Self-Adjointness of the Atomic Hamiltonian Operator

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April 19, 2013

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1 Introduction

In the realm of quantum mechanics, one of the most important properties desired is for all operators representing physical quantities to be self-adjoint in the Hilbert space theory. This property of an operator to be self-adjoint is equivalent to saying that the eigenvalue problem is completely solvable for them, that is, that there exists a complete set (discrete or continuous) of eigenfunctions.

Since the operators representing observables in quantum mechanics are typically not everywhere defined unbounded operators, it was a major mathematical problem to clarify whether (on what assumptions) they are self-adjoint. In particular, one of the most important problems of mathematical physics was to show that the Coulomb Hamiltonian (CH) operator of the many-body Schrödinger wave equation was self-adjoint. As a nice anecdote to give to light the difficulty of this problem, the undisputed expert on operator theory, John von Neumann, was unable to prove the self-adjointness of the CH operator. This grand feat

was achieved by Tosio Kato in a landmark paper published in 1951.

In this course paper, I will first review the proper background theory that is used to develop the proof for self-adjointness of the CH operator. I will then proceed with the proof that the CH operator is essentially self-adjoint.

2 Preliminaries

In this section we go over essential definitions and theorems that will be useful for developing and understanding the proof.

It is interesting to note that many of the most important operators which occur in mathematical physics are not bounded. We start with some basic definitions of unbounded operators on Hilbert spaces and some useful properties of unbounded operators on Hilbert spaces.

Definition 2.1: An unbounded **operator** T will only be defined on a dense linear subset of the Hilbert space $\mathcal{H}$. Thus an **operator** on $\mathcal{H}$ is a linear map from its domain, a linear subspace of $\mathcal{H}$, into $\mathcal{H}$. Such a subspace, which we denote by $D(T)$, is called the **domain** of the operator T.

Remark: For the remainder of this paper, we will only consider the domain of opreators to be dense. In order to identify an unbounded operator on $\mathcal{H}$, one must first give the domain on which it acts and then specify how it acts on that subspace.

The next definition was first introduced by von Neumann and it has become quite essential in the study of unbounded operators in mathematical physics and in general.

Definition 2.2: The **graph** of the linear transformation T is the set of pairs

$$\{\langle \varphi, T\varphi \rangle | \varphi \in D(T)\}$$

The graph of T, denoted by $\Gamma(T)$, is thus a subset of $\mathcal{H} \times \mathcal{H}$ which is a Hilbert space with inner product

$$\big(\langle \varphi_1, \psi_1 \rangle, \langle \varphi_2, \psi_2 \rangle\big) = \big(\varphi_1, \varphi_2\big) + \big(\psi_1, \psi_2\big)$$

T is called a **closed** operator if $\Gamma(T)$ is a closed subset of $\mathcal{H} \times \mathcal{H}$.

Definition 2.3: Let T_1 and T be operators on $\mathcal{H}$. If $\Gamma(T_1) \supset \Gamma(T)$, then T_1 is said to be an **extension** of T and we write $T_1 \supset T$. Equivalently, $T_1 \supset T$ if and only if $D(T_1) \supset D(T)$ and $T_1\varphi = T\varphi$ for all $\varphi \in D(T)$

Definition 2.4: An operator T is **closable** if it has a closed extension. Every closable operator has a smallest closed extension, called its **closure**, which we denote by $\overline{T}$.

One should note that a natural way to try to obtain a closed extension of an operator, T, is to take the closure of its graph in $\mathcal{H} \times \mathcal{H}$.

Proposition 2.5: If T is closable, then $\Gamma(\overline{T}) = \overline{\Gamma(T)}$

Proof. Suppose that S is a closed extension of T. Then $\overline{\Gamma(T)} \subset \Gamma(S)$ so if $\langle 0, \psi \rangle \in \overline{\Gamma(T)}$ then $\psi = 0$. Define R with $D(R) = \{\psi | \langle \psi, \phi \rangle \in \overline{\Gamma(T)} \text{ for some } \phi\}$ by $R\psi = \phi$ where $\phi \in \mathcal{H}$ is the unique vector so that $\langle \psi, \phi \rangle \in \overline{\Gamma(T)}$. Then $\Gamma(R) = \overline{\Gamma(T)}$ so R is clsed extension of T. But $R \subset S$ which is an arbitrary closed extension, so $R = \overline{T}$ □

For unbounded operators we can also define the notion of an adjoint operator by extending the definition from the bounded case to the unbounded case.

Definition 2.6: Let T be a densely defined linear operator on $\mathcal{H}$. Let $D(T^*)$ be the set of $\varphi \in \mathcal{H}$ for which there is an $\eta \in \mathcal{H}$ with

$$\big(T\psi, \varphi\big) = \big(\psi, \eta\big) \qquad \text{for all} \quad \psi \in D(T)$$

For each such $\varphi \in D(T^*)$, we define $T^*\varphi = \eta$. $T*$ is called the **adjoint** of T. By the Riesz lemma, $\varphi \in D(T^*)$ if and only if $\big|\big(T\psi, \varphi\big)\big| \leqslant C\|\psi\|$ for all $\psi \in D(T)$. We note that $S \subset T$ implies $T^* \subset S^*$.

For this definition, notice that η needs to be uniquely determined by $\big(T\psi, \varphi\big) = \big(\psi, \eta\big)$ we need the fact that $D(T)$ is dense. Unlike the case of bounded operators, the domain of T^* may not be dense. As a matter of fact it is possible to have $D(T^*) = 0$. If the domain of T^* is dense, then we can define $T^{**} = (T^*)^*$. There is a simple relationship between the notions of adjoint and closure expressed in the next theorem.

Theorem 2.7: Let T be a densely defined operator on $\mathcal{H}$. Then:
(a) T^* is closed.
(b) T is closable if and only if $D(T^*)$ is dense in which case $\overline{T} = T^{**}$.
(c) If T is closable, then $(\overline{T})^* = T^*$.

The proof of Theorem 2.7 can be found in [1] on Pg. 253. I won't prove it here as it is not one of the most important theorems we will be using, but it is ncessary to establish in order to realize properties of unbounded operators.

Definition 2.8: A densely defined operator T on $\mathcal{H}$ is called **symmetric** (or **Hermitian**) if $T \subset T^*$, that is, if $D(T) \subset D(T^*)$ and $T\varphi = T^*\varphi$ for all $\varphi \in D(T)$. Equivalently, T

is symmetric if and only if

$$\big(T\varphi, \psi\big) = \big(\varphi, T\psi\big) \quad \text{for all} \quad \varphi, \psi \in D(T)$$

Definition 2.9: T is called **self-adjoint** if $T = T^*$, that is if and only if T is symmetric and $D(T) = D(T^*)$.

Remark: A symmetric operator is always closable, since $D(T_*) \supset D(T)$ is dense in $\mathcal{H}$. If T is symmetric, T^* is a closed extension of T, so the smallest closed extension T^{**} of T must be contained in T^*. Thus for symmetric operators, we have

$$T \subset T^{**} \subset T^*$$

For closed symmetric operators,

$$T = T^{**} \subset T^*$$

And, for self-adjoint operators,

$$T = T^{**} = T^*$$

As one can see, a closed symmetric operator T is self-adjoint if and only if T^* is symmetric. The distinction between closed symmetric operators and self-adjoint operators is very important for it is only the self-adjoint operators that the spectral theorem holds.

