matrix vector, all of rank 2. The trial function ψ is a four-component spinor that can be written as

$$\psi = \begin{pmatrix} u \\ l \end{pmatrix}, \tag{24}$$

where u and l are two-component spinors like the one-electron functions due to Pauli. One may define the variable operator by

$$\mathbf{Q} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \Omega \end{pmatrix}, \tag{25}$$

where Ω is a trial operator matrix of rank 2, and choose the reference function

$$\phi = \begin{pmatrix} u \\ u \end{pmatrix} \tag{26}$$

such that the formation of the trial function $\psi = \mathbf{Q}\phi$ gives rise to the mutual dependence of the upper and the lower component functions, $l = \Omega u$.

For a specific u, the lower component function l changes with Ω. When the expectation value $\langle \mathbf{H}_D \rangle$ is varied as a functional of Ω, stationarity is achieved for the optimized coupling operator [6]

$$\Omega^0[u] = c(E[u] + c^2 - V)^{-1}\sigma \cdot \mathbf{p}, \tag{27}$$

where $E[u]$, the stationary value, is a functional of u. This stationary value satisfies the integral equation

$$\big(u, (E[u] - c^2 - V)u\big) = c^2\big(u, \sigma \cdot \mathbf{p}(E[u] + c^2 - V)^{-1}\sigma \cdot \mathbf{p}u\big). \tag{28}$$

It has been shown [6–10] that the coupling operator given by eq. (27) *unambiguously generates a maximum under certain precisely defined conditions*, viz.,

$$V < 0, 0 > (V)_u > 2c^2 \quad \text{and} \quad E > c^2 + (V)_u, \tag{29}$$

where $(V)_u = (u, Vu)/(u, u)$. These conditions also make $E[u]$ manifestly greater than $-c^2$. When $E[u]$ as given by eq. (28) is made stationary for *all* variations δu, one obtains one of the discrete eigenvalues $E_{i,+}$ belonging to the positive-energy spectrum and the eigenvalue equation in the separated form

$$(E_{i,+} + c^2 - V)l_{i,+} = c\sigma \cdot \mathbf{p}u_{i,+} \quad (\text{from } (27)) \tag{30}$$

and

$$(E_{i,+} - c^2 - V)u_{i,+} = c\sigma \cdot \mathbf{p} l_{i,+} \quad (\text{from } (28))$$

where $u_{i,+}$ and $l_{i,+}$ are the upper and the lower components of the eigenspinor $\psi_{i,+}$. A negative-energy eigenvalue is never obtained from the variation since $E[u]$ always remains greater than $-c^2$. Incidentally, the direct separation of the Dirac equation *for eigenspinors* into the two equations in (30) is known as the first step of the elimination method due to Pauli. Here, however, the separation has been achieved from a variational approach.

That the variation of $E[u]$ can never lead to an eigenvalue of negative energy [6, 10] indicates that for any u belonging to the group of upper component functions which satisfy $(V)_u > -2c^2$, (rather, $E[u] > -c^2$), the lower component function $l^0 = \Omega^0 u$ gives rise to a four-component spinor ψ^0 that belongs to the subspace spanned by the positive-energy eigenfunctions. For the usual potentials, (for instance, for Coulomb potentials with $Z < c$), the condition $E[u] > -c^2$ is satisfied by normalizable us. Therefore, an arbitrary variation of the energy maximum with respect to u generates an upper bound to the *ground state energy*, the least value among the discrete eigenvalues [6–10]. This result is known as the min-max theorem in relativistic quantum mechanics. It is shown in the following that the same conclusion can be reached by starting directly from eqs (8a) and (8b).

In general, a variation of Ω while keeping u fixed can mix in or get rid of the contributions from the negative-energy eigenspinors. This fact allows the following observations to be made.

PROPOSITION 5.1

The operator $\mathbf{Q}$ *in eq.* (25) *is in the general form.*

Proof. $\mathbf{Q}$ does not commute with $\mathbf{H}_D$ unless Ω is the unit matrix of rank 2, that is, unless $\mathbf{Q}$ is the unit matrix of rank 4.

Remark. In general, $\mathbf{Q}$ is not even hermitean. For instance, $\Omega^{0\dagger} \neq \Omega^0$.

