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Spectral Concentration for the Helium Schrödinger Operator

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1. Introduction

According to a well known discovery of Stark the spectral lines of an atom in an electric field split. For the case of the hydrogen atom, Schrödinger [1] used his perturbation theory to compute these split levels. His results coincided with the experiments with great accuracy. Then Oppenheimer pointed out [2] that according to physical intuition the entities computed by Schrödinger cannot be point eigen-values of the corresponding Schrödinger operator. Later this intuition was established rigorously by Titchmarsh. At the same time he proposed an asymptotic description of Schrödinger's problem.

It was observed by Riddell [13, 14] and elsewhere [11] that the phenomenon of spectral concentration holds for a large class of abstract operators, including the family of Schrödinger operators corresponding to hydrogen in an electric field.

In this paper we show that the phenomenon of spectral concentration also holds for the family of Schrödinger operators corresponding to helium in an electric field. Actually instead of the helium atom we could consider a heavier atom but we shall not be concerned with this fact. Specifically we show that near any isolated eigen-value of the helium Schrödinger operator we have concentration of order p, for each positive integer p. For the important special case of $p = 1$, this is implied by a theorem of Hunziker [20c] which says that the point eigen-functions corresponding to isolated eigen-values of multiparticle Schrödinger operators die out at infinity faster than any power of the independent variable. Another special case was treated elsewhere [21].

In Section 2 we summarize some known facts about the helium Schrödinger operator. Then we apply the abstract concentration theorem [11, 13, 14] to the family of Schrödinger operators corresponding to helium in a weak homogeneous electric field. This application is carried out in Theorem 2.1. The key assumption of this theorem is that near each isolated eigenvalue, for each integer p, the first p formal perturbation equations do admit solutions.

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In the short Section 3 we consider an abstract perturbation problem and formulate two lemmas. They are versions of two other lemmas formulated elsewhere [21a].

In Section 4 we return to the proof of Theorem 2.1. In Theorem 4.1 we formulate a property of our perturbation problem which allows the application of Lemma 3.2. This yields the validity of the key assumption of Theorem 2.1. Roughly speaking, it describes the effect of each of the electron-nucleus potentials on the helium bound states. For special circumstances Theorem 4.1 was formulated elsewhere [21b]. The novelty of the present Theorem 4.1 is its generality. In particular that it holds for each isolated eigen-value. Its proof uses an elegant observation of Combes [22b] concerning commutators of abstract operators. At the same time we make essential use of Lemma 4.1. The proof of this lemma, in turn, makes essential use of the fact that the electron-electron potential is repulsive.

For related work on spectral concentration we refer to the forthcoming papers of Veselic.

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2. Formulation of the Concentration Theorem

For the unperturbed operator we take the helium-Schrödinger operator. To describe it in more specific terms let $\dot{\mathfrak{C}}_\infty(\mathcal{E}_3)$ denote the class of infinitely differentiable functions with bounded support in $\mathcal{E}_3$, the real Euclidean space of dimension 3. The Schrödinger operator in atomic units [5], corresponding to the helium ion He$^+$, is given on $\dot{\mathfrak{C}}_\infty(\mathcal{E}_3)$ by

$$(\dot{\mathrm{He}}^+)\, f = -\frac{1}{2}\,\Delta f - 2\,M\left(\frac{1}{r}\right) f\,, \quad f \in \dot{\mathfrak{C}}_\infty(\mathcal{E}_3)\,. \tag{2.1}$$

Here and in the following we use a dot to emphasize that a given operator is defined on $\dot{\mathfrak{C}}_\infty(\mathcal{E}_3)$. In equation (2.1) Δ denotes the Laplacian and $M(1/r)$ denotes the operator of multiplication by the function

$$\frac{1}{r}\,(x) = \frac{1}{|x|}\,, \quad x \in \mathcal{E}_3\,.$$

According to Kato [3, 13i] the operator $\dot{\mathrm{He}}^+$ is essentially self-adjoint on $\dot{\mathfrak{C}}_\infty(\mathcal{E}_3)$ and the domain of its closure equals the domain of the closure of Δ. That is

$$\mathfrak{D}(\mathrm{He}^+) = \mathfrak{D}(\Delta)\,.$$

Next define the function q on $\mathcal{E}_6$ by

$$q(x) = ((x_6 - x_3)^2 + (x_5 - x_2)^2 + (x_4 - x_1)^2)^{-1/2} \tag{2.2}$$

and let $M(\dot{q})$ on $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$ be the operator of multiplication by this function. Using the usual notations for the Kroneker product of operators [17], the helium-Schrödinger operator in atomic units is given on $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$ by [5b]

$$\dot{\mathrm{He}} = \dot{\mathrm{He}}^+ \otimes I + I \otimes \dot{\mathrm{He}}^+ + \dot{M}(q)\,, \tag{2.3}$$

where I denotes the identity operator on $\mathfrak{L}_2(\mathcal{E}_3)$. Actually, it would be sufficient to define this operator on

$$\dot{\mathfrak{C}}_\infty(\mathcal{E}_3) \otimes \dot{\mathfrak{C}}_\infty(\mathcal{E}_3) \subset \dot{\mathfrak{C}}_\infty(\mathcal{E}_6) ,$$

but we shall not be concerned with this fact. Remembering definition (2.1), we see that

$$\dot{\mathrm{He}} = -\frac{1}{2}[\dot{\varDelta} \otimes I + I \otimes \dot{\varDelta}] + -2 M\left(\frac{1}{r}\right) \otimes I - 2 I \otimes M\left(\frac{1}{r}\right) + \dot{M}(q) .$$