Definition 2.10: A symmetric operator T is called **essentially self-adjoint** if its closure $\overline{T}$ is self-adjoint. If T is closed, a subset $D \subset D(T)$ is called a **core** for T if $\overline{T|_D} = T$. The notation $\overline{T|_D}$ means the closure of T restricted to domain D.

Remark: If T is essentially self-adjoint, then it has one and only one self-adjoint extension, for suppose that S is a self-adjoint extension of T. Then, S is closed and thereby, since $S \supset T, S \supset T^{**}$. Thus, $S = S^* \subset (T^{**})^* = T^{**}$, and so $S = T^{**}$. The converse is also true; namely, if T has one and only one self-adjoint extension, then T is essentially self-adjoint. Since $T^* = \overline{T}^* = T^{***}$, T is essentially self-adjoint if and only if

$$T \subset T^{**} = T^*$$

Let us have some unbounded operator B. We say B is a self-adjoint operator, then to specify A uniquely one need not give the exact domain of B (which is often difficult), but just some core for B.

The following theorem combines the definitions and propositions thus far stated in formulating basic criterion for self-adjointness of unbounded operators. We will state it without proof for general reference and will make use of it when we shall discuss discuss self-adjoint extensions of symmetric operators. Proof can be found in [1] Pg. 256.

Theorem 2.11: Let T be a symmetric operator on $\mathcal{H}$. Then the following three statements are equivalent:
(a) T is self-adjoint
(b) T is closed and $Ker\big(T^* \pm i\big) = \{0\}$
(c) $Ran\big(T \pm i\big) = \mathcal{H}$

Following this theorem, an immediate corollary can be found by formulating the theorem for the case of essentially self-adjointness.

Corollary 2.12: Let T be a symmetric operator on a $\mathcal{H}$. Then the following are equivalent:
(a) T is essentially self-adjoint
(b) $Ker\big(T^* \pm i\big) = \{0\}$
(c) $Ran\big(T \pm i\big)$ are dense

We will directly be using the following proposition in proving the kinetic energy operator term of the CH operator is essentially self-adjoint. This particular proposition will help us show that a multiplication operator for L^2-norm defined for some measurable functions on some measure space with finite measure is self-adjoint and that the spectrum of such an operator is defined as an essential range of the measurable functions. Proof of this proposition can be found in [1] Pg. 260 as we only need this for quick tool.

Proposition 2.13: Let $\langle M, \mu \rangle$ be a measure space with μ a finite measure. Suppose that f is a measurable, real-valued function on M which is finite a.e.$[\mu]$. Then the operator $(T_f) : \varphi \rightarrow f\varphi$ on $L^2(M, \mu)$ with domain

$$D(T_f) = \big\{\varphi | f\varphi \in L^2(M, \mu)\big\}$$

is self-adjoint and the **spectrum** of T_f is the **essential range** of f

The proof of Proposition 2.13 can be done by noting that if T_f is symmetric we can then take some function that is in domain of T_f^* and let T_f^* act on such a function. We can then apply the monotone convergence theorem by defining a cutoff function of the form of the characteristic function $\chi_N(m)$ and multiply that with T_f^*, thereby allowing us to define the norm of T_f^* acting on some function by a limit of $\chi_N(m)T_f^*$ acting on some function.

Now that we have some nice properties and definitions for unbounded operators, specifically for symmetric unbounded operators, we can now discuss both a key point regarding symmetric unbounded operators on some $\mathcal{H}$ and some motivation behind this key point that generated the possibility of the proof of the CH operator being essentially self-adjoint by Kato.

As stated in [4] the reasoning behind discussing symmetric, non-self-adjoint operators arises from the physical reasoning of quantum mechanics. Such reasoning gives a formal

expression for the Hamiltonian of the system; it usually is a partial differental operator on an appropriate L^2 space. By formal, we mean that the domain of such a Hamiltonian is not specified. Even if the domain of the Hamiltonian operator is not defined, it is usually quite easy to find a dense domain on which the formal Hamiltonian is a well-defined and symmetric operator H. We note that, if the closure of H, denoted $\overline{H}$, is self-adjoint then we can use $\overline{H}$ to describe the quantum dynamics occuring (by Stone's theorem). But if $\overline{H}$ is not self-adjoint, then one must ask: Does $\overline{H}$ have self-adjoint extensions? And if it has several, which one shall one choose to generate the dynamics? For the case of several extensions, one can surely note that the extensions can be distinguished by the physics of the system being described. Thus, one can see that the problem of finding the one particular slef-adjoint extension is not just a mathematical objective, but is intimately linked to physics as well.

The study of symmetric operators and their extensions are done by von Neumann's theory of deficiency indices. By von Neumann's theory, one can thus understand when symmetric operators have self-adjoint extensions, and how such extensions are characterized. Kato used the particular conditions set by Neumann's theory of deficiency indices to aid in the development of his proof that the CH operator is essentially self-adjoint. Kato noted that if one imposes a requirement that the entire CH operator is symmetric, this then allows the domain of the operator to not be too artificially restricted. If the domain of the operator was too artificially restricted then one will see that essential self-adjointness of the operator can be lost as the operator could be extended in infinitely many ways. Thus he realized

Definition 2.14: Suppose that A is a symmetric operator. Let

$$\mathcal{K}_{+} = Ker(i - A^*) = Ran(i + A)^{\perp} \tag{2.1}$$

$$\mathcal{K}_{-} = Ker(i + A^*) = Ran(-i + A)^{\perp} \tag{2.2}$$

$\mathcal{K}_{+}$ and $\mathcal{K}_{-}$ are called the **deficiency subspaces** of A. The pair of numbers n_+, n_-, given by $n_+(A) = dim[\mathcal{K}_{+}], n_-(A) = dim[\mathcal{K}_{-}]$ are called the **deficiency indices** of A. The deficiency indices are allowed to be any pair of nonnegative integers and it is possible for n_+ or n_- (or both) to be equal to infinity.

Kato made use of the following Corollary 2.15, by noting that if we know that the CH operator is symmetric (or Hermitian) and real, then CH operator can certainly be extended to a self-adjoint operator. Along with this Corollary, Kato develops a Theorem that we shall state and prove in Section 3 that allows him to utilize this Corollary along with von Neumann's theorem for symmetric operator self-adjoint extensions (Theorem 2.17), to show that CH operator has *only one* self-adjoint extension for a domain that is not too artificially restricted, meaning that he could find a specific *core* such that the CH operator is essentially self-adjoint.

Corollary 2.15: Let A a closed symmetric operator with deficiency indices n_+ and n_-. Then,

(a) A is self-adjoint if and only if $n_+ = 0 = n_-$.
(b) A has self-adjoint extensions if and only if $n_+ = n_-$. There is a one-one correspondence between self-adjoint extension of A and unitary maps from $\mathcal{K}_+$ onto $\mathcal{K}_-$.
(c) If either $n_+ = 0 \neq n_-$ or $n_- = 0 \neq n_+$, then A has no nontrivial symmetric extensions (such operators are called **maximal symmetric**).

The following theorem gives a simple and useful criterion for a symmetric operator to have self-adjoint extensions and is denoted as von Neumann's theorem [4]. Before that we make note of a definition that will be used for the theorem.

