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Smoothed Coulomb potentials for quantum mechanics

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Abstract. We consider the quantum systems of N point particles moving in $\mathbb{R}^3$ under the influence of either their mutual Coulomb potential V or a smooth potential V_n equal to V whenever all interparticle distances are greater than $1/n$ and equal to zero whenever all interparticle distances are less than $1/n - 1/n^2$. We prove that the dynamical theory based on V_n converges to that based on V as n increases indefinitely.

The fundamental interaction at the atomic level is the Coulomb force, and elementary quantum mechanics is its study. Other potentials are considered in quantum mechanics as well. They correspond to various complex phenomena, idealised, which are ultimately derivable from Coulomb forces, in principle at least. These idealisations, whilst important for descriptive purposes, sometimes introduce mathematical singularities which are not present in the underlying Coulombic description. For example, there are no infinitely deep wells, no infinitely high barriers, and no absolutely hard walls. Moreover, there are no perfectly square wells or barriers. These are convenient replacements for very deep wells, very high walls, and rounded edges on the potentials.

Another type of derived singularity is encountered in molecular theory. Here one finds potentials of the form $\sim r^{-6}$. However, such an expression is an effective potential obtained from Coulomb forces under certain approximations.

Consideration of these and other standard examples leads us to the view that the analytic properties of all quantum mechanical quantities for elementary quantum systems are derivable from the generic system of N point particles of masses m_i moving in $\mathbb{R}^3$ under the influence of their mutual Coulomb interactions $(i, j \leq N)$

$$v_{ij}(x_i - x_j) = e_i e_j / |x_i - x_j|. \tag{1}$$

By elementary quantum systems we mean the aspects of quantum theory valid for a finite number of degrees of freedom, and for energies less that those of nuclear theory. For larger energies a transition to quantum field theory occurs, and the mathematical considerations are quite different.

The Coulomb potentials (1) are not actually compatible with this energy limit. More precisely, effects arising from distances less than, say, the radius of a nucleon are outside the province of elementary quantum mechanics as we have defined it. We propose, therefore, to replace the Coulomb potential by a smoothly cut-off approximation. This will be justified only if we can prove that the cut-off theory converges to the Coulomb theory as the cut-off is removed. A proof of this convergence is the purpose of this paper.

Before proving our assertion, we wish to remark that an important consequence of our work relates to the rigged Hilbert space formulation of quantum mechanics.

Briefly, we take our space of wavefunctions to be the Schwartz space $\mathscr{S}(\mathbb{R}^d)$ of C^∞-functions of polynomial decrease at infinity, so that $\mathscr{S}(\mathbb{R}^d) \subset L^2(\mathbb{R}^d) \subset \mathscr{S}'(\mathbb{R}^d)$ forms a rigged triple. The algebra of observables may then be taken to be the set $\mathscr{A}$ of linear operators from $\mathscr{S}(\mathbb{R}^d)$ to itself whose adjoints also map $\mathscr{S}(\mathbb{R}^d)$ to itself. This is a unital topological *-algebra of unbounded operators when equipped with the topology inherited as a subspace, via kernels, of $\mathscr{S}'(\mathbb{R}^{2d})$. Recall that the kernel representation associates a distribution $B \in \mathscr{S}'(\mathbb{R}^{2d})$ to every observable $b \in \mathscr{A}$ through the formula

$$(bf)(x) = \int B(x, y) f(y)\, \mathrm{d}y, \qquad f \in \mathscr{S}(\mathbb{R}^d).$$

The coordinates and momenta are operators in $\mathscr{A}$, and the usual operator equations of quantum mechanics can be justified as continuous maps from $\mathscr{S}(\mathscr{R}^d)$ to itself.