According to Kato [3, 13g] this operator is essentially self-adjoint on $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$ and the domain of its closure equals the domain of the Laplacian. More specifically for the domains of the closures of these operators we have the following inclusions,

$$\mathfrak{D}(\mathrm{He}) = \mathfrak{D}\,(\varDelta \otimes I + I \otimes \varDelta) , \tag{2.4}$$

$$\mathfrak{D}(\mathrm{He}) \subset \mathfrak{D}\left(M\left(\frac{1}{r}\right) \otimes I\right), \quad \mathfrak{D}(\mathrm{He}) \subset \mathfrak{D}\left(I \otimes M\left(\frac{1}{r}\right)\right), \tag{2.5)^{(1)(2)}$$

$$\mathfrak{D}(\mathrm{He}) \subset \mathfrak{D}(M(q)) . \tag{2.6}$$

For brevity, we shall set

$$M^{(1)}\left(\frac{1}{r}\right) = M\left(\frac{1}{r}\right) \otimes I , \tag{2.7)^{(1)}$$

$$M^{(2)}\left(\frac{1}{r}\right) = I \otimes M\left(\frac{1}{r}\right) \tag{2.7)^{(2)}$$

and

$$\varDelta^{(1,2)} = \varDelta \otimes I + I \otimes \varDelta . \tag{2.8}$$

Note that superscripts correspond to the decomposition

$$\mathfrak{L}_2(\mathcal{E}_6) = \overline{\mathfrak{L}_2(\mathcal{E}_3) \otimes \mathfrak{L}_2(\mathcal{E}_3)} .$$

For the perturbation V we take the operator corresponding to a homogeneous electric field. More specifically it is the closure of the operator $\dot{V}$ given by

$$\dot{V} f(x) = (x_3 + x_6)\, f(x) , \quad x \in \mathcal{E}_6 , \quad f \in \dot{\mathfrak{C}}_\infty(\mathcal{E}_6) . \tag{2.9}$$

We define the family of perturbed operators on $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$ by setting

$$\dot{\mathrm{He}}(\varepsilon) = \dot{\mathrm{He}} + \varepsilon \dot{V} . \tag{2.10}$$

More specifically, we denote by $\mathrm{He}(\varepsilon)$ an arbitrary self-adjoint extension of this operator. Since the operators $\dot{\mathrm{He}}(\varepsilon)$ commute with conjugation, the existence of such an extension is ensured by a theorem of von Neumann [8]. We do not know whether such an extension is unique or not. The corresponding question for the hydrogen Schrödinger operator was treated by Ikebe and Kato [9]. They showed that in this case the extension is unique. Note that at least formally, the operator $\mathrm{He}(\varepsilon)$ is the Schrödinger operator corresponding to the helium atom in a homogeneous electric field of intensity ε [5c].

Next let $H(\varepsilon)$ be a given family of self-adjoint operators acting in an abstract Hilbert space. For a given Borel subset $\mathcal{B}_\varepsilon$ of the real line let $E(\varepsilon, \mathcal{B}_\varepsilon)$ denote the spectral projector of $H(\varepsilon)$ over $\mathcal{B}_\varepsilon$. Following a terminology used elsewhere [11], we shall say that near a given point λ_0, the spectrum of the family of operators $H(\varepsilon)$ is concentrated to order p, if there is a family of sets $\mathcal{B}_\varepsilon$, such that

$$E(\varepsilon, \mathcal{B}_\varepsilon) \to E(0, \{\lambda_0\}) \text{ as } \varepsilon \to 0 ,$$

and

$$|\mathcal{B}_\varepsilon| = o(\varepsilon^p) \text{ at } \varepsilon = 0 .$$

Here, the left member, denotes the Lebesgue measure of $\mathcal{B}_\varepsilon$ and convergence means strong convergence.

After these preparations we return to the family of Schrödinger operators in (2.10). The theorem that follows is our main theorem and it says that near isolated eigen-values of the helium Schrödinger operator the spectra of these operators is concentrated in this technical sense.

Theorem 2.1. *Let the helium Schrödinger operator* He *be defined by equation* (2.3) *and let the family of operators* He(ε) *be defined by equation* (2.8). *Suppose that λ is an isolated point eigen-value of* He. *Then for each positive integer p, near the point λ the spectra of the family of operators* He(ε) *is concentrated to order p.*

According to a theorem obtained by Riddell [14, 13i] and elsewhere [11], the phenomenon of spectral concentration occurs under general circumstances. To describe these circumstances, following Kato [13a], we say that a given subset $\mathfrak{S}$ of $\mathfrak{D}(T)$, is a core of the given operator T if the closure of its restriction to $\mathfrak{S}$ equals T. In particular, if T is essentially self-adjoint on $\mathfrak{S}$ then $\mathfrak{S}$ is a core of T. Using this notion the assumptions of the abstract spectral concentration theorem adapted to our operators, are implied by the following;

λ is an isolated point eigen-value of He *of finite m-multiplicity,* (2.11)

as ε converges to zero, the operators He(ε) *converge strongly to* He *on a set which is a core of the unperturbed operator* He, (2.12)

the first p formal perturbation equations corresponding to the family He(ε) *at the point λ admit m linearly independent solutions for each positive integer p.* (2.13)

Thus to establish Theorem 2.1 it suffices to establish these three conditions.

To verify condition (2.11) we need a theorem of Zhiclin [7] and Hunziker [20]. This says that the essential spectrum of the operator He consists of an interval. Hence each isolated point eigen-value is of finite multiplicity and condition (2.11) follows.

To verify condition (2.12) recall that according to Kato the operator He is essentially self-adjoint on $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$. It is clear from definition (2.10) that for each vector f of this set

$$\lim_{\varepsilon \to 0} \mathrm{He}(\varepsilon)\, f = \mathrm{He}\, f .$$

Hence condition (2.12) follows.

It remains to verify condition (2.13) which we shall do in the two sections that follow.

