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RECURSIVITY IN QUANTUM MECHANICS

BY

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ABSTRACT. The techniques of effective descriptive set theory are applied to the mathematical formalism of quantum mechanics in order to see whether it actually provides effective algorithms for the computation of various physically significant quantities, e.g. matrix elements. Various Hamiltonians are proven to be recursive (effectively computable) and shown to generate unitary groups which act recursively on the Hilbert space of physical states. In particular, it is shown that the n-particle Coulombic Hamiltonian is recursive, and that the time evolution of n-particle quantum Coulombic systems is recursive.

Introduction. Computable analysis [**1**] and effective descriptive set theory [**3**] study mathematical processes to see whether they can be done effectively, e.g. by computer programs. Kreisel [**2**] has raised the possibility of applying these branches of mathematics to mathematical physics. Since the goal of physics is to be able to predict phenomena, it is of interest to see whether physical theories provide effective algorithms for making quantitative predictions. In Kreisel's words, "We consider theories, by which we mean such things as classical or quantum mechanics, and ask *if every sequence of natural numbers or every real number which is well defined* (observable) *according to the theory must be recursive*, or, more generally, *recursive in the data* (which, according to the theory, determine the observations considered)."

In [**4**], Pour-El and Richards study the classical wave equation in $\mathbf{R}^3$ and show that even when recursive initial conditions are given the solution may not be a recursive function. In this paper I will show, among other things, that the quantum-mechanical Coulombic Hamiltonian

$$H = -\sum_{i=1}^{n} \frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_{1\leq i<j\leq n} \frac{q_i q_j}{|\vec{x}_i - \vec{x}_j|}$$

generates a unitary group $\exp(-iHt/\hbar)$ which acts on $L^2(\mathbf{R}^{3n})$ in a manner that is recursive in the data m_i, q_i, $\hbar$. Since I deal with wave-functions as vectors in $L^2(\mathbf{R}^{3n})$ rather than pointwise-defined continuous functions, nonrecursivity of the type found by Pour-El and Richards, in which the solutions of the classical wave equations are not computable on certain sets of measure zero in $\mathbf{R}^3$, cannot occur. Treating wave-functions as vectors in a Hilbert space would be artificial in the context of the classical wave equation, but this is natural in the framework of quantum mechanics, where the expectation values of all observables depend only on the vector in Hilbert space representing the physical state. Thus it seems as if nonrecursivity may

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be less of a problem in quantum mechanics than in classical mechanics. There are, however, interesting unresolved questions about the recursivity of spectra of quantum-mechanical Hamiltonians, which I will discuss in the Conclusion.

Preliminaries. In this section I will introduce the Kleene pointclasses and recursive functions on recursively presented separable metric spaces. Moschovakis discusses this material in detail in [3], so I will follow his definitions and notation closely.

Let M be a separable metric space with metric $d\colon M \times M \to \mathbf{R}$. A "recursive presentation" of M is a dense sequence of points $(r_i)_{i \in \mathbf{N}}$ of M such that the relations

$$d(r_i, r_j) \leqslant m/(k+1) \quad \text{and} \quad d(r_i, r_j) < m/(k+1)$$

are recursive. (Requiring that $d(r_i, r_j) < m/(k+1)$ and $d(r_i, r_j) > m/(k+1)$ be recursively enumerable relations is in fact sufficient, but this need not concern us here.) The recursively presented space will be denoted either by the ordered pair $(M, (r_i))$ or simply by M.

Given a recursively presented space, we can enumerate a base for its topology as follows. Let $(p_i)_{i \in \mathbf{N}}$ be the sequence of prime numbers in increasing order, and define

$$\langle k_0, \dots, k_n \rangle = p_0^{k_0+1} \cdots p_n^{k_n+1}$$

so that $\langle \cdot \rangle$ effectively assigns a unique integer to each finite sequence of integers. Next define

$$(a)_i = \begin{cases} k_i & \text{if } a = \langle k_0, \dots, k_n \rangle \text{ for some } k_0, \dots, k_n, \\ 0 & \text{otherwise,} \end{cases}$$

so that $\Phi_n\colon \mathbf{N} \to \mathbf{N}^{n+1}$ defined by

$$\Phi_n(a) = ((a)_0, \dots, (a)_n)$$

is onto (though not one-to-one). Then given the recursively presented space $(M, (r_i))$, defining

$$B_k(M, (r_i)) = \{ x \in M \colon d(r_{(k)_0}, x) < (k)_1 / ((k)_2 + 1) \}$$

gives an enumerated base of balls $(B_k(M, (r_i)))_{k \in \mathbf{N}}$ for the topology of M.