The states of the system, in this formulation, are the positive trace-normalised continuous linear functionals on $\mathscr{A}$. It is a mathematical consequence that all states are given through density matrices; the wavefunctions, the elements of $\mathscr{S}(\mathbb{R}^d)$, are exactly the extremal states. States also have a kernel representation. The kernel of a state ρ will be a smooth function $R \in \mathscr{S}(\mathbb{R}^{2d})$. Written in terms of kernels, the expectation value of an observable b in the state ρ is

$$\rho(b) = \int\int R(x, y) B(x, y)\, \mathrm{d}x\, \mathrm{d}y.$$

Note that every observable has a finite expectation value in every state (cf Lassner 1972, 1980, Lassner and Uhlmann 1978, Lassner 1978, Roberts 1966a, b, Schmüdgen 1978, 1979, Sherman 1968, Woronowicz 1970).

Suppose we replace the Coulomb potential by a potential in the class

$$\Phi = \{V \in C^\infty(\mathbb{R}^d) \colon \sup_{x \in \mathbb{R}^d} |\partial^n f(x)| < \infty,\ n \in \mathbb{N}^d\}. \tag{2}$$

Then (Hunziker 1966) the Hamiltonian is an element of $\mathscr{A}$, and the Hamiltonian generates a time translation group under which $\mathscr{S}$ is invariant. In the Heisenberg picture, the dynamics is described by an automorphism group of $\mathscr{A}$.

We start our analysis with some necessary definitions.

Definition 1. Let $h_n \in \mathscr{D}(\mathbb{R}^+)$ be a chosen function such that $h_n \equiv 1$ on $[0, 1/n - 1/n^2]$ and $h_n \equiv 0$ on $[1/n, \infty)$. The cut-off Coulomb function for given n is

$$v_{ij}^{(n)}(x_i - x_j) = [1 - h_n(|x_i - x_j|)] v_{ij}(x_i - x_j). \tag{3}$$

Letting Σ' stand for the sum over non-coincident pairs (i, j), the potentials are

$$V(x_1, \ldots, x_N) = \sum{}' v_{ij}(x_i - x_j), \tag{4a}$$

$$V_n(x_1, \ldots, x_N) = \sum{}' v_{ij}^{(n)}(x_i - x_j), \tag{4b}$$

and determine Hamiltonians $H = (T + V)^{**}$, $H_n = (T + V_n)^{**}$ respectively, where T is the kinetic energy, the self-adjoint Dirichlet Laplacian. By $U(t)$, respectively $U^{(n)}(t)$, we mean the unitary groups $(t \in \mathbb{R})$ whose generators are H, respectively H_n.

The cut-off Coulomb function $v_{ij}^{(n)}$ is seen to be equal to v_{ij} for $|x_i - x_j| > 1/n$ and is equal to zero for $|x_i - x_j| < 1/n - 1/n^2$; it is $\mathscr{S}$-class, so that $V_n \in \Phi$. It is known that V is relatively T-bounded, with T bound equal to zero; the same proof holds for V_n. Hence $D(H) = D(H_n) = D(T)$ (Kato 1966). For the purposes of our result below, just which function h_n is chosen is immaterial; it suffices to know that one such exists (Treves 1967).

Proposition 2. For every $f \in \mathscr{S}(\mathbb{R}^{3N})$ and all $t \in \mathbb{R}$, the time translations converge in the L^2 sense:

$$\lim_{n\to\infty} \|U^{(n)}(t)f - U(t)f\|_2 = 0. \tag{5}$$

Proof. We shall consider the equivalent statement

$$\lim_{n\to\infty} \|U^{(n)}(-t)U(t)f - f\|_2 = 0. \tag{5'}$$

As in Cook's method in scattering theory (Reed and Simon 1979) we have the integral inequality

$$\|U^{(n)}(-t)U(t)f-f\|_2 \leq \int_0^t \mathrm{d}s\, \|U^{(n)}(s)[V-V_n]U(s)f\|_2$$

$$\leq \sum{}' \int_0^t \mathrm{d}s\, \|(v_{ij}-v_{ij}^{(n)})U(s)f\|_2. \tag{6}$$