3. A Sufficient Condition for the Solvability of the Perturbation Equations

Let H and V be possibly unbounded symmetric operators acting in some abstract Hilbert space $\mathfrak{H}$ and assume that the intersection of their domains is dense. Define the family of operators $H(\varepsilon)$ by

$$H(\varepsilon) = H + \varepsilon V \text{ on } \mathfrak{D}(H) \cap \mathfrak{D}(V) . \tag{3.1}$$

Suppose that λ_0 is an isolated point eigen-value of H and formally set

$$\lambda(\varepsilon) \sim \sum_{j=0}^{\infty} \lambda_j \varepsilon^j \tag{3.2}$$

and

$$f(\varepsilon) \sim \sum_{j=0}^{\infty} f_j \varepsilon^j \tag{3.3}$$

and

$$H(\varepsilon) f(\varepsilon) \sim \lambda(\varepsilon) f(\varepsilon) . \tag{3.4}$$

Carrying out the multiplication of the formal power series in this relation and equating the coefficients of the like powers of ε, we obtain the following set of recursive equations,

$$(H - \lambda_0) f_0 = 0 , \tag*{$(3.5)_0$}$$

$$(H - \lambda_0) f_n = \sum_{j=0}^{n} \lambda_j f_{n-j} - V f_{n-1} , \quad n = 1, 2, \ldots . \tag*{$(3.5)_n$}$$

This set of equations is called the set of formal perturbation equations corresponding to the family $H(\varepsilon)$ at the point λ_0. Note that in general $f(\varepsilon)$ is not an eigen-vector and $\lambda(\varepsilon)$ is not eigen-value of $H(\varepsilon)$, in fact such formal power series need not exist. The lemma that follows is a version of a lemma formulated elsewhere [21a] and accordingly we state but do not prove it. It gives sufficient conditions for the solvability of these equations. These conditions are implied by the ones of Riddell [14b].

Lemma 3.1. *Let λ_0 be an isolated point eigenvalue of $\mathfrak{H}$ of finite multiplicity, and let $E\{\lambda_0\}$ denote the spectral-projector over λ_0. Suppose that there is a subset $\mathfrak{S}$ of $\mathfrak{H}$ such that*

$$E\{\lambda_0\} \mathfrak{H} \subset \mathfrak{S} \tag{3.6}$$

and

$$V \mathfrak{S} \subset \mathfrak{S} \tag{3.7}$$

and

$$(\lambda_0 - H + E\{\lambda_0\})^{-1} \mathfrak{S} \subset \mathfrak{S} . \tag{3.8}$$

Then for each positive integer n the first n formal perturbation equations corresponding to the family (3.1) *at λ_0, that is equations* $(3.5)_0$ *through* $(3.5)_n$ *do admit solutions. Furthermore, the number of linearly independent solutions equals* $\dim E\{\lambda_0\} \mathfrak{H}$.

The assumptions of Lemma 3.1 are rather general and it is difficult to verify them for specific operators. The lemma that follows, is again a version of a lemma formulated elsewhere [21a] and accordingly we state but do not prove it. It formulates assumptions which are adapted to our perturbation problem and which imply the main ones of Lemma 3.1. In it $\mathfrak{B}(\mathfrak{H})$ denotes the space of bounded operators defined on all of $\mathfrak{H}$ and $\varrho(T)$ denotes the resolvent set of a given operator T.

Lemma 3.2. *Let the operators $A_{0,1}$, be self-adjoint on the given domains $\mathfrak{D}(A_{0,1})$ in $\mathfrak{H}$ and let λ_0 in $\varrho(A_0)$ be an isolated eigen-value of $A_0 + A_1$ of finite multiplicity with spectral-projector $E\{\lambda_0\}$. Suppose that*

$$A_1 (\lambda_0 - A_0)^{-1} \in \mathfrak{B}(\mathfrak{H}) \,. \tag{3.10}$$

Suppose further that an infinite sequence of sets, $\mathfrak{B}_0 = \mathfrak{H}$, $\mathfrak{B}_1, \ldots$, is given such that for each integer n

$$A_1 (\mathfrak{B}_n \cap \mathfrak{D}(A_1)) \subset \mathfrak{B}_{n+1} \tag*{(3.11)$_n$}$$

and

$$(\lambda_0 - A_0)^{-1} \mathfrak{B}_n \subset \mathfrak{B}_n \,. \tag*{(3.12$_n$)}$$

Then the set

$$\mathfrak{S} = \bigcap_{n=0}^{\infty} \mathfrak{B}_n \tag{3.13}$$

satisfies assumptions (3.6) *and* (3.8) *of Lemma* 3.1 *with reference the operator $H = A_0 + A_1$.*

4. Application of Lemmas 3.1 and 3.2 to the Helium Schrödinger Operator

We start by defining two different splittings of the helium Schrödinger operator and applying the abstract Lemma 3.2 to each of them. To describe these splittings we introduce two operators by setting

$$\dot{F}^{(1)(2)} = \dot{\mathrm{H}}\mathrm{e} - \dot{M}^{(1)(2)} \left(\frac{1}{r}\right) \quad \text{on} \quad \dot{\mathfrak{C}}_\infty(\mathcal{E}_6) \,, \tag*{(4.1)$^{(1)(2)}$}$$

and defining $F^{(1),(2)}$ to be their closures. In analogy with previous notation we also set

$$\dot{M}_l f(x) = x_l f(x) \,, \quad x \in \mathcal{E}_6 \,, \quad f \in \dot{\mathfrak{C}}_\infty(\mathcal{E}_6) \,, \quad l = 1, 2, \ldots, 6 \tag{4.2}$$

and define the operator M_l by closure. Note that subscripts refer to the decomposition

$$\mathfrak{L}_2(\mathcal{E}_6) = \overline{\mathfrak{L}_2(\mathcal{E}_1) \otimes \mathfrak{L}_2(\mathcal{E}_1) \otimes \mathfrak{L}_2(\mathcal{E}_1) \otimes \mathfrak{L}_2(\mathcal{E}_1) \otimes \mathfrak{L}_2(\mathcal{E}_1) \otimes \mathfrak{L}_2(\mathcal{E}_1)} \,.$$

The key fact in the application of the abstract Lemma 3.2 is formulated in the theorem that follows. It extends a result formulated elsewhere for any isolated eigen-value of the hydrogen Schrödinger operator [16] and for the lowest eigen-value of the helium Schrödinger operator [21]. The proof of this theorem is based on an elegant observation of Combes [22b] used in connection with his study of the decay of the eigen-functions. In it as before for a given operator T we denote by $\varrho(T)$ the resolvent set.