Given recursively presented spaces $(M_0, (r_i^0)), \dots, (M_n, (r_i^n))$ with metrics $d_k\colon M_k \times M_k \to \mathbf{R}$, the product space $M_0 \times \cdots \times M_n$ is a separable metric space when given the metric d defined by

$$d((x_0, \dots, x_n), (y_0, \dots, y_n)) = \sum_{k=0}^{n} d_k(x_k, y_k).$$

$M_0 \times \cdots \times M_n$ has a canonical recursive presentation $((r^0 \otimes \cdots \otimes r^n)_i)$ given by

$$(r^0 \otimes \cdots \otimes r^n)_i = \left(r^0_{(i)_0}, \dots, r^n_{(i)_n} \right)$$

(cf. [3, Exercise 3B.3]).

We will take $(0, 1, 2, \dots)$ as a recursive presentation of $\mathbf{N}$ with the metric

$$d(i, j) = \begin{cases} 0 & \text{if } i = j, \\ 1 & \text{if } i \neq j. \end{cases}$$

We will take (q_i) as a recursive presentation of **R**, where

$$q_i = (-1)^{(i)_0}(i)_1/((i)_2 + 1),$$

and we will consider **C** to be $\mathbf{R} \times \mathbf{R}$ so that it gets the canonical recursive presentation (c_i), where

$$c_i = q_{(i)_0} + \sqrt{-1}\, q_{(i)_1}.$$

A set $S \subseteq M$ is said to be "semirecursive" with respect to the recursive presentation (r_i) of M if for some recursive $f: \mathbf{N} \to \mathbf{N}$

$$S = \bigcup_{n \in \mathbf{N}} B_{f(n)}(M, (r_i)).$$

The class of semirecursive subsets of M is denoted by $\Sigma_1^0(M)$, and the class of sets of the form

$$\{x \in M : \exists n[(x, n) \notin S]\},$$

where $S \in \Sigma_n^0(M \times \mathbf{N})$, is denoted by $\Sigma_{n+1}^0(M)$. The class of sets with $M - S \in \Sigma_n^0(M)$ is denoted by $\Pi_n^0(M)$. Also, we write

$$\Delta_n^0(M) = \Pi_n^0(M) \cap \Sigma_n^0(M).$$

Σ_n^0, Π_n^0, and Δ_n^0 are known as the "Kleene pointclasses" and satisfy the inclusions:

$$\begin{array}{ccccccc} \Delta_1^0 & \subsetneq & \Sigma_1^0 & \subsetneq & \Delta_2^0 & \subsetneq & \Sigma_2^0 \cdots \\ & \subsetneq & \Pi_1^0 & \subsetneq & & \subsetneq & \Pi_2^0 \cdots \end{array}$$

In the case $M = \mathbf{N}$ this is just the arithmetical hierarchy.

Given $f: M \to N$, where $(M, (r_i))$ and $(N, (s_i))$ are recursively presented spaces, the "neighborhood (nbhd) diagram" of f, a set $G^f \subseteq M \times \mathbf{N}$, is defined by

$$G^f = \{(x, k) : f(x) \in B_k(N, (s_i))\}.$$

We say f is "Σ_n^0-recursive" if $G^f \in \Sigma_n^0(M \times \mathbf{N})$, and if f is Σ_1^0-recursive we say simply that f is "recursive." (If $f: \mathbf{N} \to \mathbf{N}$, this definition of "recursive" coincides with the usual definition.) If $f: M \to N$ is recursive, we can effectively compute arbitrarily good approximations to $f(x)$ by choosing n and searching for k such that $f(x) \in B_k(N)$ and $B_k(N)$ has radius less than $1/n$. Note that recursive functions are always continuous, since their nbhd diagrams must be open.

Recursive real-valued functions can be characterized as follows:

PROPOSITION 1. *$f: M \to \mathbf{R}$ is recursive iff the relation*

$$q_i < f(x) < q_j$$

is semirecursive as a subset of $M \times \mathbf{N}^2$ (cf. [3, Exercise 3D.9]). □

In [1], many standard real and complex functions are proved to be recursive. From now on we shall use such results without special mention.

The following closure properties are extremely useful and will also be used without special mention.

PROPOSITION 2. *Let Γ be a Kleene pointclass. If $S, T \in \Gamma(M)$ then $S \cup T \in \Gamma(M)$ and $S \cap T \in \Gamma(M)$. If $S \in \Gamma(M \times \mathbf{N})$ then*

$$\{(x, n) : \exists k \leq n[(x, k) \in S]\} \in \Gamma(M \times \mathbf{N})$$

and

$$\{(x, n) : \forall k \leq n[(x, k) \in S]\} \in \Gamma(M \times \mathbf{N}).$$

If $f: M \to N$ is recursive and $S \in \Gamma(N)$, $f^{-1}(S) \in \Gamma(M)$. Also, if $S \in \Sigma_n^0(M \times \mathbf{N})$,

$$\{x : \exists n[(x, n) \in S]\} \in \Sigma_n^0(M)$$

and if $S \in \Pi_n^0(M \times \mathbf{N})$

$$\{x : \forall n[(x, n) \in S]\} \in \Pi_n^0(M)$$

Lastly, $S \in \Delta_n^0(M)$ implies $M - S \in \Delta_n^0(M)$ (cf. [3, Corollary 3E.2]). □

