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Invariant Domains for the Time-Dependent Schrödinger Equation*

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1. INTRODUCTION

It is often stated, with some justification, that existence proofs in quantum dynamics are simpler than the corresponding results in classical dynamics. For example, the famous result of Kato [3] proves that the Coulomb Hamiltonian

$$H = -\sum_{j=1}^{N} (2m_j)^{-1} \Delta_j + \sum_{j<k} \lambda_{jk} \mid \mathbf{x}_j - \mathbf{x}_k \mid^{-1}$$

on $L^2(\mathbb{R}^{3N})$ is essentially self adjoint on $C_0^\infty(\mathbb{R}^{3N})$, so that the evolution operators $\exp(-iHt)$ are unambiguously defined as a one parameter unitary group. The corresponding classical dynamical question is still open; i.e., it is unknown (for $N \geqslant 5$, $\lambda_{jk} < 0$) whether or not for almost every initial condition the Hamilton equations associated with

$$h = \sum_{j=1}^{N} (2m_j)^{-1} p_j^2 + \sum_{j<k} \lambda_{jk} \mid \mathbf{x}_j - \mathbf{x}_k \mid^{-1}$$

have global solutions. Results of Saari [9] and Sperling [11] imply, however, that the basic problem in proving this classical result would be the proof that, for almost every initial condition, $\mathbf{x}(t)^2 \equiv \sum_{j=1}^{N} \mathbf{x}_j(t)^2$ cannot become infinite in finite time. Interestingly enough, while Kato's result "solves" the dynamical existence question in the quantum case, it says nothing about the question of $\mathbf{x}(t)^2$ remaining finite in time! From its physical interpretation, proof of such a regularity property is clearly desirable.

The problem to which we address ourselves here is, therefore, that of finding a dense set of physically reasonable states, f, such that $\langle \exp(-iHt)f, \mathbf{x}^2 \exp(-iHt)f \rangle$ remains finite in finite time. The solution of this problem is not

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difficult; in fact for each fixed t, $\exp(-iHt)$ can be shown to be a bounded map on the set (equipped with the obvious norm) of those f such that

$$\langle f, (-\Delta + \mathbf{x}^2)f\rangle < \infty.$$

This result can be found in Section 2. To emphasize that the behavior in time of moments in position or momentum can be counterintuitive, we give some examples in Section 3, including a state, f, with the following properties: (a) At $t = 0$, all moments in position are finite; (b) Under the free evolution the fourth moment of position diverges for all $t \neq 0$; (c) Under an evolution with a purely repulsive potential, the fourth moment of position remains finite in finite time. In Section 4 we discuss in more detail the effect of local singularities in the potential on the behavior in time of moments in position.

2. Main Results

Let H_0 be the self-adjoint operator $-\Delta$ on $L^2 \equiv L^2(\mathbb{R}^m)$ (by a linear change of coordinates $\sum_{j=1}^N (-2m_j)^{-1} \Delta_j$ can be brought to this form), and let V be a real valued measurable function of $\mathbf{x} = (x_1, ..., x_m) \in \mathbb{R}^m$. Using freely the perturbation theoretic language of [4, 7] we consider the two cases: (a) V is H_0-form bounded with relative bound smaller than one, i.e. the operator domain $D(|V|^{1/2})$ contains $D(H_0^{1/2})$ and, for some $a < 1$, $b > 0$, and all f in $D(H_0^{1/2})$:

$$\langle |V|^{1/2}f, |V|^{1/2}f\rangle \leqslant a\langle H_0^{1/2}f, H_0^{1/2}f\rangle + b\langle f,f\rangle \tag{1}$$

and (b) V is H_0-operator bounded with relative bound smaller than one, i.e. $D(H_0) \subset D(V)$ and for some $\tilde{a} < 1$, $\tilde{b} > 0$ and all f in $D(H_0)$:

$$\| Vf \| \leqslant \tilde{a} \| H_0 f \| + \tilde{b} \| f \|. \tag{2}$$

Wide classes of potentials obey (1) or (noting that (2) implies (1)) both (1) and (2), including the Coulomb potential; see [4, 7]. Our main result is:

THEOREM 2.1. *Let V obey* (1) *and let $H = H_0 + V$ as a sum of forms* [4, 7]. *Let $S_1 \equiv \{f \in L^2 \mid |\mathbf{x}| f \in L^2, \ |\mathbf{k}| \hat{f} \in L^2\}$ where $|\mathbf{x}| \equiv (\mathbf{x}^2)^{1/2}$, $|\mathbf{k}| \equiv (\mathbf{k}^2)^{1/2}$, $\hat{f}(\mathbf{k})$ is the Fourier transform of $f(\mathbf{x})$, and equip S_1 with the norm*

$$\begin{aligned} |||f|||_1 &= (\|f\|^2 + \| |\mathbf{x}| f\|^2 + \| |\mathbf{k}| \hat{f}\|^2)^{1/2} \\ &= (\|f\|^2 + \| |\mathbf{x}| f\|^2 + \| H_0^{1/2} f\|^2)^{1/2}. \end{aligned}$$

Then $\exp(-iHt)$ *maps S_1 onto S_1 and*

$$||| e^{-iHt} f |||_1 \leqslant (c + d|t|) |||f|||_1 \tag{3}$$

for suitable c and d.