Theorem 4.1. *Let the operators $F^{(1),(2)}$ be defined by equations* (4.1)$^{(1)(2)}$. *Suppose that the real number λ is an isolated eigen-value of the helium Schrödinger operator* He. *Then,*

$$\lambda \in \varrho(F^{(1)}) \cap \varrho(F^{(2)}) \tag{4.3}$$

and for each positive integer n

$$(\lambda - F^{(1),(2)})^{-1}\, \mathfrak{D}(M_l^n) \subset \mathfrak{D}(M_l^n)\,. \tag{4.4}^n$$

To verify conclusion (4.3) we need a result of Zhislin [7] and Hunziker [20a]. This says that the essential spectrum of the helium Schrödinger operator is given by

$$\sigma_e(\mathrm{He}) = [\inf \sigma(\mathrm{He}^+), \infty)$$

Hence for the isolated points of the spectrum we have

$$\lambda < \inf \sigma(\mathrm{He}^+) \tag{4.5}$$

At the same time it follows that λ is of finite multiplicity, although we shall not make use of this fact. As is well known [23], under circumstances more general than ours, the spectrum of a Kronecker sum is the sum of the spectra. This yields

$$\sigma\left(-\frac{1}{2}\Delta \otimes I + I \otimes \mathrm{He}^+\right) = [\inf \sigma(\mathrm{He}^+), \infty)\,.$$

Remembering that the operator $M(q)$ is positive we obtain from these relations that

$$\sigma(F^{(1)}) \subset [\inf \sigma(\mathrm{He}^+), \infty) \tag{4.6}$$

Insertion of this relation in (4.5) shows that λ is in $\varrho(F^{(1)})$. A repetition of this argument, that we shall not carry out, shows that λ is also in $\varrho(F^{(2)})$. This establishes the validity of conclusion (4.3).

To verify conclusion $(4.4)^n$ we first note that for each positive integer n

$$(i + M_l)^{-n}\, \mathfrak{L}_2(\mathcal{E}_6) = \mathfrak{D}\,(i + M_l)^n = \mathfrak{D}(M_l^n)\,.$$

Next in analogy with Section 2 we denote by $\mathfrak{B}(\mathfrak{L}_2(\mathcal{E}_6))$ the space of bounded operators defined on all of $\mathfrak{L}_2(\mathcal{E}_6)$. Hence remembering the definition of the product of unbounded operators we see that conclusion $(4.4)^n$ is implied by

$$(i + M_l)^n\, (\lambda - F^{(1),(2)})^{-1}\, (i + M_l)^{-n} \in \mathfrak{B}(\mathfrak{L}_2(\mathcal{E}_6))\,. \tag{4.7}^n$$

To verify the validity of this relation for $n = 1$, following Combes [22b] we note that there is an elementary relation between the commutator of the inverse operator $(\lambda - F^{(1)})^{-1}$ and the commutator of the original operator $(\lambda - F^{(1)})$. Specifically we have

$$[(i + M_l), (\lambda - F^{(1)})^{-1}] = (\lambda - F^{(1)})^{-1}\, [(i + M_l), (\lambda - F^{(1)})]\, (\lambda - F^{(1)})^{-1}, \tag{4.8}$$

on $(\lambda - F^{(1)})\, \dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$.

Remembering definition $(4.1)^{(1)}$ we see that

$$[(i + M_l), (\lambda - F^{(1)})] = [(i - M_l), \Delta^{(1,2)}] \text{ on } \dot{\mathfrak{C}}_\infty(\mathcal{E}_6)\,. \tag{4.9}$$

Combining these two relations we obtain

$$[(i + M_l), (\lambda - F^{(1)})^{-1}] = (\lambda - F^{(1)})^{-1}\, [(i + M_l), \Delta^{(1,2)}]\, (\lambda - F^{(1)})^{-1}, \tag{4.10}^1$$

on $(\lambda - F^{(1)})\, \dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$.

Next we define a set $\mathfrak{C}^{(1)}$ by setting

$$\mathfrak{C}^{(1)} = (i + M_l)\,(\lambda - F^{(1)})\,\dot{\mathfrak{C}}_\infty(\mathcal{E}_6) \tag{4.11^1}$$

and an operator $Q^{(1)}(\lambda)$ on it by setting

$$Q^{(1)}(\lambda) = (\lambda - F^{(1)})^{-1} + (\lambda - F^{(1)})^{-1}\,[(i + M_l)\,,\Delta^{(1,2)}]\,(\lambda - F^{(1)})^{-1}\,(i + M_l)^{-1} \tag{4.12^1}$$

Inserting these two definitions in equation (4.10)[1] we arrive at

$$(i + M_l)\,(\lambda - F^{(1)})^{-1}\,(i + M_l)^{-1} = Q^{(1)}(\lambda) \ \text{ on } \mathfrak{C}^1\,. \tag{4.13^1}$$

The lemma that follows will imply that this set is dense. In it, for a given set $\mathfrak{S}$ we denote by $\bar{\mathfrak{S}}$ its closure.

Lemma 4.1.[2]) *Suppose that the number λ is an isolated eigen-value of the helium Schrödinger operator* He. *Then for each positive integer n*

$$(i + M_l)^n\,(\lambda - F^{(1)(2)})\,\dot{\mathfrak{C}}_\infty(\mathcal{E}_6) = \mathfrak{L}_2(\mathcal{E}_6)^{2})\,. \tag{4.14$^{(1)(2)}$}$$

To verify this lemma we introduce some notations. Let $\mathcal{B}_r$ denote the ball in $\mathcal{E}_6$ of radius r, specifically set

$$\mathcal{B}_r = \{x\colon |x| \leqslant r\,,\ x \in \mathcal{E}_6\}\,.$$

In analogy with previous notation we define the class $\dot{\mathfrak{C}}_\infty(\mathcal{B}_r)$ and the space $\mathfrak{L}_2(\mathcal{B}_r)$. For a given operator T we denote by T_r the $\mathfrak{L}_2(\mathcal{B}_r)$ closure of its restriction to $\dot{\mathfrak{C}}_\infty(\mathcal{B}_r)$. As is well known [13d] a densely defined symmetric operator does admit a closure.