PROPOSITION 3. *If $f: M \to N$ and $g: N \to O$ are Σ_n^0-recursive, then $g \circ f: M \to O$ is Σ_n^0-recursive (cf. [3, Theorem 3D.4]).* □

PROPOSITION 4. *$f: M \to N_0 \times \cdots \times N_k$ is Σ_n^0-recursive iff $f(x) = (f_0(x), \ldots, f_k(x))$ for some Σ_n^0-recursive functions $f_i: M \to N_i$, $0 \leq i \leq k$ (cf. [3, Theorem 3D.3]).* □

The following propositions will also be useful:

PROPOSITION 5. *The metric $d: M \times M \to \mathbf{R}$ is recursive for any recursively presented space M (cf. [3, Exercise 3D.10]).* □

PROPOSITION 6. *The sequence (r_i) considered as a function from $\mathbf{N}$ to M is recursive for any recursively presented space $(M, (r_i))$ (cf. [3, Exercise 3D.8]).* □

Recursive operators. Operators occuring in quantum mechanics are often given in the form $A : D(A) \to L^2(\mathbf{R}^n)$, where $D(A)$ is a "core" for A, i.e. a dense subspace of $L^2(\mathbf{R}^n)$ on which A is essentially selfadjoint. "Weighted Sobolev spaces" will be useful because they are cores for some important operators. If $r, s \in \mathbf{N}$ and $\varphi : \mathbf{R}^n \to \mathbf{C}$ is measurable with a well-defined Fourier transform $\hat{\varphi} : \mathbf{R}^n \to \mathbf{C}$, and

$$\|\varphi\|_{r,s} = \int_{\mathbf{R}^n} (1 + |x|^2)^r |\varphi(x)|^2 \, dx + \int_{\mathbf{R}^n} (1 + |x|^2)^s |\hat{\varphi}(x)|^2 \, dx$$

is finite, we say φ is in the "weighted Sobolev space" $W_{r,s}(\mathbf{R}^n)$.

The spaces $W_{0,s}(\mathbf{R}^n)$ are often called "Sobolev spaces"; the spaces $W_{r,0}(\mathbf{R}^n)$ are called "weighted L^2 spaces"; $W_{0,0}(\mathbf{R}^n)$ is just $L^2(\mathbf{R}^n)$. $\varphi \in W_{r,s}(\mathbf{R}^n)$ iff for all multiindices α, β with $|\alpha| \leq r$, $|\beta| \leq s$, we have $x^\alpha \varphi \in L^2(\mathbf{R}^n)$ and $D^\beta \varphi \in L^2(\mathbf{R}^n)$, where derivatives are taken in the sense of distributions. $W_{r,s}(\mathbf{R}^n)$ is a Hilbert space with the inner product $(\cdot, \cdot)_{r,s}$ naturally associated to the norm $\|\cdot\|_{r,s}$ via the polarization identity. If $r \leq r'$ and $s \leq s'$, $W_{r',s'}(\mathbf{R}^n)$ is a dense subspace of $W_{r,s}(\mathbf{R}^n)$. (For these and other results of functional analysis stated without proof see, e.g., [5].)

$W_{0,2}(\mathbf{R}^3)$ is a core for the free Hamiltonian; by the Kato-Rellich theorem $W_{0,2}(\mathbf{R}^{3n})$ is a core for the n-particle Coulombic Hamiltonian. $W_{2,2}(\mathbf{R}^n)$ is a core for the harmonic oscillator Hamiltonian. Furthermore, these Hamiltonians are bounded as operators from $W_{r,s}(\mathbf{R}^n)$ (with appropriate r, s, n) to $L^2(\mathbf{R}^n)$. This is important because recursivity only makes sense for continuous functions. Indeed, the only unbounded selfadjoint operators we will be considering are those which have some $W_{r,s}(\mathbf{R}^n)$ as a core and restrict to a bounded operator from $W_{r,s}(\mathbf{R}^n)$ to $L^2(\mathbf{R}^n)$. We will often describe this situation simply by saying "$A : W_{r,s}(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$ is essentially selfadjoint."