Proof. From Eq. (1), one sees that, as form inequalities,

$$H_0 + V \leqslant (1 + a)H_0 + b$$

and

$$H_0 \leqslant (1 - a)^{-1}(H_0 + V + b).$$

Thus, if $f_t \equiv \exp(-iHt)f$, we have that $\| f_t \| = \| f \|$ and

$$\begin{aligned} \| H_0^{1/2} f_t \|^2 &\leqslant (1 - a)^{-1} \|(H_0 + V + b)^{1/2} f_t \|^2 \\ &\leqslant (1 - a)^{-1} \|(H_0 + V + b)^{1/2} f \|^2 \\ &\leqslant (1 - a)^{-1}((1 + a)\| H_0^{1/2} f \|^2 + 2b \| f \|^2). \end{aligned}$$

Therefore we need only show that if $f \in S_1$ then $f_t \in D(| \mathbf{x} |)$ and $\| | \mathbf{x} | f_t \| \leqslant (c_0 + | t | d_0) ||| f |||_1$.

We will first give a formal proof and then a rigorous one of these two facts. Let $\mathbf{x}(t) = \exp(iHt)\mathbf{x} \exp(-iHt)$, so that we want to show that $\langle f, \mathbf{x}(t)^2 f \rangle^{1/2}$ remains finite and in fact grows no more than linearly in t. Now formally the time derivative $\mathbf{x}'(t) = t[H, \mathbf{x}(t)] = 2\mathbf{p}(t)$, where $\mathbf{p}$ is the momentum $-i\nabla$, so that $(\mathbf{x}(t)^2)' = 2(\mathbf{x}(t) \cdot \mathbf{p}(t) + \mathbf{p}(t) \cdot \mathbf{x}(t))$ and therefore by the Schwarz inequality

$$\frac{d}{dt} \langle f, \mathbf{x}(t)^2 f \rangle \leqslant 4 \langle f, \mathbf{x}(t)^2 f \rangle^{1/2} \langle f, \mathbf{p}(t)^2 f \rangle^{1/2}.$$

Equivalently,

$$\frac{d}{dt} \langle f, \mathbf{x}(t)^2 f \rangle^{1/2} \leqslant 2 \langle f, \mathbf{p}(t)^2 f \rangle^{1/2}$$

or

$$\langle f, \mathbf{x}(t)^2 f \rangle^{1/2} \leqslant \langle f, \mathbf{x}(0)^2 f \rangle^{1/2} + \int_0^t 2 \langle f, \mathbf{p}(s)^2 f \rangle^{1/2} \, ds. \tag{4}$$

But by our previous considerations, $\langle f, \mathbf{p}(t)^2 f \rangle = \| H_0^{1/2} f_t \|^2 \leqslant \tilde{c} ||| f |||_1$, so (4) implies that $\langle f, \mathbf{x}(t)^2 f \rangle^{1/2}$ grows at most linearly in t.

To make the above rigorous we define the function $F_\epsilon(y) = (\mathbf{y}^2/(1 + \epsilon \mathbf{y}^2)$ and the corresponding operators $F_\epsilon(\mathbf{x})$, and $F_\epsilon(\mathbf{x}(t)) = \exp(iHt) F_\epsilon(\mathbf{x}) \exp(-iHt)$. $F_\epsilon(\mathbf{x}(t))$ is a bounded operator, so if we prove that for $f \in S_1$

$$\langle f, F_\epsilon(\mathbf{x}(t)) f \rangle^{1/2} \leqslant (c_0 + d_0 | t |) ||| f |||_1 \tag{5}$$

independently of ϵ, then taking ϵ to zero $\exp(-iHt) f \in D(| \mathbf{x} |)$ and

$$\langle f, \mathbf{x}(t)^2 f \rangle^{1/2} \leqslant (c_0 + d_0 | t |) ||| f |||_1 .$$