[2]) *Added in proof.*
Since $F^{(1)(2)}$ is essentially self-adjoint on $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$ it follows from conclusion (4.3) of Theorem 4.1 that

$$\overline{(\lambda - F^{(1)(2)})\,\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)} = \mathfrak{L}_2(\mathcal{E}_6)\,.$$

In other words this set is dense. It is an interesting fact observed by McCarthy that the operator $(i + M_l)^n$ need not map any dense subset of its domain onto a dense set. The following counter-example is due to him. For brevity let $n = 1$ and let M denote the multiplication operator on $\mathfrak{L}_2(\mathcal{E}_1)$. Define the set $\mathfrak{M}$ by

$$\mathfrak{M} = \left\{ f\colon f \in \mathfrak{L}_2(\mathcal{E}_1) \text{ and the support of } f \text{ is compact and } \int_{-\infty}^{\infty} f(x)\,dx = 0 \right\}.$$

An elementary argument that we shall not carry out shows that $\mathfrak{M}$ is dense. At the same time we see that for every f in $\mathfrak{M}$ we have

$$\int_{-\infty}^{\infty} (i + M)\,f(x) \cdot \frac{1}{i+x}\,dx = 0\,.$$

In other words the function

$$g(x) = \frac{1}{i-x}$$

is orthogonal to the set $(i + M)\,\mathfrak{M}$. Therefore this set is not dense.

We first maintain that in analogy with relation (4.6) we have

$$\sigma(F_r^{(1)}) \subset [\inf \sigma(\mathrm{He}^+), \infty) \,. \tag{4.16$_r$}$$

For, according to a result of Kato [13g] to each positive number ε there is a number $\gamma(\varepsilon)$ such that for every function f in $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$, in particular in $\dot{\mathfrak{C}}_\infty(\mathcal{B}_r)$,

$$\left\| \left(-2\, M^{(2)} \left(\frac{1}{r} \right) + M(q) \right) f \right\| \leqslant \varepsilon \, \|\Delta^{(1,2)} f\| + \gamma(\varepsilon) \, \|f\| \,. \tag{4.15}$$

In other words, the restriction of the operator on the left is ε-bounded with reference the restriction of the operator on the right. As is well known [13g] the restriction of $\Delta^{(1,2)}$ to $\dot{\mathfrak{C}}_\infty(\mathcal{B}_r)$ is essentially self-adjoint in $\mathfrak{L}_2(\mathcal{B}_r)$. According to a theorem of Rellich and Kato [13e], these two facts together imply that the sum of these two operators is essentially self-adjoint on $\dot{\mathfrak{C}}_\infty(\mathcal{B}_r)$ in $\mathfrak{L}_2(\mathcal{B}_r)$. At the same time it follows that in this case the closure of the sum is the sum of the closures. Remembering definitions $(4.1)^{(1)}$ and (2.1) we obtain the essential self-adjointness of $F_r^{(1)}$ on $\dot{\mathfrak{C}}_\infty(\mathcal{B}_r)$ in $\mathfrak{L}_2(\mathcal{B}_r)$.

We see from this essential self-adjointness that the numerical range of $F_r^{(1)}$ is contained in the closure of the numerical range of its restriction to $\dot{\mathfrak{C}}_\infty(\mathcal{B}_r)$. Since $F^{(1)}$ is essentially self-adjoint on $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$ and $\dot{\mathfrak{C}}_\infty(\mathcal{B}_r)$ is a subset of $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$, we obtain that the closure of the numerical range of $F_r^{(1)}$ is contained in the closure of the numerical range of $F^{(1)}$. In symbols,

$$\overline{\nu(F_r^{(1)})} \subset \overline{\nu(F^{(1)})} \,.$$

It is an elementary consequence of the spectral theorem that the convex hull of the spectrum of a self-adjoint operator is closed and that it equals the closure of the numerical range. Applying this fact to the operator $F^{(1)}$ we obtain,

$$\nu(F^{(1)}) \subset [\inf \sigma(\mathrm{He}^+), \infty) \,.$$

These two relations together yield

$$\overline{\nu(F_r^{(1)}} \subset [\inf \sigma(\mathrm{He}^+), \infty) \,.$$

Combining this relation with the essential self-adjointness of $F_r^{(1)}$ we arrive at the validity of relation (4.15).

Relations (4.5) and (4.15) together imply that λ is the resolvent set of $F_r^{(1)}$. This, in turn, implies that

$$\overline{(\lambda - F^{(1)}) \, \dot{\mathfrak{C}}_\infty(\mathcal{B}_r)} = \mathfrak{L}_2(\mathcal{B}_r) \tag{4.16}$$

if we remember that $F_r^{(1)}$ is essentially self-adjoint on $\dot{\mathfrak{C}}_\infty(\mathcal{B}_r)$ and that on this set the operators $F_r^{(1)}$ and $F^{(1)}$ are equal. Clearly for each positive integer n the restriction of the operator $(i + M_l)^n$ to $\mathfrak{L}_2(\mathcal{B}_r)$ is bounded and admits a bounded inverse. Hence this operator maps a given dense subset of $\mathfrak{L}_2(\mathcal{B}_r)$ onto another dense subset. Inserting this fact in relation (4.10) we obtain

$$\overline{(i + M_l)^n \, (\lambda - F^{(1)}) \, \dot{\mathfrak{C}}_\infty(\mathcal{B}_r)} = \mathfrak{L}_2(\mathcal{B}_r) \,.$$

From this, in turn, we obtain

$$\overline{(i + M_l)^n (\lambda - F^{(1)}) \dot{\mathfrak{C}}_\infty(\mathcal{E}_6)} \supset \bigcup_{r=0}^{\infty} \mathfrak{L}_2(\mathcal{B}_r) \tag{4.17}$$

if we remember that the closure of a union equals the union of the closures and that

$$\bigcup_{r=0}^{\infty} \dot{\mathfrak{C}}_\infty(\mathcal{B}_r) = \dot{\mathfrak{C}}_\infty(\mathcal{E}_6) .$$

Since the right member of (4.10) is dense in $\mathfrak{L}_2(\mathcal{E}_6)$ we arrive at

$$\overline{(i + M_l)^n (\lambda - F^{(1)}) \dot{\mathfrak{C}}_\infty(\mathcal{E}_6)} = \mathfrak{L}_2(\mathcal{E}_6) .$$

That is to say, conclusion $(4.14)^{(1)}$ holds.