To study recursive operators on weighted Sobolev spaces we need recursive presentations for these spaces. A handy one involves tensor products of the Hermite functions $\Omega_i : \mathbf{R} \to \mathbf{R}$. Let

$$\eta_i^n(x_1,\ldots,x_n) = \Omega_{(i)_0}(x_1)\cdots\Omega_{(i)_{n-1}}(x_n)$$

and

$$\psi_i^n = \sum_{l=0}^{\infty} c_{(i)_l}\eta_l^n.$$

Note that this sum is always effectively finite since if $l > i$ then $(i)_l = 0$ so $c_{(i)_l} = 0$. $(\eta_i^n)_{i\in\mathbf{N}}$ is an orthonormal basis for $L^2(\mathbf{R}^n)$ and for any r, s $(\psi_i^n)_{i\in\mathbf{N}}$ is dense in $W_{r,s}(\mathbf{R}^n)$; indeed we have

PROPOSITION 7. *(ψ_i^n) is a recursive presentation of $W_{r,s}(\mathbf{R}^n)$.*

PROOF. Since $\|\psi_i^n - \psi_j^n\|_{r,s}$ is effectively computable in terms of rational functions and square roots using Hermite function identities, the relations

$$\|\psi_i^n - \psi_j^n\|_{r,s} \leq m/(k+1)$$

and

$$\|\psi_i^n - \psi_j^n\|_{r,s} < m/(k+1)$$

are recursive. □

In what follows I will often use the abbreviations W for $W_{r,s}(\mathbf{R}^n)$, $(\cdot,\cdot)_w$ for $(\cdot,\cdot)_{r,s}$, $\|\cdot\|_w$ for $\|\cdot\|_{r,s}$, $(\cdot,\cdot)$ for $(\cdot,\cdot)_{0,0}$, $\|\cdot\|$ for $\|\cdot\|_{0,0}$, (ψ_i) for (ψ_i^n), and (η_i) for (η_i^n).

PROPOSITION 8. *The following functions are recursive*: $\|\cdot\|_w : W \to \mathbf{R}$, $+: W\times W \to W$, $\mu : \mathbf{C}\times W \to W$ *defined by* $\mu(x,\varphi) = x\varphi$, *and* $(\cdot,\cdot)_w : W\times W \to \mathbf{C}$.

PROOF. By Propositions 5 and 6 and the fact that $\|\varphi\|_w = \|\varphi - \psi_0\|_w$, it follows that $\|\cdot\|_w : W \to \mathbf{R}$ is recursive.

By standard recursion-theoretic techniques there is a recursive $\alpha : \mathbf{N}\to\mathbf{N}$ such that

$$+\left((\psi\otimes\psi)_i\right) = +\left(\psi_{(i)_0}, \psi_{(i)_1}\right) = \psi_{(i)_0} + \psi_{(i)_1} = \psi_{\alpha(i)}.$$

Note that $\varphi + \varphi' \in B_k(W)$ iff

$$\|(\varphi+\varphi') - \psi_{(k)_0}\|_w < \frac{(k)_1}{(k)_2+1}.$$

Since $((\psi\otimes\psi)_i)$ is dense in $W\times W$, this means that $\varphi+\varphi' \in B_k(W)$ iff

$$(1)\quad \exists i\left[\|\varphi - \psi_{(i)_0}\|_w + \|\varphi' - \psi_{(i)_1}\|_w + \|\psi_{\alpha(i)} - \psi_{(k)_0}\|_w < (k)_1/((k)_2+1)\right].$$

By Propositions 1, 5, and 6 we see that (1) defines a set in $\Sigma_1^0(W \times W \times \mathbf{N})$. This set is precisely the nbhd diagram of $+: W \times W \to W$, so $+$ is recursive.

There is also a recursive $\beta : \mathbf{N} \to \mathbf{N}$ such that

$$\mu((c \otimes \psi)_i) = \mu\big(c_{(i)_0}, \psi_{(i)_1}\big) = c_{(i)_0}\psi_{(i)_1} = \psi_{\beta(i)}.$$

Note that $x\varphi \in B_k(W)$ iff

$$\|x\varphi - \psi_{(k)_0}\|_w < \frac{(k)_1}{(k)_2 + 1}.$$

Since $((c \otimes \psi)_i)$ is dense in $\mathbf{C} \times W$, this means $x\varphi \in B_k(W)$ iff

(2)

$$\exists i\big[|x - c_{(i)_0}|\|\varphi\|_w + |c_{(i)_0}|\|\varphi - \psi_{(i)_1}\|_w + \|\psi_{\beta(i)} - \psi_{(k)_0}\|_w < (k)_1/\left((k)_2 + 1\right)\big].$$

By Propositions 1, 5, and 6 we see that (2) defines a set in $\Sigma_1^0(\mathbf{C} \times W \times \mathbf{N})$. This set is precisely the nbhd diagram of $\mu : \mathbf{C} \times W \to W$. Thus μ is recursive.