Definition 2.16: An antilinear map $C : \mathcal{H} \to \mathcal{H}$ $\big(C\big(\alpha\varphi + \beta\psi\big) = \overline{\alpha}C\varphi + \overline{\beta}C\psi\big)$ is called a **conjugation** if it is norm-preserving and $C^2 = I$.

Theorem 2.17: Let A be a symmetric operator and suppose that there exists a conjugation C with $C : \ D(A) \to D(A)$ and $AC = CA$. Then A has equal deficiency indices and therefore has self-adjoint extensions.

Proof of Theorem 2.17 is found in [4] Pg. 143-144. We only need to state the theorem for our purposes, as we will not be using this result directly, rather we use it as method for orienting our proof of self-adjointness in the right direction.

We now have enough definitions and properties to officially demonstrate that the CH operator is indeed essentially self-adjoint.

3 Essential Self-Adjointness of the Coulomb Hamiltonian Operator

In this section, we will follow what Kato had done for the first few steps in his paper, and outline in detail a few of his arguments that he had developed. We will then prove an equivalently defined CH operator is essentially self-adjoint using a slightly different approach that is essentially what Kato had done. This slightly different approach will enable us to define what Kato potentials are [6], and make use of the most important theorem of this course paper, The Kato-Rellich theorem for perturbation of unbounded operator self-adjoint operators. With this theorem, we will show how the equivalently defined CH operator is essentially self-adjoint.

Definition 1.1: The Coulomb Hamiltonian (CH) for a system of N electrons and A atomic

nuclei may be written as

$$\mathbf{H} = \sum_{g}^{A} \frac{\mathbf{p}_g^2}{2m_g} \; + \; \frac{e^2}{8\pi\epsilon_0} \sum_{1 \leqslant g < h \leqslant A} \frac{Z_g Z_h}{|r_g - r_h|} \; + \; \sum_{i=1}^{N} \left(\frac{\mathbf{p}_i^2}{2m} - \frac{e^2}{4\pi\epsilon_0} \sum_{g=1}^{A} \frac{Z_g}{|r_i - r_g|} \right) + \; \frac{e^2}{8\pi\epsilon_0} \sum_{1 \leqslant i < j \leqslant N} \frac{1}{|r_i - r_j|} \tag{3.1}$$

where the kinetic energy terms are written in terms of the momentum operator and r_i, r_j, r_g are position coordinates respective to ith-,jth-,gth-particle (be it electron or nucleus for each respective index). One can note that each individual term in (3.1) has obvious classical interpretations; the charges and masses of the electrons and nuclei are regarded as parameters to be taken from experimental data. N and A are undetermined positive integers.

As stated earlier, in 1951 Kato [5] had proved that CH, $\mathbf{H}$, is essentially self-adjoint. This property, which is stronger than Hermiticity, guarantees that the time evolution

$$\Psi(t) = e^{\frac{-i\mathbf{H}t}{\hbar}} \Psi(0)$$

of a Schrödinger wavefunction is unitary, and so conserves probability. This is not true for operators that are Hermitian but not self-adjoint. Thirring [8] showed a nice example: the radial momentum operator $-i\hbar\frac{\partial}{\partial r}$ acting on functions $\phi(r), \phi(0) = 0$ with $0 \leqslant r < \infty$.

One of the first steps that Kato did was to separate out the centre-of-mass (COM) motion from (3.1). In classical mechanics it is easy to separate off the COM motion of a system of point masses. Classically the motion of the COM is uncoupled from the other motions. The COM moves uniformly (i.e., with constant velocity) through space as if it were a point particle with mass equal to the sum Mtot of the masses of all the particles.

In quantum mechanics a free particle has as state function a plane wave function, which is a non-square-integrable function of well-defined momentum. The kinetic energy of this particle can take any positive value. The position of the COM is uniformly probable everywhere, in agreement with the Heisenberg uncertainty principle.

All that is needed to remove the COM motion from the full molecular Hamiltonian is a linear point transformation symbolised by

$$(\mathbf{t}\boldsymbol{\xi}) = \mathbf{x}\mathbf{V} \tag{3.2}$$

In (3.2) M_T is the total mass of all the particles in the system, $\mathbf{t}$ is a 3 by $N_T - 1$ matrix ($N_T = N + A$) and $\boldsymbol{\xi}$ is a 3 by 1 matrix, so that the combined (bracketed) matrix on the left of (3.2) is 3 by N_T. $\mathbf{V}$ is an N_T by N_T matrix which, from the structure of the left side of (3.2), has a special last column whose elements are

$$V_{iN_T} = M_T^{-1} m_i, \quad M_T = \sum_{i=1}^{N_T} m_i \tag{3.3}$$

Hence $\boldsymbol{\xi}$ is the standard COM coordinate

$$\boldsymbol{\xi} = M_T^{-1} \sum_{i=1}^{N_T} m_i \mathbf{x}_i \tag{3.4}$$

As the coordinates $\mathbf{t}_j$, $j = 1, 2, \ldots, N_T - 1$ are to be translationally invariant,

$$\sum_{i=1}^{N_T} V_{ij} = 0, \quad j = 1, 2, \ldots, N_T - 1 \tag{3.5}$$

on each remaining column of $\mathbf{V}$ and it is easy to see that (3.5) forces $\mathbf{t}_j \to \mathbf{t}_j$ as $\mathbf{x}_i \to \mathbf{x}_i + \mathbf{a}$ for all i.

The $\mathbf{t}_i$ are independent if the inverse transformation

$$\mathbf{x} = (\mathbf{t}\boldsymbol{\xi})\mathbf{V}^{-1} \tag{3.6}$$

exists. The structure of the right hand side of (3.6) shows that the bottom row of $\mathbf{V}^{-1}$ is special and, WLOG, its elements may be equired to be

$$\left(\mathbf{V}^{-1}\right)_{N_T i} = 1 \qquad i = 1, 2, \ldots, N_T \tag{3.7}$$

The inverse requirement on the remainder of $\mathbf{V}^{-1}$ implies that

$$\sum_{i=1}^{N_T} \left(\mathbf{V}^{-1}\right)_{ij} m_i = 0 \qquad j = 1, 2, \ldots, N_T - 1 \tag{3.8}$$

The Hamiltonian (3.1) in the new coordinates becomes

$$\begin{aligned} \mathbf{H}(\mathbf{t}, \boldsymbol{\xi}) &= -\frac{\hbar^2}{2} \sum_{i=1}^{N_T - 1} \frac{1}{\mu_{ii}} \nabla^2(\mathbf{t}_i) \; - \frac{\hbar^2}{2} \sum_{1 \leqslant g < h \leqslant N_T - 1} \frac{1}{\mu_{ij}} \vec{\nabla}(\mathbf{t}_i) \dot{\nabla}(\mathbf{t}_j) \\ &+ \frac{e^2}{8\pi\epsilon_0} \sum_{1 \leqslant i < j \leqslant N_T} \frac{Z_i Z_j}{r_{ij}} - \frac{\hbar^2}{2M_T} \nabla^2(\boldsymbol{\xi}) \\ &= \mathbf{H}'(\mathbf{t}) - \frac{\hbar^2}{2M_T} \nabla^2(\boldsymbol{\xi}) \end{aligned} \tag{3.9}$$