Replacing the operator $F^{(1)}$ by $F^{(2)}$ in the present argument we arrive at the validity of conclusion $(4.14)^{(2)}$. This completes the proof of Lemma 4.1.

In conclusion let us remark that this lemma extends a result of Combes [22c], inasmuch as his result shows that the intersection of the ortho-complement of the set in (4.14) with $\mathfrak{D}\,(i + M_l)$ consists of the zero vector only.

We return to the proof of conclusion $(4.4)^1$. First we claim that the closure of the operator $Q^{(1)}(\lambda)$ of definition $(4.12)^{(1)}$ is bounded and it is defined on all of $\mathfrak{L}_2(\mathcal{E}_6)$. That is to say,

$$\overline{Q^{(1)}(\lambda)} \in \mathfrak{B}(\mathfrak{L}_2(\mathcal{E}_6)) . \tag{4.18^1}$$

To verify this relation we first note that

$$[(i + M_l, \Delta^{(1,2)}] = -D_l \ \ on \ \ \dot{\mathfrak{C}}_\infty(\mathcal{E}_6) .$$

Insertion of this fact in definition $(4.12)^1$ yields

$$Q^1(\lambda) = (\lambda - F^{(1)})^{-1} - (\lambda - F^{(1)})^{-1} D_l (\lambda - F^{(1)})^{-1} (i + M_l)^{-1}, \ on \ \mathfrak{C}^1 . \tag{4.19^1}$$

As is well known [13, 18] the operator D_l is bounded with reference to the operator $\Delta^{(1,2)}$. Relations (4.16) and (4.6) together with definition (2.1) show that the operator $F^{(1)}$ is bounded with reference the operator $\Delta^{(1,2)}$. Combining these two facts we obtain

$$\overline{(\lambda - F^{(1)})^{-1} D_l} \in \mathfrak{B}(\mathfrak{L}_2(\mathcal{E}_6)) . \tag{4.20}$$

Inserting this fact in relation $(4.19)^1$ we arrive at the boundedness of $Q^{(1)}(\lambda)$ on $\mathfrak{C}^1$. From this, in turn, we arrive at the validity of relation $(4.19)^1$ if we remember that according to Lemma 4.1 the set $\mathfrak{C}^1$ is dense.

Next we insert relation $(4.18)^1$ in the key equation $(4.13)^1$. This shows that

$$(i + M_l)\ (\lambda - F^{(1)})^{-1}\ (i + M_l)^{-1} \ is\ bounded\ in\ \mathfrak{C}^1 .$$

To complete the proof of relation $(4.7)^1$ we need an observation of Kato [13b]. This implies that if the closure of the operator A on $\mathfrak{A}$ admits a bounded inverse and C on $\mathfrak{C}$ is closable and such that

$$C\,\mathfrak{C} \subset \mathfrak{A} ,$$

then the closure of the product of A and C equals the product of the closures, that is

$$\overline{AC} = \bar{A} \cdot \bar{C} \, .$$

Applying this abstract proposition to

$$A = (i + M_l) \, , \quad \mathfrak{A} = \dot{\mathfrak{C}}_\infty(\mathcal{E}_6) \, ,$$

$$C = (\lambda - F^{(1)})^{-1} (i + M_l)^{-1} \, , \quad \mathfrak{C} = (i + M_l) (\lambda - F^{(1)})^{-1} \dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$$

we obtain that the $\mathfrak{C}^1$-closure of the above triple product equals the product of the closures. Remembering that this triple product is bounded on $\mathfrak{C}^1$ and that $\mathfrak{C}^1$ is dense we arrive at

$$(i + M_l) (\lambda - F^{(1)})^{-1} (i + M_l)^{-1} \in \mathfrak{B}(\mathfrak{L}_2(\mathcal{E}_6)) \, .$$

This establishes the validity of relation $(4.7)^1$ if we observe that in the arguments leading to it the operator $F^{(1)}$ can be replaced by $F^{(2)}$.

To verify relation $(4.7)^n$ in the general case we employ induction on n. We have already seen that it holds for $n = 1$. Accordingly assume that it holds for $n = k - 1$ and we show that it also holds for $n = k$. To verify this we first need a generalization of relation $(4.10)^1$. Specifically we need that for each positive integer k

$$[(i + M_l)^k, (\lambda - F^{(1)})^{-1}] = (\lambda - F^{(1)})^{-1} [i + M_l)^k, \Delta^{(1,2)}] (\lambda - F^{(1)})^{-1} \qquad (4.10)^k$$

on $(\lambda - F^{(1)}) \dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$.