Having proved that $\|\cdot\|_w$, $+$, and μ are recursive, to see that $(\cdot,\cdot)_w$ is recursive we need only note the polarization identity:

$$(\varphi, \varphi')_w = \tfrac{1}{4}\left(\|\varphi + \varphi'\|_w^2 - \|\varphi - \varphi'\|_w^2\right) + \tfrac{1}{4i}\left(\|\varphi + i\varphi'\|_w^2 - \|\varphi - i\varphi'\|_w^2\right). \quad \square$$

We now turn our attention to operators from W to $L^2(\mathbf{R}^n)$. We shall study not only operators but "parametrized operators," that is, continuous functions $T: M \times W \to L^2(\mathbf{R}^n)$ such that for each $x \in M$, $T_x : W \to L^2(\mathbf{R}^n)$ is an operator. Operators in physics are often parametrized, the parameters being either physical constants or variables such as time.

Note that Proposition 8 implies that if $T: M \times W \to L^2(\mathbf{R}^n)$ is a recursive parametrized operator the function $(\varphi, T_x\varphi')$ from $M \times L^2(\mathbf{R}^n) \times W$ to $\mathbf{C}$ is recursive. This is desirable in quantum mechanics, where such matrix elements have physical significance.

The following proposition characterizes uniformly bounded parametrized operators.

PROPOSITION 9. *Let $T: M \times W \to L^2(\mathbf{R}^n)$ be a uniformly bounded parametrized operator. T is recursive iff there are recursive functions $f: M \times \mathbf{N}^2 \to \mathbf{C}$ and $g: M \times \mathbf{N} \to \mathbf{R}$ such that*

$$f_x(i, j) = (\eta_j, T_x\eta_i) \quad \textit{and} \quad g_x(i) = \|T_x\eta_i\|.$$

PROOF. If T is recursive, f and g are recursive by Proposition 8 and the recursivity, easily seen, of the sequence (η_i) considered as a function from $\mathbf{N}$ to W (or to $L^2(\mathbf{R}^n)$).

For the converse, assume f and g are recursive and $\|T_x\| \leqslant K \in \mathbf{N}$ for all $x \in M$. Let $F: \mathbf{N} \to \mathbf{N}$ be a recursive function such that $j > F(k)$ implies $(k)_j = 0$, hence

$c_{(k)_j} = 0$. Since (η_i) is an orthonormal basis for $L^2(\mathbf{R}^n)$ we have

$$\begin{aligned}\|T_x\eta_i - \psi_k\|^2 &= \left\| \sum_{j=0}^{\infty} \left((\eta_j, T_x\eta_i) - c_{(k)_j} \right) \eta_j \right\|^2 = \sum_{j=0}^{\infty} |f_x(i,j) - c_{(k)_j}|^2 \\ &= \sum_{j=0}^{F(k)} |f_x(i,j) - c_{(k)_j}|^2 + \sum_{j=F(k)+1}^{\infty} |f_x(i,j)|^2 \\ &= \sum_{j=0}^{F(k)} \left(|f_x(i,j) - c_{(k)_j}|^2 - |f_x(i,j)|^2 \right) + \sum_{j=0}^{\infty} |f_x(i,j)|^2 \\ &= \sum_{j=0}^{F(k)} \left(|f_x(i,j) - c_{(k)_j}|^2 - |f_x(i,j)|^2 \right) + g_x(i)^2.\end{aligned}$$

Thus $T_x\eta_i \in B_k(L^2(\mathbf{R}^n))$ iff

$$\text{(3)} \qquad \sum_{j=0}^{F(k)} \left(|f_x(i,j) - c_{(k)_j}|^2 - |f_x(i,j)|^2 \right) + g_x(i)^2 < \left(\frac{(k)_1}{(k)_2 + 1} \right)^2.$$

Since f, g, and F are recursive, (3) defines a set in $\Sigma_1^0(M \times \mathbf{N}^2)$. This set is just the nbhd diagram of $T_x\eta_i$ as a function from $M \times \mathbf{N}$ to $L^2(\mathbf{R}^n)$, so $T_x\eta_i$ is a recursive function.

Since

$$T_x\psi_i = \sum_{j=0}^{F(i)} c_{(i)_j} T_x\eta_j$$

we can conclude that $T_x\psi_i$ is also recursive as a function from $M \times \mathbf{N}$ to $L^2(\mathbf{R}^n)$.

For $\varphi \in W$, $T_x\varphi \in B_k(L^2(\mathbf{R}^n))$ iff

$$\|T_x\varphi - \psi_{(k)_0}\| < \frac{(k)_1}{(k)_2 + 1}$$

and since (ψ_i) is dense in W and $\|T_x\| \leq K$, this holds iff

$$\text{(4)} \qquad \exists i \left[K\|\varphi - \psi_i\|_w + \|T_x\psi_i - \psi_{(k)_0}\| < (k)_1 / ((k)_2 + 1) \right].$$

Since $T_x\psi_i$ is a recursive function and $K \in \mathbf{N}$, (4) defines a set in $\Sigma_1^0(M \times W \times \mathbf{N})$ which is the nbhd diagram of $T: M \times W \to L^2(\mathbf{R}^n)$. Thus T is recursive. □

This has as a corollary:

PROPOSITION 10. *An operator $T: W \to L^2(\mathbf{R}^n)$ is recursive iff there are recursive functions $f: \mathbf{N}^2 \to \mathbf{C}$ and $g: \mathbf{N} \to \mathbf{R}$ such that $f(i, j) = (\eta_j, T\eta_i)$ and $g(i) = \|T\eta_i\|$.*

PROOF. Take M to be a one-point space in Proposition 9 and use the existence of a natural recursive bijection between W and $M \times W$. □

Define an "essentially selfadjoint (ess. s.a.) parametrized operator" to be a parametrized operator $A: M \times W \to L^2(\mathbf{R}^n)$ such that for each $x \in M$ A_x is essentially selfadjoint. We will show that a recursive ess. s.a. parametrized operator A generates a unitary group $\exp(iA_x t)$ which acts recursively on $L^2(\mathbf{R}^n)$. First, however, we need a lemma on resolvents.

If $A_x : W \to L^2(\mathbf{R}^n)$ is essentially selfadjoint, there is an operator $(A_x + i)^{-1}: L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$ such that $(A_x + i)^{-1}(A_x + i)$ is the identity on W (cf. [5, Theorem VIII.3]). If $A : M \times W \to L^2(\mathbf{R}^n)$ is an ess. s.a. parametrized operator, we can define a parametrized operator $(A + i)^{-1} : M \times L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$ by

$$(A + i)_x^{-1} = (A_x + i)^{-1}.$$

$(A + i)^{-1}$ is called the "resolvent" of A. We always have $\|(A + i)_x^{-1}\| \leq 1$.

Proposition 11. *If $A : M \times W \to L^2(\mathbf{R}^n)$ is a recursive ess. s.a. parametrized operator, then the resolvent $(A + i)^{-1} : M \times L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$ is a recursive parametrized operator.*

Proof. Suppose $(A + i)_x^{-1}\varphi \in B_k(L^2(\mathbf{R}^n))$, i.e.

$$\|(A + i)_x^{-1}\varphi - \psi_{(k)_0}\| < \frac{(k)_1}{(k)_2 + 1}.$$

Then since W is a core for A_x, we can find ψ_j making both $\|(A + i)_x^{-1}\varphi - \psi_j\|$ and $\|(A + i)_x^{-1}\varphi - \psi_j\|_w$ simultaneously as small as we like, so we know by the triangle inequality that

$$\exists j\left[\|A_x + i\| \|(A + i)_x^{-1}\varphi - \psi_j\|_w + \|\psi_j - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1)\right].$$

This in turn implies

(5) $$\exists j\left[\|\varphi - (A_x + i)\psi_j\| + \|\psi_j - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1)\right].$$

Conversely, suppose (5) holds. Then since $\|(A + i)_x^{-1}\| \leq 1$, we have

$$\exists j\left[\|(A + i)_x^{-1}\varphi - \psi_j\| + \|\psi_j - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1)\right]$$

which implies

$$\|(A + i)_x^{-1}\varphi - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1),$$

i.e. $(A + i)_x^{-1}\varphi \in B_k(L^2(\mathbf{R}^n))$. Thus (5) defines a subset of $M \times L^2(\mathbf{R}^n) \times \mathbf{N}$ which is the nbhd diagram of $(A + i)^{-1} : M \times L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$. If A is recursive (5) defines a semirecursive set, which implies that $(A + i)^{-1}$ is recursive. □

Theorem 12. *If $A : M \times W \to L^2(\mathbf{R}^n)$ is a recursive ess. s.a. parametrized operator, the parametrized operator $U: M \times \mathbf{R} \times L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$ defined by $U_{x,t} = \exp(iA_x t)$ is recursive.*

Proof. Define the parametrized operators $R, R^* : M \times L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$ by

$$R_x = (A + i)_x^{-1}, \quad R_x^* = \left((A + i)_x^{-1}\right)^* = -(-A + i)_x^{-1}.$$

Since A and $-A$ are recursive ess. s.a. parametrized operators, R and R^* are recursive parametrized operators by Proposition 11. The proof will proceed by using the functional calculus for normal operators to approximate $U_{x,t}$ with polynomials in R_x and R_x^*. Define a "recursively parametrized polynomial" to be a function $P : N \times \mathbf{C} \to \mathbf{C}$ (N being a recursively presented space) such that for $\alpha \in N$ $P_\alpha : \mathbf{C} \to \mathbf{C}$ is a polynomial in $\lambda, \bar{\lambda} \in \mathbf{C}$ whose degree and coefficients are recursive functions of α. Using standard recursion-theoretic techniques one can see that if P is a recursively parametrized polynomial, the corresponding parametrized operator $P(R): M \times N \times L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$ given by the functional calculus is recursive. (For all $x \in M$ and $\alpha \in N$, $P_\alpha(R_x)$ is a polynomial in R_x and R_x^*.)