Let a pair (i,j) be fixed; by introducing the new variables $y_k = x_k$ $(k \neq i,j)$, $y_i = x_i - x_j$, $y_j = (x_i + x_j)/2$, each term in the integrand can be reduced to an $\mathbb{R}^3$ expression by integrating over all variables except y_i. If we write

$$|f_{i,s}(y_i)|^2 = \int |[U(s)f](y_1,\ldots,y_N)|^2\,\mathrm{d}y_1\ldots\mathrm{d}\hat{y}_i\ldots\mathrm{d}y_N,$$

the circumflex indicating omission, then

$$\|(v_{ij}-v_{ij}^{(n)})U(s)f\|_2 = \|(v_{ij}-v_{ij}^{(n)})f_{i,s}\|_2'.$$

The prime indicates that only the variable y_i is under consideration. Now as $v_{ij}-v_{ij}^{(n)}$ has support in the compact ball $\{x\in\mathbb{R}^3\colon |x|\leq 1/n\}$, we can write

$$\|(v_{ij}-v_{ij}^{(n)})f_{i,s}\|_2' \leq \|(v_{ij}-v_{ij}^{(n)})\|_2'\|f_{i,s}\|_\infty'.$$

Now we use the elementary inequality (cf Simon 1971 for one dimension)

$$\|g\|_\infty' \leq \pi(2\pi)^{-3/2}(\|g\|_2' + \|\Delta_i g\|_2').$$

This is obtained from $\|g\|_\infty' \leq (2\pi)^{-3/2}\|\tilde{g}\|_1'$ for the Fourier transform, by multiplying and dividing $\tilde{g}$ by $1+|p_i|^2$, using the Cauchy-Schwarz inequality and inverting the Fourier transform. From the relative T boundedness of V, $U_s f \in D(T)$ and so we have existence for

$$\|(v_{ij}-v_{ij}^{(n)})U(s)f\|_2 \leq (2n)^{-1/2}(\|f_{i,s}\|_2' + \|\Delta_i f_{i,s}\|_2) \leq (2n)^{-1/2}(\|U(s)f\|_2 + \|TU(s)f\|_2).$$

We invoke relative boundedness again: there exists a positive constant c such that for all $g\in D(T)$,

$$\|Vg\|_2 \leq \tfrac{1}{2}\|Tg\|_2 + c\|g\|_2.$$

Rearranging so as to gather all $TU(s)f$ terms together yields

$$\|TU(s)f\|_2 \leq \|HU(s)f\|_2 + \|VU(s)f\|_2, \qquad \|TU(s)f\|_2 \leq 2\|Hf\|_2 + 2c\|f\|_2.$$

Hence, recalling that $\mathscr{S} \subset D(T)$,

$$\|(v_{ij} - v_{ij}^{(n)}) U(s)f\|_2 \leqslant 2(2n)^{-1/2}[\|Hf\|_2 + (c+1)\|f\|_2]. \tag{7}$$

Summing over (i, j) pairs yields

$$\|U^{(n)}(-t)U(t)f - f\|_2 \leqslant (N-1)!t(2n)^{-1/2}[\|Hf\|_2 + (c+1)\|f\|_2];$$

the limit $n \to \infty$ now proves the assertion.

When we state that the V_n theory converges to the V theory we mean first of all proposition 1. We also mean that the time evolved expectation values of the V_n theory converge to those of the V theory. Now to each symmetric operation in $\mathscr{A}$ corresponds a generalised spectral decomposition by means of at least one positive contraction valued Borel measure $\{E(\Delta): \Delta \in \mathbb{B} \text{ or } (\mathbb{R})\}$ (cf Riesz and Sz Nagy 1960, Dubin and Sotelo 1984). The expectation values of the theory are $\langle f, E(\Delta)f\rangle$ for all $f \in \mathscr{S}$ and all such spectral families E of the theory.