Here the positive constants $\frac{1}{\mu_{ij}}$ are given by

$$\frac{1}{\mu_{ij}} = \sum_{k=1}^{N_T} m_k^{-1} V_{ki} V_{kj}, \qquad i, j = 1, 2, \ldots, N_T - 1 \tag{3.10}$$

The operator r_{ij} is the interparticle distance operator expressed as a function $\mathbf{t}_i$. Thus

$$r_{ij} = \left(\sum_{\alpha} \left(\sum_{k=1}^{N_T - 1} ((\mathbf{V}^{-1})_{kj} - (\mathbf{V}^{-1})_{ki}) \mathbf{t}_{\alpha k} \right)^2 \right)^{\frac{1}{2}} \tag{3.11}$$

In (3.9) the $\vec{\nabla}(\mathbf{t}_i)$ are grad operators expressed in the cartesian components of $\mathbf{t}_i$ and the last term represents the COM kinetic energy. Since the COM variable does not enter the potential energy term, the COM may be separated off completely so that the eigenfunctions of $\mathbf{H}$ are of the form

$$\mathbf{T}(\boldsymbol{\xi})\boldsymbol{\Psi}(\mathbf{t}) \tag{3.12}$$

where $\boldsymbol{\Psi}(\mathbf{t})$ is a wavefunction for the Hamiltonian $\mathbf{H}'(\mathbf{t})$, Eq. (3.9), which will be referred to as the **translationally invariant** Hamiltonian. It should be emphasized that different choices of $\mathbf{V}$ are unitarily equivalent so that the spectrum of $\mathbf{H}'(\mathbf{t})$ is independent of the particular form chosen for $\mathbf{V}$, provided that it is consistent with (3.3) and (3.5). In particular it is perfectly possible to put the kinetic energy into diagonal form by choosing an orthogonal matrix $\mathbf{U}$ that diagonalizes the positive definite symmetric matrix of dimension N_T-1 formed from the $\frac{1}{\mu_{ij}}$ and then replacing elements of the originally chosen $\mathbf{V}$ according to

$$\mathbf{V}_{ij} \rightarrow \sum_{k=1}^{N_T-1} \mathbf{V}_{ik}\mathbf{U}_{kj}, \qquad j = 1, 2, \ldots, N_T - 1 \tag{3.13}$$

As can be seen from (3.11), the practical problem with any choice of $\mathbf{V}$ is the complicated form given to the potential operator.

In [5], Kato considers only $\mathbf{H}'$ and he actually uses a coordinate system in which the kinetic energy operator can be written in the form

$$\frac{\hbar^2}{2}\sum_{i=1}^{N_T-1}\frac{1}{\mu_{ii}}\nabla^2(\mathbf{r}_i) + \frac{\hbar^2}{2\mu_0}\left|\sum_{i=1}^{N_T-1}|\vec{\nabla}^2(\mathbf{r}_i)|\right|^2 \tag{3.14}$$

where $\mathbf{t}$ is replaced by $\mathbf{r}$ so that it agrees with what Kato used in describing the coordinates. Each individual $\mathbf{r}_i$ is though of as being composed of three caresian coordinates (x_i, y_i, z_i) with $\mathbf{r}_i = \sqrt{(x_i^2 + y_i^2 + z_i^2)}$.

Kato then stated that if μ_0 increases without limit then one can retrieve back $\mathbf{H}$ of (3.1), but having one "particle" less, so that there is no loss of generality in choosing the form $\mathbf{H}'$.

Kato then specifies the potential energy operator as an expressible form

$$\mathbf{V}(\mathbf{r}) = \mathbf{V}'(\mathbf{r}) + \sum_{i=1}^{N_T-1}\mathbf{V}_{0i}(\mathbf{r}) + \sum_{i,j}^{N_T-1}\mathbf{V}_{ij}\big(|\mathbf{r}_i - \mathbf{r}_j|\big) \tag{3.15}$$

Kato states in his paper, "...we cannot expect such an obscure operator to be self-adjoint in the literal sense." He clarifies that $\mathbf{H}'$ (with such a defined potential energy $\mathbf{V(r)}$) has very vague specifications for a differential operator. To remove such vagueness, Kato

notes that one must specify the domain of the operator thereby specifying what sort of functions it is supposed to operator on, and one must specify the behaviour of the potential.

As noted in Section 2, Kato realizes that $\mathbf{H}'$ must be a symmetric (or Hermitian) operator, and that $\mathbf{H}$ can be applied on all functions of the form

$$g(\mathbf{r}) = P(\mathbf{r})exp\left(-\frac{1}{2}\left(\sum_{i=1}^{N_T-1} r_i^2\right)\right)$$

where P is a polynomial.

Observe that this does imply that it can only be applied to such a sort of functions. Rather, it must produce meaningful results when applied to such functions. The reason Kato chooses such functions for his proof is because he wanted to work in momentum space, and such class of functions (Hermite polynomial functions) have nice Fourier transforms. Observe that such class of functions that Kato uses are orthogonal with respect to the weight function measure and thus also form an orthogonal basis of some Hilbert space of functions that satisfy the L^2-norm that is respective to the weight function measure chosen. This class of functions belongs to a Hilbert space $\mathcal{H}$ denoted L^2 of square integrable functions. It is then seen that for $\mathbf{H}'$ to make any sense one must have the product function of $\mathbf{V}g$ must belong to the same HIlbert space.

To ensure such criteria is met, Kato requires that for two real constants C and R

$$\begin{aligned}
&|\mathbf{V}(r)| \leqslant C \\
&\int_{r\leqslant R} |\mathbf{V}_{ij}(\mathbf{r})^2 dxdydz \leqslant C^2 \\
&|\mathbf{V}_{ij}(\mathbf{r})| \leqslant C(r > R)
\end{aligned}$$

with $\mathbf{r} = \sqrt{(x_i^2 + y_i^2 + z_i^2)}$. The Coulomb potential satisfies such conditions this immediately. In fact, all inverse power potentials of the form r^{-m} satisfy such conditions provided that m is positive and $m < \frac{3}{2}$. Such conditions do not hold for inverse square potentials, making relativistic calculations in computations very tricky.

As stated in Section 2, Kato used these requirements to show that it is not necessary to specify the domain of $\mathbf{H}'$ more closely than this, as such conditions on functions and potentials enabled Kato to find a **core** for the operator such that it was not too artificially restricted. Thus, Kato showed that $\mathbf{H}'$ restricted to a core has a unique self-adjoint extension and that this extension gives back the original operator $\mathbf{H}$.

It was quite well-known that the kinetic energy operator alone is indeed self-adjoint because of their classical mechanical experience. In the 1930s M.H.Stone had shown that the multiplicative opeartors of the kind specified above are also self-adjoint but it was not

obvious that the sum of the operators would be self-adjoint because the sum of the operators is defined only on the intersection of their domains.

Through an early variation of his now well-established theorem, the Kato-Rellich theorem, Lemma 4 in [5] showed that for a specific type of potential energy operator $\mathbf{V}$ with a domain that contains the domain of the kinetic energy operator, and for any function f that was in the domain of the full kinetic energy operator, the product of $\mathbf{V}f$ is bounded above by the kinetic energy operator. This means that the Coulomb potential is small compared to the kinetic energy. This then enabled Kato to arrive at his main result of Lemma 5, stating that indeed $\mathbf{H}$ is self-adjoint and is bounded from below.