Let $\mathscr{H}_{+1}$, $\mathscr{H}_{-1}$ be the scale of Hilbert spaces associated with H_0 in the usual way [6], so that H is a bounded map from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$ and so that, by a simple calculation, $F_\epsilon(\mathbf{x})$ is a bounded map from $\mathscr{H}_{+1}$ (resp. $\mathscr{H}_{-1}$) to itself. Then as a map from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$, $F_\epsilon(\mathbf{x}(t))$ is strongly differentiable and

$$\begin{aligned}\frac{d}{dt} F_\epsilon(\mathbf{x}(t)) &= i[H, F_\epsilon(\mathbf{x}(t))] \\ &= ie^{iHt}[H, F_\epsilon(\mathbf{x})]\, e^{-iHt} \\ &= ie^{iHt}[H_0, F_\epsilon(\mathbf{x})]\, e^{-iHt} \\ &= \mathbf{G}_\epsilon(\mathbf{x}(t)) \cdot \mathbf{p}(t) + \mathbf{p}(t) \cdot \mathbf{G}_\epsilon(\mathbf{x}(t))\end{aligned}$$

where $\mathbf{G}_\epsilon(\mathbf{y}) = (\operatorname{grad} F_\epsilon)(\mathbf{y}) = 2\mathbf{y}/(1 + \epsilon\mathbf{y}^2)$. It follows that for $f \in S_1 \subset \mathscr{H}_{+1}$:

$$\frac{d}{dt} \langle f, F_\epsilon(\mathbf{x}(t)) f\rangle \leqslant 2 \| \,|\mathbf{p}|\,(t) f\| \, \| \,|\mathbf{G}_\epsilon|\,(\mathbf{x}(t)) f\|.$$

Since $\mathbf{G}_\epsilon(\mathbf{y})^2 = 4(\mathbf{y}^2/(1 + \epsilon\mathbf{y}^2))((1 + \epsilon\mathbf{y}^2)^{-1} \leqslant 4F(\mathbf{y})$, we see that

$$\begin{aligned}\frac{d}{dt} \langle f, F_\epsilon(\mathbf{x}(t)) f\rangle &\leqslant 4\langle f, F_\epsilon(\mathbf{x}(t)) f\rangle^{1/2} \| \,|\mathbf{p}|\,(t) f\| \\ &\leqslant 2c' \langle f, F_\epsilon(\mathbf{x}(t)) f\rangle^{1/2} |||f|||_1\end{aligned}$$

for a suitable constant c'. Integrating we obtain (5).

Remarks. 1. It is easy to see that (4) remains true if $\langle f, \mathbf{x}(t)^2 f\rangle$ is replaced by the variance in position,

$$\sigma_f(\mathbf{x}(t))^2 \equiv \langle f, \mathbf{x}(t)^2 f\rangle - \langle f, \mathbf{x}(t) f\rangle^2.$$

2. For scattering states $\langle f, \mathbf{x}(t)^2 f\rangle^{1/2}$ grows linearly in t as $t \to \pm\infty$, so the time behavior of (3) is best possible.

3. The results above are certainly not the first smoothness results for solutions of $i(d/dt)u = Hu$; for example, Kato [5] (see also Simon [10]) has proven that $C^\infty(H)$ is contained in the family of Holder continuous functions, under suitable conditions on V. See also [1, 2] for results resembling ours.

THEOREM 2.2. *Let V obey (2) and let $H = H_0 + V$ as a self adjoint operator sum* [4, 7]. *Let $S_2 = \{f \in L^2 \mid \mathbf{x}^2 f \in L^2, \mathbf{k}^2 \hat{f} \in L^2\}$, and equip S_2 with the norm*

$$\begin{aligned}|||f|||_2 &= (\|f\|^2 + \|\mathbf{x}^2 f\|^2 + \|\mathbf{k}^2 \hat{f}\|^2)^{1/2} \\ &= (\|f\|^2 + \|\mathbf{x}^2 f\|^2 + \|H_0 f\|^2)^{1/2}.\end{aligned}$$

Then $\exp(-iHt)$ *maps* S_2 *onto* S_2 *and for suitable* c' *and* d'

$$|||\, e^{-iHt}f \,|||_2 \leqslant (c' + d't^2)\, |||\, f \,|||_2 \,.$$

Formal proof. Since the pattern is the same as for Theorem 2.1, we only give a formal proof. As in the last theorem, one easily sees that

$$\| H_0 f_t \| \leqslant c\, |||\, f \,|||_2 \tag{6}$$

Moreover, for each j we have formally

$$\frac{d}{dt}\langle f, x_j(t)^4 f\rangle = 4\langle f, (p_j(t)\, x_j(t)^3 + x_j(t)^3 p_j(t)) f\rangle$$

so that by the Schwarz inequality

$$\begin{aligned}\frac{d}{dt}\langle f, x_j(t)^4 f\rangle &\leqslant 8\langle f, x_j(t)^4 f\rangle^{1/2}\langle f, p_j(t)\, x_j(t)^2 p_j(t) f\rangle^{1/2}\\ &\leqslant 8\langle f, x_j(t)^4 f\rangle^{1/2}(\langle f, p_j(t)^2 x_j(t)^2 f\rangle + 2i\langle f, p_j(t)\, x_j(t) f\rangle)^{1/2}\\ &\leqslant 8\langle f, x_j(t)^4 f\rangle^{1/2}(\langle f, p_j(t)^4 f\rangle + 2\langle f, p_j(t)^2 f\rangle)^{1/4}\\ &\quad\cdot (\langle f, x_j(t)^4 f\rangle + 2\langle f, x_j(t)^2 f\rangle)^{1/4}.\end{aligned}$$