PROPOSITION 5.2

The lower component function $l = \Omega^0 u$ *generates the four-component trial spinor* $\mathbf{Q}_+|\phi\rangle$ *that lies completely in the subspace spanned by the positive-energy spinors.*

Proof. The variation of Ω to maximize $\langle \mathbf{H}_D \rangle$ leads to the optimized operator

$$\mathbf{Q}_+ = \begin{pmatrix} 1 & 0 \\ 0 & \Omega^0 \end{pmatrix}.$$

Since $E[u]$ is *unambiguously* a maximum and greater than all negative-energy eigenvalues as discussed in refs [6–10], the general form of $\mathbf{Q}_+$ is given by eq. (8b), that is, $\mathbf{Q}_+$ can be written as

$$\mathbf{Q}_+ = \sum_m \sum_p |\psi_{m,+}\rangle q_{mp} \langle \psi_{p,+}| + \sum_m \sum_n |\psi_{m,+}\rangle q_{mn} \langle \psi_{n,-}|, \tag{31}$$

where $E_{m,+}$ etc. are all greater than the negative energy values, that is, $\psi_{m,+}$ etc. are all four-component eigenspinors of positive energy, whereas $\psi_{n,-}$ etc. are the negative-energy

eigenspinors. (The negative energy eigenvalues form a continuous spectrum). Hence the proposition.

Proposition 5.2 leads to the following important result.

COROLLARY 5.3

Variation of the maximum as a functional of u gives rise to an upper bound to the ground state energy $E_{0,+}$.

Proof. One observes

$$\min_{u} \max_{\Omega} \langle \mathbf{H}_D \rangle \equiv \min_{\phi} \max_{\mathbf{Q}} \langle \mathbf{H}_D \rangle.$$

By Proposition 5.2 the rhs equals the ground state energy so that

$$\min_{u} \max_{\Omega} \langle \mathbf{H}_D \rangle = E_{0,+} \tag{32}$$

which is the min-max theorem for the solution of Dirac's equation [6–10].

6. Discussion

The variation method discussed here is based on the use of a variable operator $\mathbf{Q}$. The treatment leads to two transparent conditions, one for manifestly obtaining a maximum, and the other for a minimum. But the merit of the formulation is that each condition gives rise to the possibility of carrying out a two-step variation as the reference function ϕ can also be varied. By adopting the diagonal representation for the variable operator, one can interpret the pseudopotential technique as a min-max procedure. This is a new interpretation, and its importance lies in the possibility that it may be exploited to generate *effective potentials* for systems with more than one valence electron. Effective potentials generally correspond to the sum of the pseudopotentials and analytical functions which account for the modification of the two-electron interaction. Hence they may be considered in terms of $\mathbf{Q}_v \equiv \sum_v d_v \mathbf{P}_v$ but with $d_v \neq 1$. Also, the explicit use of E spoils the hermitean nature of the pseudopotentials V_R^{GPK}, V^{PP}, and V^{PK}, whereas a variational approach can avoid this disconcerting feature. These aspects will be discussed in a future communication.

But the two-step process is more flexible. It works even when the variable operator is given an analytical form that does not manifestly involve projectors. This has been illustrated by comparing the present technique with the variational solution of Dirac's relativistic electron equation. The outcome is an alternative proof that the process of maximizing energy by varying the $u - l$ coupling operator eliminates all negative-energy contributions from a trial spinor. Then the two-step method becomes synonymous with the min-max technique.

A general account of the separation theorems and the min-max problem has been given by Epstein [11] in the context of discussing the basis set expansion technique. A number of examples of the minimax technique for the Dirac problem have been given in ref. [10]. The minimax procedure was intuitively put forward by Talman who apparently took the theorem for granted but did not supply any proof [12]. Grant and his coworkers solved the

variational problem in practice in a different way, in terms of the matrix representation of operators and operator products [13, 14].

Recently, Kutzelnigg has criticized the min-max principle and the formulation of the min-max theorem by assuming that in these procedures the upper and the lower component functions vary in such a way that their functional forms are not dependent upon each other [15]. Kutzelnigg then imposes the constraint of inter-component coupling to ensure an upper bound, and refers to the procedure as the 'strong minimax principle'. In fact, the so-called strong minimax principle is comprehensively included in Talman's suggestion [12] and in the derivation of the min-max theorem [6–10], as in both the cases the authors have explicitly considered the two components to be coupled. See the bracket Talman uses to write down the min-max principle [12].

The min-max theorems valid for both the Dirac and Dirac–Fock analyses were worked out in [6], and the relevant computational aspects were discussed in [16]. The min-max theorem for the two-electron Dirac–Coulomb equation was established in [17]. A general overview of all the three minimax procedures (Dirac, Dirac–Fock, and Dirac–Coulomb problems) is given in [18]. The present work establishes the one-electron min-max theorem on a firmer footing in the sense that the structure of the operator $\mathbf{Q}_+$ is revealed by eq. (31).

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