Rather than expanding the steps in [5] of Kato, I will present a more general and modern account of proving an equivalent formulation of $\mathbf{H}'$ in (3.9) is self-adjoint. First I will show that just the kinetic energy operator is self-adjoint. Second, I will make use of the Kato-Rellich theorem, and the definition of Kato Potentials, and a specific theorem denoted as Kato's theorem in [4] to show that the CH operator is self-adjoint. Thus, the main result of this section can be stated in the following theorem.

Theorem 3.2: Let $\mathbf{x}_1, \ldots, \mathbf{x}_n$ in $\mathbb{R}^3$ be orthogonal coordinates for $\mathbb{R}^{3n}$. Then

$$\boldsymbol{H} = -\sum_{i=1}^{n} \Delta_i - \sum_{i=1}^{n} \frac{ne^2}{|\mathbf{x}_i|} + \sum_{i<j}^{n} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \tag{3.16}$$

is essentially self-adjoint on $C_0^\infty\big(\mathbb{R}^{3n}\big)$.

We first prove that the kinetic energy operator of (3.16), $-\Delta$, is self-adjoint. We first note that $-\Delta$ as an operator on $L^2(\mathbb{R}^n)$, there are two reasonable domains to choose for $-\Delta$,

$$D_{max} = \big\{\varphi \mid \varphi \in L^2(\mathbb{R}^n) \text{ and } -\Delta\varphi \in L^2(\mathbb{R}^n) \text{ in the sense of distributions}\big\} \tag{3.17}$$

$$D_{min} = C_0^\infty\big(\mathbb{R}^n\big) \tag{3.18}$$

We denote $\Delta|_{D_{max}}$ by T_{max} and $\Delta|_{D_{min}}$ by T_{min}

Theorem 3.3: (a) $\varphi \in D_{max}$ if and only if $|\lambda|^2\hat{\varphi}(\lambda) \in L^2\big(\mathbb{R}^n\big)$ and in that case $T_{max}\varphi = \mathscr{F}^{-1}\Big(|\lambda|^2\hat{\varphi}(\lambda)\Big)$.
(b) T_{max} is self-adjoint
(c) T_{min} is essentially self-adjoint and $\overline{T}_{min} = T_{max}$.

Proof. (a) follows immediately from the formula

$$-\widehat{\Delta T} = |\lambda|^2\hat{T}$$

which is valid for arbitrary tempered distributions. By Proposition 2.13 of Section 2, multiplication by $|\lambda|^2$ is self-adjoint on

$$\left\{\varphi \in L^2\big(\mathbb{R}^n\big) |\ |\lambda|^2\varphi \in L^2\big(\mathbb{R}^n\big)\right\}$$

Since $\mathscr{F}$ is unitary and

$$T_{max} = \mathscr{F}^{-1}|\lambda|^2\mathscr{F}$$

T_{max} is self-adjoint on D_{max}.
To prove that T_{min} is essentially self-adjoint it is sufficient to show that

$$T^*_{min} = T_{max}$$

since then

$$\overline{T}_{min} = T^{**}_{min} = T_{max}$$

Suppose that $\psi \in D(T^*_{min})$. Then

$$(-\Delta\varphi, \psi) = (T_{min}\varphi, \psi) = (\varphi, T^*_{min}\psi) \text{ for all } \varphi \in C^\infty_0\big(\mathbb{R}^n\big)$$

Thus $-\Delta\psi \in L^2\big(\mathbb{R}^n\big)$ in the sense of distributions, so $\psi \in D_{max}$ and

$$T^*_{min}\psi = -\Delta\psi = T_{max}\psi$$

Conversely, suppose that $\psi \in D_{max}$. Then

$$-\Delta\psi \in L^2\big(\mathbb{R}^n\big)$$

so that for all $\varphi \in C^\infty_0$,

$$\big(-\Delta\varphi, \psi\big) = \big(\varphi, -\Delta\psi\big)$$

Thus, $\psi \in D(T^*_{min})$ and $T^*_{min}\psi = -\Delta\psi$. □

We denote $-\Delta$ with the domain D_{max} by H_0 and call it the **free Hamiltonian**. We now prove a theorem that gives further properties of the functions in $D(H_0)$ so that we may complete the proof of the self-adjointness of the kinetic energy operator of $\boldsymbol{H}$ of (3.16).

Since H_0 is self-adjoint, its powers H^m_0 are also self-adjoint. Since $H^m_0 = \mathscr{F}^{-1}|\lambda|^{2m}\mathscr{F}$, the domain of H^m_0 is just the Sobolev space W^{2m}. By Sobolev's Lemma (cf.[4] Pg.52) immediately implies:

Proposition 3.4: A vector $\varphi \in L^2\big(\mathbb{R}^n\big)$ is in $C^\infty\big(H_0\big) = \bigcap_{m=1}^\infty D(H^m_0)$ if and only if $\varphi \in C^\infty\big(\mathbb{R}^n\big)$ and $D^\alpha\varphi \in L^2\big(\mathbb{R}^n\big)$ for each α.
More importantly, the vectors in $D(H_0)$ itself have the following properties:

Theorem 3.5: Let $\varphi \in L^2\big(\mathbb{R}^n\big)$ be in $D(H_0)$. Then
(a) If $n \leqslant 3$, φ is a bounded continous function and for any $a > 0$, there is a b, independent of φ, so that

$$\|\varphi\|_\infty \leqslant a\|H_0\varphi\| + b\|\varphi\| \tag{3.19}$$

(b) If $n \geqslant 4$ and $2 \leqslant q < \frac{2n}{(n-4)}$, then $\varphi \in L^q\big(\mathbb{R}^n\big)$ and for any $a > 0$, there is a b (depending only on $q, n,$ and a) so that

$$\|\varphi\|_\infty \leqslant a\|H_0\varphi\| + b\|\varphi\| \tag{3.20}$$

Proof. By the Riemann-Lebesgue lemma and the Plancherel theorem, (a) will follow if we can prove that $\hat{\varphi} \in L^1\big(\mathbb{R}^n\big)$ and

$$\|\hat{\varphi}\|_1 \leqslant a\|\lambda^2\hat{\varphi}\|_2 + b\|\hat{\varphi}\|_2 \tag{3.21}$$

We will prove (3.21) in the case $n = 3$. Suppose $\varphi \in D(H_0)$, then $(1 + \lambda^2)\hat{\varphi}$ and $(1 + \lambda^2)^{-1}$ are in $L^2\big(\mathbb{R}^3\big)$ so $\hat{\varphi} \in L^1\big(\mathbb{R}^3\big)$ and by the Schwarz inequality

$$\|\hat{\varphi}\|_1 \leqslant c\|(\lambda^2 + 1)\hat{\varphi}\|_2 \leqslant c(\|\hat{\varphi}\|_2 + \|\lambda^2\hat{\varphi}\|_2) \tag{3.22}$$

where $c^2 = \int(1 + \lambda^2)^{-2}d\lambda$. For any $r > 0$, let $\hat{\varphi}_r(\lambda) = r^3\hat{\varphi}(r\lambda)$. Then

$$\|\hat{\varphi}_r\|_1 = \|\hat{\varphi}\|_1, \|\hat{\varphi}_r\|_2 = r^{\frac{3}{2}}\|\hat{\varphi}\|_2 \tag{3.23}$$

$$\text{and } \|\lambda^2\hat{\varphi}_r\|_2 = r^{-\frac{1}{2}}\|\lambda^2\hat{\varphi}\|_2 \tag{3.24}$$

Thus, using (3.22) for $\hat{\varphi}_r$, and using (3.23) and (3.24), we obtain

$$\|\hat{\varphi}\|_1 \leqslant cr^{-\frac{1}{2}}\|\lambda^2\hat{\varphi}\|_2 + cr^{\frac{3}{2}}\|\hat{\varphi}\|_2 \tag{3.25}$$

for any $r > 0$. If we choose r large enough, (3.21) follows.