A repetition of the arguments leading to relation $(4.10)^1$ shows the validity of this relation and for brevity we skip the details of the proof. In analogy with definition $(4.11)^1$ define the set $\mathfrak{C}^k$ by

$$\mathfrak{C}^k = (i + M_l)^k (\lambda - F^{(1)}) \dot{\mathfrak{C}}_\infty(\mathcal{E}_6) \, , \qquad (4.11)^k$$

and the operator $Q^{(k)}(\lambda)$ on it by setting

$$Q^{(k)}(\lambda) = (\lambda - F^{(1)})^{-1} + (\lambda - F^{(1)})^{-1} [(i + M_l)^k, \Delta^{(1,2)}] (\lambda - F^{(1)})^{-1} (i + M_l)^{-k} \qquad (4.12)^k$$

Inserting these two definitions in equation $(4.10)^k$ we arrive at

$$(i + M_l)^k (\lambda - F^{(1)})^{-1} (i + M_l)^{-k} = Q^{(k)}(\lambda) \text{ on } \mathfrak{C}^k. \qquad (4.13)^k$$

Remembering definition $(4.11)^k$ we see from Lemma 4.1 that the set $\mathfrak{C}^k$ is dense. Next we maintain that the operator $Q^{(k)}(\lambda)$ is bounded on it. More specifically we maintain that

$$\overline{Q^{(k)}(\lambda)} \in \mathfrak{B}(\mathfrak{L}_2(\mathcal{E}_6)) \, . \qquad (4.18)^k$$

For, it is an elementary fact that

$$[(i + M_l)^k, \Delta^{(1,2)} = -k (i + M_l)^{k-1} D_l - k (k - 1) (i + M_l)^{k-2} \textit{ on } \dot{\mathfrak{C}}_\infty(\mathcal{E}_6) \, .$$

Inserting this fact in definition $(4.12)^k$ we obtain

$$Q^{(k)}(\lambda) = (\lambda - F^{(1)})^{-1} - k (\lambda - F^{(1)})^{-1} (i + M_l)^{k-1} D_l (\lambda - F^{(1)})^{-1} (i + M_l)^{-k}$$

$$- k (k - 1) (\lambda - F^{(1)})^{-1} (i + M_l)^{k-2} (\lambda - F^{(1)})^{-1} (i + M_l)^{-k} \, . \qquad (4.19)^k$$

We see from the induction hypothesis that the third term on the right is a bounded operator. To see the boundedness of the second term, note that

$$[(i + M_l)^{k-1}, D_l] = -(k-1)\,(i + M_l)^{k-2} \text{ on } \dot{\mathfrak{C}}_\infty(\mathcal{E}_6)\,.$$

Hence on $\mathfrak{C}^k$ we have

$$(\lambda - F^{(1)})^{-1}\,(i + M_l)^{k-1}\,D_l\,(\lambda - F^{(1)})^{-1}\,(i + M_l)^{-k} =$$
$$= (\lambda - F^{(1)})^{-1}\,D_l\,(i + M_l)^{k-1}\,(\lambda - F^{(1)})^{-1}\,(i + M_l)^{-k} -$$
$$- (k-1)\,(\lambda - F^{(1)})^{-1}\,(i + M_l)^{k-2}\,(\lambda - F^{(1)})^{-1}\,(i + M_l)^{-k}\,.$$

The induction hypothesis together with relation (4.20) shows that each of the two operators on the right are bounded. Hence the second term on the right of equation $(4.14)^k$ is also bounded and according to the already established conclusion (4.3) so is the first term. Inserting this fact in equation $(4.19)^k$ we arrive at the boundedness of the operator $Q^k(\lambda)$ on $\mathfrak{C}^k$. From this, in turn, we arrive at the validity of $(4.18)^k$. Relation $(4.18)^k$ implies relation $(4.7)^k$ similarly to the way relation $(4.18)^1$ did imply relation $(4.7)^1$. Thus relation $(4.4)^n$ holds for each positive integer n and this establishes the validity of conclusion $(4.7)^n$. This completes the proof of Theorem 4.1.

Next we derive the main Theorem 2.1 from Theorem 4.1 and from the abstract Lemma 3.2. According to the arguments of Section 2 it suffices to verify condition (2.12) only. To verify this, in turn, we first maintain that the assumptions of Lemma 3.2 hold for the pair of operators

$$A_0^{(1)} = F^{(1)} \quad \text{and} \quad A_1^{(1)} = -2\,M^{(1)}\left(\frac{1}{r}\right) \tag{4.21$^{(1)}$}$$

with reference to the sequence of sets

$$\mathfrak{B}^{(1)(k)} = \mathfrak{D}\,(i + M_3)^k \qquad k = 0, 1, 2, \ldots \tag{4.22$^{(1)(k)}$}$$

For, we see from conclusion (4.3) of Theorem 4.1 and from relations (2.4) and $(2.5)^{(1)}$ that

$$M^{(1)}\left(\frac{1}{r}\right)(\lambda - F^{(1)})^{-1} \in \mathfrak{B}(\mathfrak{L}_2(\mathcal{E}_6))\,.$$

That is to say assumption (3.10) holds at each eigen-value λ of the helium Schrödinger operator He. The validity of assumption (3.12) is the statement of the other conclusion of Theorem 4.1. To see the validity of assumption (3.11) we first claim that

$$f \in \mathfrak{D}\left(M^{(1)}\left(\frac{1}{r}\right)\right) \quad \text{implies} \quad M^{(1)}\left(\frac{1}{r}\right) f \in \mathfrak{D}\,(i + M_3)\,. \tag{4.23$^{(1)(1)}$}$$

For, the elementary inequality

$$\frac{1 + x_3^2}{x_1^2 + x_2^2 + x_3^2} \leqslant 1 + \frac{1}{x_1^2 + x_2^2 + x_3^2}$$

yields for each g in $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$,

$$\| (i + M_3 \| M^{(1)} \left(\frac{1}{r}\right) g \|^2 \leqslant \| g \|^2 + \| M^{(1)} \left(\frac{1}{r}\right) g \|^2 . \tag{4.24)^{(1)(1)}$$

Since by definition $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$ is a core for each of these two unbounded closed operators, the validity of $(4.22)^1$ on all of $\mathfrak{D}(M^{(1)}(1/r))$ follows by closure. Next we claim that for each positive integer k and each f in $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$

$$\| (i + M_3)^k M^{(1)} \left(\frac{1}{r}\right) f \|^2 \leqslant \sum_{l=0}^{k-1} \| (i + M_3)^1 f \|^2 + \| M^{(1)} \left(\frac{1}{r}\right) f \|^2 . \tag{4.44)^{(1)(k)}$$