By the functional calculus we know

$$U_{x,t} = \exp\big(it\big(R_x^{-1} - i\big)\big)$$

or if we let $f_t(\lambda) = \exp(it(\lambda^{-1} - i))$,

$$U_{x,t} = f_t(R_x).$$

Let

$$p_{l,t}(\lambda) = \begin{cases} 0 & \text{if } |\lambda| \leqslant 1/(l+1), \\ f_t(\lambda)((l+1)|\lambda| - 1) & \text{if } 1/(l+1) \leqslant |\lambda| \leqslant 2/(l+1), \\ f_t(\lambda) & \text{if } |\lambda| \geqslant 2/(l+1). \end{cases}$$

The spectrum of R_x is a subset of $D = \{\lambda \in \mathbf{C} : |\lambda| \leqslant 1\}$, and zero is not in the pure point spectrum of R_x. Thus $s\text{-}\lim_{l\to\infty} p_{l,t}(R_x) = f_t(R_x)$, since $\lim_{l\to\infty} p_{l,t} = f_t$ pointwise on $D - \{0\}$ and $\|p_{l,t}\|_\infty \leqslant 1$ for all l, t. Thus for all $\varphi \in L^2(\mathbf{R}^n)$ we have $\lim_{l\to\infty} p_{l,t}(R_x)\varphi = U_{x,t}\varphi$, but at first glance this convergence does not seem effective. However, since $U_{x,t}$ is unitary

$$\|(p_{l,0}(R_x) - I)\varphi\| = \|U_{x,t}(p_{l,0}(R_x) - I)\varphi\| = \|(f_t(R_x)p_{l,0}(R_x) - U_{x,t})\varphi\|$$

and since $f_t p_{l,0} = p_{l,t}$ this implies

(6) $$\|(p_{l,0}(R_x) - I)\varphi\| = \|(p_{l,t}(R_x) - U_{x,t})\varphi\|.$$

This will allow us to effectively compute how close $p_{l,t}(R_x)\psi$ is to $U_{x,t}\psi$.

By standard analytical techniques we can find a recursively parametrized polynomial $P : \mathbf{N}^2 \times \mathbf{R} \times \mathbf{C} \to \mathbf{C}$ such that for all l, m, t

(7) $$\sup_{\substack{\lambda \in D \\ \tau = 0, t}} |P_{l,m,\tau}(\lambda) - p_{l,\tau}(\lambda)| < \delta_{m,t}$$

where $\delta : \mathbf{N} \times \mathbf{R} \to \mathbf{R}$ is a recursive function with $\lim_{m\to\infty} \delta_{m,t} = 0$ for all t. By the preceding remarks we know that $P(R) : \mathbf{N}^2 \times \mathbf{R} \times L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$ is a recursive parametrized operator. Since the spectrum of R_x is in D, (7) implies

(8) $$\|P_{l,m,0}(R_x) - p_{l,0}(R_x)\| < \delta_{m,t}$$

and

(9) $$\|P_{l,m,t}(R_x) - p_{l,t}(R_x)\| < \delta_{m,t}.$$

Now suppose $U_{x,t}\varphi \in B_k(L^2(\mathbf{R}^n))$, i.e.

$$\|U_{x,t}\varphi - \psi_{(k)_0}\| < \frac{(k)_1}{(k)_2 + 1}.$$

Then since $s\text{-}\lim_{l\to\infty} p_{l,t}(R_x) = U_{x,t}$, we know

$$\exists l\big[\|U_{x,t}\varphi - p_{l,t}(R_x)\varphi\| + \|p_{l,t}(R_x)\varphi - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1)\big].$$

By (6) this implies

$$\exists l\left[\|p_{l,0}(R_x)\varphi - \varphi\| + \|p_{l,t}(R_x)\varphi - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1)\right].$$

Since $\lim_{m\to\infty}\delta_{m,t} = 0$ this implies

$$\exists m\exists l\left[4\delta_{m,t}\|\varphi\| + \|p_{l,0}(R_x)\varphi - \varphi\| + \|p_{l,t}(R_x)\varphi - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1)\right].$$

By (8), (9) and the triangle inequality this implies

$$(10)\qquad \exists m\exists l\big[2\delta_{m,t}\|\varphi\| + \|P_{l,m,0}(R_x)\varphi - \varphi\| + \|P_{l,m,t}(R_x)\varphi - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1)\big].$$