For (b), we use the Hausdorff-Young inequality and the Plancherel theorem, and note that we only need to show that for any p satisfying $\frac{2n}{(n+4)} < p \leqslant 2$ and $a > 0$ there is a b so that

$$\|\hat{\varphi}\|_p \leqslant a\|\lambda^2\hat{\varphi}\|_2 + b\|\hat{\varphi}\|_2 \tag{3.26}$$

The Hölder inequality implies that

$$\|\hat{\varphi}\|_p^p \leqslant \|(1 + \lambda^2)^{-p}\|_r\|(1 + \lambda^2)^p|\hat{\varphi}|^p\|_s \tag{3.27}$$

where $\frac{1}{r} + \frac{1}{s} = 1$. Choosing $s = \frac{2}{p}$, the triangle inequality shows that

$$\|(1 + \lambda^2)^p|\hat{\varphi}|^p\|_s = \big(\|(1 + \lambda^2)|\hat{\varphi}|\|_2\big)^p \tag{3.28}$$

$$\leqslant \big(\|\hat{\varphi}\|_2 + \|\lambda^2\hat{\varphi}\|_2\big)^p \tag{3.29}$$

Thus if $\|(1+\lambda^2)^{-p}\|_{\frac{2}{(2-p}} = c_1 < \infty$, we have

$$\|\hat{\varphi}\|_p \leqslant c_1^{\frac{1}{p}} \left(\|\lambda^2 \hat{\varphi}\|_2 + \|\hat{\varphi}\|_2\right) \tag{3.30}$$

But

$$\|(1+\lambda^2)^{-p}\|_{\frac{2}{(2-p}}^{\frac{2}{(2-p}} = \int \frac{d\lambda}{(1+\lambda^2)^{\frac{2p}{(2-p}}} < \infty \tag{3.31}$$

if $\frac{4p}{(2-p)} > n$, i.e. $if p > \frac{2n}{(4+n}$. The method of proving that the constant in front of $\|\lambda^2\hat{\varphi}\|$ can be chosen arbitrarily small is the same as in part (a). □

The present the following definition that will be used in the Kato-Rellich theorem, and other theorems in this section as well.

Definition 3.6: Let A and B be densely defined operators on a Hilbert space $\mathcal{H}$. We say that B is A-**bounded** if
(i) $D(B) \supset D(A)$
(ii) There exist real numbers a and b such that

$$\|B\varphi\| \leqslant a\|A\varphi\| + b\|\varphi\| \qquad \forall \varphi \in D(A) \tag{3.32}$$

Notice if

$$\|B\varphi\|^2 \leqslant a^2\|A\varphi\|^2 + b^2\|\varphi\|^2 \tag{3.33}$$

then (3.32) holds. On the other hand, if (3.32) holds, then

$$\|B\varphi\|^2 \leqslant a^2\|A\varphi\|^2 + b^2\|\varphi\|^2 + 2ab\|A\varphi\|\|\varphi\| \tag{3.34}$$

Writing $ab = (a\varepsilon)(\frac{b}{\varepsilon})$ we get

$$2ab\|A\varphi\|\|\varphi\| \leqslant a^2\varepsilon^2\|A\varphi\|^2 + \frac{b^2}{\varepsilon^2}\|\varphi\|^2$$

So, (3.32) implies (3.33) with a replaced by $a+\varepsilon$ and b replaced by $b+\frac{1}{\varepsilon}$. Thus the infimum of a over all (a,b) such that (3.32) holds is the same as the infimum of a over all (a,b) such that (3.33) holds. This common infimum is called the **relative bound** of B with respect to A. If this relative bound is 0 we say that B is **infinitesimally small** with respect to A. In verifying (3.32) or (3.33) it is sufficient to do so for all φ belonging to a core of A

We now present the Kato-Rellich theorem. This theorem was proved by Rellich in 1939 and was extensively used by Kato in the 1960's and is now known as the Kato-Rellich theorem.

Theorem 3.7 **(the Kato-Rellich theorem)**: Suppose that A is a self-adjoint, B is symmetric, and B is A-bounded with relative bound $a < 1$. Then $A+B$ is self-adjoint on $D(A)$ and essentially self-adjoint on any core of A. Further, if A is bounded below by M, then $A+B$ is bounded below by $M - max\{\frac{b}{(1-a)}, a|M| + b\}$ where a and b are given by (3.32).

Proof. We will show that $Ran(A + B \pm i\mu_0) = \mathcal{H}$ for some $\mu_0 > 0$. For $\varphi \in D(A)$, we have

$$\|(A + i\mu)\varphi\|^2 = \|A\varphi\|^2 + \mu^2\|\varphi\|^2 \tag{3.35}$$

Letting $\varphi = (A + i\mu)^{-1}\psi$, and rewriting (3.35) (with $\pm = +$) as

$$\|\psi\|^2 = \|A(A + i\mu)^{-1}\psi\|^2 + \mu^2\|(A + i\mu)^{-1}\psi\|^2 \tag{3.36}$$

In particular,

$$\|A(A + i\mu)^{-1}\psi\| \leqslant \|\psi\| \quad \text{and} \quad \|(A + i\mu)^{-1}\psi\| \leqslant \frac{1}{\mu}\|\psi\| \tag{3.37}$$

Therefore, applying (3.32) with $\varphi = (A + i\mu)^{-1}\psi$, we find that

$$\|B(A + i\mu)^{-1}\psi\| \leqslant a\|A(A + i\mu)^{-1}\psi\| + b(A + i\mu)^{-1}\psi\| \tag{3.38}$$

$$\leqslant \left(a + \frac{b}{\mu}\right)\|\psi\| \tag{3.39}$$

Thus, for μ_0 large, $C = B(A+i\mu_0)^{-1}$ has norm less than one, since $a < 1$ by assumption. This implies that -1 is not in the spectrum of C and so $I+C$ is invertible and so $Ran(I+C) = \mathcal{H}$. Also, $Ran(A + i\mu_0) = \mathcal{H}$ since A is self-adjoint. Thus the equation

$$(I + C)(A + i\mu_0)\varphi = (A + B + i\mu_0)\varphi \qquad \text{for} \quad \varphi \in D(A) \tag{3.40}$$

implies that $Ran(A + B + i\mu_0) = \mathcal{H}$. The proof that $Ran(A + B - i\mu_0) = \mathcal{H}$ is the same. Thus by Theorem 2.11 in Section 2, which describes the fundamental criterion for symmetric operators, $A + B$ is self-adjoint on $D(A)$.