For, evidently for each positive integer l,

$$(i + M_3)^l M^{(1)} \left(\frac{1}{r}\right) = (i + M_3) M^{(1)} \left(\frac{1}{r}\right) (i + M_3)^{l-1}, \text{ on } \dot{\mathfrak{C}}_\infty(\mathcal{E}_6) . \tag{4.25}$$

Hence for f in $\dot{\mathfrak{C}}_\infty(\mathcal{E}_6)$ setting

$$g = (i + M_3)^{l-1} f$$

in relation $(4.22)^1$ we obtain

$$\| (i + M_3)^l M^{(1)} \left(\frac{1}{r}\right) f \|^2 \leqslant \| (i + M_3)^{l-1} f \|^2 + \| M^{(1)} \left(\frac{1}{r}\right) (i + M_3)^{l-1} f \|^2 .$$

The validity of relation $(4.22)^k$ follows by induction if we use relation (4.23) again. From this, in turn, it follows by closure that for each integer k

$$f \in \mathfrak{D}\left(M^{(1)}\left(\frac{1}{r}\right)\right) \cap \mathfrak{D}\left((i + M_3)^k\right) \text{ implies } M^{(1)}\left(\frac{1}{r}\right) f \in \mathfrak{D}\left((i + M_3)^{k+1}\right) . \tag{4.23)^k$$

That is to say assumption (3.11) of Lemma 3.2 holds for the pair of operators $(4.21)^{(1)}$ with reference the sequence of sets of definition $(4.22)^{(1)(k)}$. Thus we see from Lemma 3.2 that setting

$$\mathfrak{S}^{(1)} = \bigcap_{l=0}^{\infty} \mathfrak{D}\, (i + M_3)^l \tag{4.26}$$

we have

$$E\{\lambda\}\, \mathfrak{S}^{(1)} \subset \mathfrak{S} \tag{4.27)^{(1)}$$

and

$$(\lambda - \mathrm{He} + E\{\lambda\})^{-1\,(1)}\, \mathfrak{S} \subset \mathfrak{S}^{(1)} . \tag{4.28)^{(1}$$

A similar argument, that we shall not carry out, shows that Lemma 3.2 applies to the pair of operators

$$A_0^{(2)} = F^{(2)} \text{ and } A_1^{(2)} = -2\, M^{(2)} \left(\frac{1}{r}\right) \tag{4.21)^{(2)}$$

with reference to the sequence of sets

$$\mathfrak{B}^{(2)(k)} = \mathfrak{D}\,(i + M_6)^k \tag{4.22$^{(2)(k)}$}$$

Thus we see from Lemma 3.2 that setting

$$\mathfrak{S}^{(2)} = \bigcap_{l=0}^{\infty} \mathfrak{D}\,(i - M_6)^l \tag{4.26$^{(2)}$}$$

we have

$$E\{\lambda\}\,\mathfrak{S}^{(2)} \subset \mathfrak{S}^{(2)} \tag{4.27$^{(2)}$}$$

and

$$(\lambda - \mathrm{He} + E\{\lambda\})^{-1}\,\mathfrak{S}^{(2)} \subset \mathfrak{S}^{(2)}\,. \tag{4.28$^{(2)}$}$$

Combining definitions $(4.26)^{(1)}$, $(4.26)^{(2)}$ and relations $(4.27)^{(1)}$, $(4.27)^{(2)}$, $(4.28)^{(1)}$, $(4.28)^{(2)}$, we see that setting

$$\mathfrak{S} = \mathfrak{S}^{(1)} \cap \mathfrak{S}^{(2)} \tag{4.26}$$

we have

$$E\{\lambda\}\,\mathfrak{S} \subset \mathfrak{S} \tag{4.27}$$

and

$$(\lambda - \mathrm{He} + E\{\lambda\})^{-1}\,\mathfrak{S} \subset \mathfrak{S}\,. \tag{4.28}$$

In other words, at the isolated eigen-value λ the operator He satisfies the assumptions (3.6) and (3.8) of Lemma 3.1 with reference the set of definition (4.26).

Note that relation (4.27) is a version of a result of Hunziker [20b] inasmuch as our set S is larger than his. Actually he showed that this holds for a class of potentials including the Coulomb potential, but we shall not be concerned with this fact.

Finally we maintain that with reference to this set assumption (3.7) of Lemma 3.1 holds for the perturbation V of definition (2.7). For, suppose that f is in S, which in view of definition (4.26) means that for each positive integer k

$$\int [(1 + x_3^2)^k + (1 + x_6^2)^k]\,|f(x)|^2\,dx \subset \infty\,. \tag{4.29}$$

Since

$$(x_3 + x_6)^2 \leqslant 2\,(x_3^2 + x_6^2)$$

and

$$2\,x_{3,6}^2\,(1 + x_{6,3}^2)^k \leqslant x_{3,6}^4 + (1 + x_{6,3}^2)^{2k}$$

we see that

$$(x_3 + x_6)^2\,[(1 + x_3^2)^k + (1 + x_6^2)^k] \leqslant 2\,[(1 + x_3^2)^{2k} + (1 + x_6^2)^{2k}]\,.$$

Insertion of this inequality in assumption (4.29) yields, for each integer k,

$$\int (x_3 + x_6)^2\,[(1 + x_3^2)^k + (1 + x_6^2)^k]\,|f(x)|^2\,dx \subset \infty\,.$$

Remembering definitions (2.7) and (4.26) this estimate says that $V f$ is in $\mathfrak{S}$. Hence

$$V \mathfrak{S} \subset \mathfrak{S},$$

that is to say, assumption (3.7) holds as we have maintained.

Therefore we can conclude from Lemma 3.1 that for each positive integer n the first n formal perturbation equations corresponding to the family $\mathrm{He}(\varepsilon)$ of definition (2.8) do admit solutions. In other words we have established the validity of condition (2.12). This completes the proof of Theorem 2.1.

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Addendum

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