Conversely, assume (10) is true. Then (8), (9) and the triangle inequality imply

$$\exists l\left[\|p_{l,0}(R_x)\varphi - \varphi\| + \|p_{l,t}(R_x)\varphi - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1)\right]$$

which by (6) implies

$$\exists l\left[\|U_{x,t}\varphi - p_{l,t}(R_x)\varphi\| + \|p_{l,t}(R_x)\varphi - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1)\right]$$

so that

$$\|U_{x,t}\varphi - \psi_{(k)_0}\| < (k)_1/((k)_2 + 1),$$

i.e. $U_{x,t}\varphi \in B_k(L^2(\mathbf{R}^n))$. Thus (10) holds iff $U_{x,t}\varphi \in B_k(L^2(\mathbf{R}^n))$, so (10) defines a subset of $M \times \mathbf{R} \times L^2(\mathbf{R}^n) \times \mathbf{N}$ which is precisely the nbhd diagram of $U\colon M \times \mathbf{R} \times L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$. Since δ is recursive and $P(R)$ is a recursive parametrized operator, the set (10) defines is semirecursive. Thus U is recursive. □

Recursivity of Hamiltonians. The recursivity of a number of physically important Hamiltonians follows directly from Proposition 10. For example, we can prove the recursivity of the n-particle Coulombic Hamiltonian, which for convenience we parametrize using the "reciprocal masses" $\mu_i = 1/m_i$.

PROPOSITION 13. *If one defines* $H\colon \mathbf{R}^{2n+1} \times W_{0,2}(\mathbf{R}^{3n}) \to L^2(\mathbf{R}^{3n})$ *by*

$$H_{\mu_1,\ldots,\mu_n,q_1,\ldots,q_n,\hbar} = -\sum_{i=1}^{n}\frac{1}{2}\hbar^2\mu_i\nabla_i^2 + \sum_{1\le i<j\le n}\frac{q_iq_j}{|\vec{x}_i - \vec{x}_j|}$$

where

$$\nabla_i^2\varphi = \left(\frac{\partial^2}{\partial x_{3i-2}^2} + \frac{\partial^2}{\partial x_{3i-1}^2} + \frac{\partial^2}{\partial x_{3i}^2}\right)\varphi$$

and

$$\vec{x}_i = (x_{3i-2}, x_{3i-1}, x_{3i})$$

then H is a recursive parametrized operator.

PROOF. $\nabla_i^2 : W_{0,2}(\mathbf{R}^{3n}) \to L^2(\mathbf{R}^{3n})$ is a bounded linear operator, and by the Kato-Rellich theorem so is $1/|\vec{x}_i - \vec{x}_j| : W_{0,2}(\mathbf{R}^{3n}) \to L^2(\mathbf{R}^{3n})$ (cf. [**5**, Theorem X.16]). A simple application of Proposition 10 implies these operators are recursive. Thus the parametrized linear combination

$$H_{\mu_1,\ldots,\mu_n,q_1,\ldots,q_n,\hbar} = -\sum_{i=1}^{n} \frac{1}{2}\hbar^2\mu_i\nabla_i^2 + \sum_{1\leq i<j\leq n} \frac{q_i q_j}{|\vec{x}_i - \vec{x}_j|}$$

is a recursive parametrized operator. □

An important corollary of this is the following

THEOREM 14. *If one defines* $U: \mathbf{R}^{2n+2} \times L^2(\mathbf{R}^{3n}) \to L^2(\mathbf{R}^{3n})$ *by*

$$U_{\mu_1,\ldots,\mu_n,q_1,\ldots,q_n,\hbar,\tilde{t}} = \exp\left(-itH_{\mu_1,\ldots,\mu_n,q_1,\ldots,q_n,\hbar}\right)$$

where $H_{\mu_1,\ldots,\mu_n,q_1,\ldots,q_n,\hbar}$ *is defined as above and* $\tilde{t} = t/\hbar$, *then* U *is a recursive parametrized operator.*

PROOF. A corollary of Theorem 12 and Proposition 13. □

This says that the time evolution of an n-particle quantum Coulombic system is recursive in the initial conditions and the data μ_i, q_i, $\hbar$.

If we set all the q_i equal to zero in Proposition 13 and Theorem 14, we obtain recursivity results for the n-particle free Hamiltonian. One can easily derive similar results for the harmonic oscillator Hamiltonian and other operators with weighted Sobolev spaces for cores.

Conclusion. The results obtained here make it seem that quantum mechanics is a fairly tractable theory from the point of view of recursivity. In particular, the methods used here to prove the recursivity of Hamiltonians and the unitary groups they generate seem easily generalizable.

An interesting possibility for further research lies in characterizing the spectra of selfadjoint operators in terms of the Kleene pointclasses. This idea is implicit in a remark of Kreisel [**2**]: "Suppose we find a Schrödinger equation of a—presumably large—molecule such that the (dimensionless) ratio λ_2/λ_1 of its second to its first eigenvalue is not recursive (in the data). Then there is no difficulty in finding a corresponding experimental setup to show that quantum theory is nonmechanistic in the sense of this note." It is possible, using methods similar to the proof of Proposition 12, to show that the spectrum of a recursive essentially selfadjoint operator with a weighted Sobolev space for its core must be in $\Pi_2^0(\mathbf{R})$. Sharper results will require more specialized methods suited to the particular operators being studied.

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