If D_0 is a core of A then it follows from (3.32) that $D(\overline{(A + B)|_{D_0}}) \supset D(\overline{A|_{D_0}})$. This shows that $A + B$ is essentially self-adjoint on any core of A.

For proving the semiboundedness statement, let us suppose that $t \in \mathbb{R}$ and $-t < M$. Then $Ran(A + t) = \mathcal{H}$ and the same estimates as before show that $\|B(A + t)^{-1}\| < 1$ if

$$-t < M - max\left\{\frac{b}{(1 - a)}, a|M| + b\right\} \tag{3.41}$$

Thus for such t, $Ran(A + B + t) = \mathcal{H}$ and $(A + B + t)^{-1} = (A + t)^{-1} \times (I + C)^{-1}$ which implies that $-t$ is an element of the resolvent set of $(A + B)$.

□

We come now to Kato's basic application of the Kato-Rellich theorem to $\boldsymbol{H}$ defined in Theorem 3.2. First, we define some new classes of functions.

Definition 3.8: Let $\langle M, \mu \rangle$ be a measure space. The set of measurable functions f on M which can be written $f = f_1 + f_2$ where $f_1 \in L^r\big(M, d\mu\big)$ and $f_2 \in L^s\big(M, d\mu\big)$ will be denoted by $L^r\big(M, d\mu\big) + L^s\big(M, d\mu\big)$.

In [4], it is stated that one needs a theorem that describes the behavior of the potential energy term of $\boldsymbol{H}$ when it is an element of $L^2\big(\mathbb{R}^3\big) + L^2\big(\mathbb{R}^3\big)$ which is always true for Coulomb type potentials as we shall see shortly. The reason V is in this space has to do with how Kato expressed the potential energy operator in an expressible form (3.15), splitting it into essentially a sum of three terms. Before we dive into the theorem that shows $-\Delta + \mathbf{V(x)}$ is essentially self-adjoint on D_{min} defined when proving the free Hamiltonian is self-adjoint (Theorem 3.3), we give a very useful definition that will help us place more general conditions on the potential energy operator.

Definition 3.9 **(Kato Potentials)**: Let $X = \mathbb{R}^n$ for some n. A locally L^2 real-valued function on X is called a **Kato Potential** if for any $\alpha > 0$ there is $\beta = \beta(\alpha)$ such that

$$\|V\varphi\| \leqslant \alpha\|\Delta\varphi\| + \beta\|\varphi\| \tag{3.42}$$

for all $\varphi \in C_0^\infty$. Clearly the set of all Kato potentials on X form a real vector space.

Lemma 3.10: We prove that $V \in L^2\big(\mathbb{R}^3\big)$ is a Kato potential, which is apart of the proof of Theorem 3.11.

Proof. Suppose that $X = \mathbb{R}^3$ and $V \in L^2(X)$. We claim that V is a Kato potential. Indeed,

$$\|V\varphi\| := \|V\varphi\|_2 \leqslant \|V\|_2\|\varphi\|_\infty \tag{3.43}$$

So, we will be done if we show that for any $a > 0$ there is a $b > 0$ such that

$$\|\varphi\|_{/infty} \leqslant \|\Delta\varphi\|_2 + b\|\varphi\|_2 \tag{3.44}$$

By the Fourier inversion formula, we have

$$\|\varphi\|_\infty \leqslant \|\hat{\varphi}\|_1 \tag{3.45}$$

where $\hat{\varphi}$ denotes the Fourier transform of φ. Now the Fourier transform of $\Delta\psi$ (it's just a positive version of our free Hamiltonian, it is easily changeable to negative depending on how you physically view the system) is the function

$$\xi \mapsto \|\xi\|^2\|\hat{\varphi}(\xi)\| \tag{3.46}$$

where $\|\xi\|$ denotes the Euclidean norm of ξ. Since $\hat{\varphi}$ belongs to the Schwartz space $\mathcal{S}$, the function

$$\xi \mapsto (1 + \|\xi\|^2)\|\hat{\varphi}(\xi)\| \tag{3.47}$$

belongs to L^2 as does the function $\xi \mapsto (1+\|\xi\|^2)^{-1}\|\hat{\varphi}(\xi)\|$ in three dimensions. Let λ denote the function $\xi \mapsto \|\xi\|$. By the Cauchy-Schwarz inequality we have (basically following the proof from Theorem 3.5)

$$\|\hat{\varphi}\|_1 = |((1+\lambda^2)^{-1}, (1+\lambda^2)\hat{\varphi}) \leqslant c\|(\lambda^2+1)\hat{\varphi}\| \leqslant c\|\lambda^2\hat{\varphi}\|_2 + c\|\hat{\varphi}\|_2 \tag{3.48}$$

where

$$c^2 = \|(1+\lambda^2)^{-1}\|_2 \tag{3.49}$$

As in Theorem 3.5, for any $r > 0$ and any function $\psi \in \mathcal{S}$ let ψ_r be defined by

$$\hat{\phi}_r(\xi) = r^3\hat{\phi}(r\xi) \tag{3.50}$$

Then

$$\|\hat{\psi}_r\|_1 = \|\hat{\psi}\|_1, \quad \|\hat{\psi}_r\|_2 = r^{\frac{3}{2}}\|\hat{\psi}\|_2, \quad \textit{and} \quad \|\lambda^2\hat{\psi}_r\|_2 = r^{-\frac{1}{2}}\|\lambda^2\hat{\psi}\|_2 \tag{3.51}$$

Applied to φ this gives

$$\|\hat{\varphi}\|_1 \leqslant cr^{-\frac{1}{2}}\|\lambda^2\hat{\phi}\|_2 + cr^{\frac{3}{2}}\|\hat{\phi}\|_2 \tag{3.52}$$

By Plancherel theorem

$$\|\lambda^2\hat{\phi}\|_2 = \|\Delta\varphi\|_2 \quad \textit{and} \quad \|\hat{\varphi}\|_2 = \|\varphi\|_2 \tag{3.53}$$

□

This shows that any $V \in L^2(\mathbb{R}^3)$ is a Kato potential. We also note that for $V \in L^infty(X)$, that

$$\|V\varphi\|_2 \leqslant \|V\|_\infty\|\varphi\| \tag{3.54}$$

If we put these two Kato potentials together, we see that if $V = V_1 + V_2$ where $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$ then V is a Kato potential. Now we state and prove Theorem 3.10. Theorem 3.10 essentially is utilizes the notion of Kato potential, hence why we defined it first, for generality purposes.

Theorem 3.11: Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ be real-valued. Then $-\Delta + V(\mathbf{x})$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ and self-adjoint on $D(-\Delta)$.