Proposition 3. For all f, t, E, Δ

$$\lim_{n\to\infty} \langle U^{(n)}(t)f, E(\Delta)U^{(n)}(t)f\rangle = \langle U(t)f, E(\Delta)U(t)f\rangle. \tag{8}$$

Proof. For brevity we introduce the notation

$$G_n(t) = U^{(n)}(t)f - U(t)f.$$

Now

$$\langle G_n(t), E(\Delta)G_n(t)\rangle = \langle U^{(n)}(t)f, E(\Delta)U^{(n)}(t)f\rangle + \langle U(t)f, E(\Delta)U(t)f\rangle$$
$$- \langle U^{(n)}(t)f, E(\Delta)U(t)f\rangle - \langle U(t)f, E(\Delta)U^{(n)}(t)f\rangle.$$

By the Cauchy-Schwarz inequality, the last two terms each converge to $\langle U(t)f, E(\Delta)U(t)f\rangle$, from proposition 1. In the same way, since $G_n(t) \to 0$, the left side converges to zero, and so (8) follows.

Finally, the convergence of the V_n to the V theory also means the convergence of the spectra of the Hamiltonians in the following sense.

Proposition 4. In the generalised strong sense of Kato (1966),

$$H_n \to H,$$

and the resolvents converge similarly, provided $\mathrm{Im}(z) \neq 0$:

$$R_n(z) \to R(z).$$

Hence every open subset of $\mathbb{R}$ containing a point of the spectrum of H contains at least one point of the spectrum of H_n for large enough n. The corresponding spectral projections converge in the strong sense: $P_n(t_n) \to P(t)$ for all $t_n \to t$.

For the case of two particles, consider the relative motion. To each eigenvalue $-1/n^2$ (n is now the principle quantum number), there corresponds n eigenvalues $E^{(p)}(1, n), \ldots, E^{(p)}(n, n)$ of H_p in the neighbourhood of $-1/n^2$. Thus, the n^2-fold degeneracy of $-1/n^2$ is partially broken, each $E^{(p)}$ being n-fold degenerate due to rotational symmetry. For $p \to \infty$, $E^{(p)}(j, n) \to -1/n^2$, for all j.

Proof. Our estimate (7) with $s=0$ implies that $\|(H-H_n)f\|_2 \to 0$ for all $f \in \mathscr{S}$. As $\mathscr{S}$ is a core for H and H_n, the first part follows from Kato (1966, VIII.1, Cor 1.6). The second part then follows from Kato (1966, VIII.2, th. 1.14). For two-particle relative motion, the spectrum of H below zero consists only of isolated eigenvalues of finite multiplicity. Moreover the forms associated with the H_n increase to the H form. Hence th. 3.15 of Kato (1966, VIII.4) applies.

We have not analysed the $N \geqslant 3$ case for the stability of isolated eigenvalues.

In conclusion, then, we have shown that the H_n theory converges to the H theory. If we use the H_n theory we can utilise the rigged Hilbert space formalism, which is H_n dynamically stable.

In essentially all physics literature, it is taken as axiomatic that Hilbert space is the proper arena for quantum mechanics. We pointed out at the beginning of this note that there are cogent reasons for using the rigged Hilbert space formalism, based on choosing the wavefunctions to be smooth functions belonging to Schwartz space. This ensures finite expectation values for all observables: position, momentum, energy, etc, in any state.

The significance of the result given in this paper is that for the Coulomb potential, arguably the most fundamental potential, one can remain within the Schwartz space by a physically justified cut-off at small distances. This cut-off does not affect the elementary quantum properties derived within the usual Hilbert space context, and the numerical values of the cut-off theory converge to those of the pure Coulomb theory as the cut-off is removed.

Were we to consider potential wells and barriers, the same technique used in the proof of proposition 2 shows that the rounded well, or barrier, theory converges to that of the square well, or barrier, theory as the smoothing is removed.

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