Proof. Since V is real-valued, the opeartor of multiplication by V is self-adjoint on

$$D(V) = \{\varphi | \varphi \in L^2(\mathbb{R}^3), V\varphi \in L^2(\mathbb{R}^3)\} \tag{3.55}$$

Let $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$. Then

$$\|V\varphi\|_2 \leqslant \|V_1\|_2\|\varphi\|_\infty + \|V_2\|_\infty\|\varphi\|_2 \tag{3.56}$$

so $D(V) \supset C_0^\infty(\mathbb{R}^3)$. By Theorem 3.5 and more relevantly, Lemma 3.10, given any $a > 0$, there is $b > 0$ so that

$$\|\varphi\|_\infty \leqslant a\|\Delta\varphi\|_2 + b\|\varphi\|_2 \tag{3.57}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^3)$. This inequality and (3.56) give

$$\|V\varphi\|_2 \leqslant a\|V_1\|_2\| - \Delta\varphi\|_2 + \big(b + \|V_2\|_\infty\big)\|\varphi\|_2 \tag{3.58}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^3)$. Thus V is $-\Delta$-bounded with arbitrarily small bound on $C_0^\infty(\mathbb{R}^3)$. Since $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$, then by the Kato-Rellich theorem (Theorem 3.7) implies that $-\Delta + V$ is also essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ □

We note that Coulomb type potentials satisfy this Lemma 3.9 and Theorem 3.11.

The function

$$V(\mathbf{x}) = \frac{}{\|\mathbf{x}\|} \tag{3.59}$$

on $\mathbb{R}^3$ can be written as a sum $V = V_1 + V_2$ where $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$ and so is a Kato potential.

Suppose that $X = X_1 \oplus X_2$ and V depends only on the X_1 component where it is a Kato potential. Then by Fubini's theorem implies that V is a Kato potential if and only if V is a Kato potential on X_1. So, if $X = \mathbb{R}^{3n}$ and we write $\mathbf{x} \in X$ as $\mathbf{x} = (r_1, \ldots, x_N)$ where $x_i \in \mathbb{R}^3$ then

$$V_{ij} = \frac{1}{\|x_i - x_j\|} \tag{3.60}$$

are Kato potentials as are any linear combination of them. So, the total Coulomb potential of any system of charged partiles is a Kato potential. We note that $\boldsymbol{H}$ is the translationally invariant, and separated operator. Thus the restriction of this potential to the subspace $\{\mathbf{x}|\sum m_i x_i = 0\}$ is a Kato potential. This is the "atomic potential" about the COM.

We now come down to the final theorem that will now aid in synthesizing everything we've done in this Section and thereby proving Theorem 3.2. The theorem is called Kato's theorem as mentioned in [4]. This is the main synthetic argument that Kato implements to imply that $\boldsymbol{H}$ in (3.16) is self-adjoint.

Theorem 3.12 **(Kato's theorem)**: Let $\{V_k\}_{k=1}^m$ be a collection of real-valued measurable functions each of which is in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Let $V_k(\mathbf{y}_k)$ be the multiplication operator on $L^2(\mathbb{R}^{3n})$ obtained by choosing $\mathbf{y}_k$ to be three coordinates of $\mathbb{R}^{3n}$. Then $-\Delta + \sum_{k=1}^m V_k(\mathbf{y}_k)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3n})$, where Δ denotes the Laplacian on $\mathbb{R}^{3n}$.

Proof. First we consider one of the functions V_k separately. By rotation of variables we may assume the variables in $V_k(\cdot)$ are x_1, x_2, x_3. (This is because $\|\cdot\|_2, \|\cdot\|_\infty$, and $-\Delta$ are invariant under rotations of coordinates.) Let Δ_1 denote the Laplacian with respect to x_1, x_2, x_3. By the estimate (3.57), together with the "equivalence" of the bounds in (3.32) and (3.33), we

have for all $\varphi \in C_0^\infty(\mathbb{R}^{3n})$,

$$\begin{aligned}\|V_k\varphi\|^2_{L^2\left(\mathbb{R}^{3n}\right)} \leqslant & a^2 \int |-\Delta_1\varphi(x_1,\ldots,x_{3n}|^2 dx_1\cdots dx_{3n} \\ & + b^2 \int |\varphi(x_1,\ldots,x_{3n})|^2 dx_1\cdots dx_{3n}\end{aligned} \tag{3.61}$$

$$= a^2 \int \left|\sum_{i=1}^{3} p_i^2 \hat{\varphi}(p_1,\ldots,p_{3n})\right|^2 dp_1\cdots dp_{3n} + b^2\|\varphi\|^2 \tag{3.62}$$

$$\leqslant a^2 \int \left|\sum_{i=1}^{n} p_i^2 \hat{\varphi}(p_1,\ldots,p_{3n})\right|^2 dp_1\cdots dp_{3n} + b^2\|\varphi\|^2 \tag{3.63}$$

$$= a^2\|-\Delta\|^2 + b^2\|\varphi\|^2 \tag{3.64}$$

Thus, using the Schwarz inequality, one easily concludes that

$$\left\|\sum_{k=1}^{m} V_k(\mathbf{y}_k)\varphi\right\|^2 \leqslant m^2a^2\|-\Delta\varphi\|^2 + m^2b^2\|\varphi\|^2 \tag{3.65}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^{3n})$. Since a may be chosen as small as we like, we conclude that $\sum_{k=1}^m V_k(\mathbf{y}_k)$ is infinitesimally small with respect to $-\Delta$. Thus, by the Kato-Rellich theorem, $-\Delta + \sum_{k=1}^m V_k(\mathbf{y}_k)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$

□

The proof that $\boldsymbol{H}$ is essentially self-adjoint on $C_0^\infty\left(\mathbb{R}^{3n}\right)$ follows from Theorem 3.12 by just inducting the argument for all V_k and substituting $n = 3n$ in $C_0^\infty(\mathbb{R}^n)$ the core of $-\Delta$.

4 Concluding Remarks

The self-adjointness of the Coulomb Hamiltonian operator was one of the most foundational properties that needed to be established in many-body quantum physics and quantum chemistry, as a lot of pertinent calculations and experimental treatments of the subject relied on it. One may still ask, why worry about this property of the Coulomb Hamiltonian being essentially self-adjoint? Well if the operator is not self-adjoint then it could support solutions interpretable as a particle falling into a singularity or getting to infinity in a finite time, and these are unacceptable as physical solutions. Another reason is that now one can apply von Neumann's spectral theory for unbounded operators, thereby developing some mathematical and physical understanding of the system.

References

[1] *Methods of Modern Mathematical Physics-Functional Analysis Vol. 1*, Michael Reed and Barry Simon, 1980

[2] *John Von Neumann: Selected Letters*, Miklos Redei, 2005, Pg. 14-25

[3] *The Fundamental Principles of Quantum Mechanics*, Edwin C. Kemble, 1937, Pg. 196-215

[4] *Methods of Modern Mathematical Physics-Fourier Analysis, Self-Adjointness Vol. 2*, Michael Reed and Barry Simon, 1975

[5] *Fundamental Properties of Hamiltonian Operators of Schrodinger Type*, Tosio Kato, Transactions of the American Mathematical Society, 1951, Pg. 195-211 `http://www.jstor.org/stable/1990366`

[6] *Bound States and Scattering States, The Kato-Rellich Theorem, Kato Potentials*, Shlomo Sternberg, `http://isites.harvard.edu/fs/docs/icb.topic255424.files/212b0811handout.pdf`

[7] *What Mathematicians know about the solutions of Schrodinger Coulomb Hamiltonian. Should chemists care?*, Brian T. Sutcliffe, Journal of Mathematical Chemistry, Volume 44, Pg. 988-1008 `http://link.springer.com/content/pdf/10.1007%2Fs10910-008-9358-7.pdf`

[8] *Schrdinger, Centenary Celebrations of a Polymath*, Walter Thirring, Cambridge University Press, Pg. 65, 1987