Therefore

$$\frac{d}{dt}\langle f, (x_j(t)^4 + 1) f\rangle \leqslant \tilde{c}\langle f, (x_j(t)^4 + 1) f\rangle^{3/4}$$

i.e., $\langle f, x_j(t)^4 f\rangle^{1/4}$ is linearly bounded in t, and

$$\| \mathbf{x}(t)^2 f \|^2 \leqslant \sum_{j=1}^{N} \| x_j(t)^2 f \|^2 = \sum_{j=1}^{N} \langle f, x_j(t)^4 f\rangle.$$

3. Some Examples

We first want to show that for the atomic case there are f in Schwartz space such that $\langle f_t, |\mathbf{p}|^5 f_t\rangle$ blows up in finite time even though we know (see (6)) that $\langle f_t, |\mathbf{p}|^4 f_t\rangle$ is uniformly bounded in time.

Theorem 3.1. *Let* $V(\mathbf{x}) = -|\mathbf{x}|^{-1}$, $H = -\Delta + V$ *on* $L^2(\mathbb{R}^3)$. *Let* $f \in C_0^\infty(\mathbb{R}^3)$ *with* f *identically zero near* $\mathbf{x} = 0$, $f \geqslant 0$, $f \not\equiv 0$. *Then* $|\mathbf{k}|^{5/2}\hat{f}_t \notin L^2$ *for almost all real* t.

Proof. As a preliminary let $g \in C^\infty(H)$. Then g is, in particular, a Hölder continuous function since $C^\infty(H) \subseteq D(-\Delta)$ [5]. Suppose that $g(0) \neq 0$. Then we claim that $\langle g, |\mathbf{p}|^5 g\rangle = \infty$. For

$$\Delta g(\mathbf{x}) = -(Hg)(\mathbf{x}) - |\mathbf{x}|^{-1} g(\mathbf{x})$$

and by a result of Kato [3], Hg and g have gradients bounded as $\mathbf{x} \to 0$ so $\nabla(\Delta g(\mathbf{x})) = |\mathbf{x}|^{-3}\mathbf{x}g(0) + O(|\mathbf{x}|^{-1})$. Since $\Delta g(\mathbf{x}) = -|\mathbf{x}|^{-1} g(0) + O(1)$, we see that

$$\overline{\Delta g(\mathbf{x})}\, \nabla(\Delta g(\mathbf{x})) = -|\mathbf{x}|^{-4}\mathbf{x}\, |g(0)|^2 + O(|\mathbf{x}|^{-2})$$

which is not in L^1.

By the above, we only need to show that $f_t(0) \neq 0$ for almost all t. Let $h(t) = (\exp(-iHt)f)(0)$, defined for $\operatorname{Im} t \leqslant 0$. Then $h(t)$ is analytic in $\operatorname{Im} t < 0$, continuous and uniformly bounded in $\operatorname{Im} t \leqslant 0$ since $t \to \exp(-iHt)f$ has these properties as a $C^\infty(H)$ valued function and $f \to f(0)$ is a continuous linear map from $C^\infty(H)$ to $\mathbb{C}$. Also $h(t) \neq 0$ for $t = -ia$, $a > 0$, since $\exp(-aH)$ has a strictly positive integral kernel in the Feynman–Kac formula [7]. Thus $h(t) \neq 0$ for almost all real t by (a conformal mapping and) Fatou's theorem [8, Theorem 17.18] that a function in H^∞ of the disk which is not identically zero can only have zero boundary values on a set of measure zero.

Since $\langle f, |\mathbf{p}(t)|^5 f\rangle = \infty$ for most t and $\mathbf{x}'(t) = i[H, \mathbf{x}(t)] = 2\mathbf{p}(t)$, one might expect that $\langle f, |\mathbf{x}(t)|^5 f\rangle$ would be infinite, but this is not true as we shall see in the next section. One way of seeing that this intuition is not reliable is to consider an s-wave eigenfunction g: for that case, $\langle g, |\mathbf{p}|^5 g\rangle = \infty$ but $\langle g, |\mathbf{x}|^5 g\rangle < \infty$. One might feel that the failure of the intuition depends on the (Coulomb) force being attractive, for the following argument is alluring: If $\langle g, |\mathbf{p}(0)|^5 g\rangle = \infty$ and $\langle g, |\mathbf{x}(0)|^5 g\rangle < \infty$, then for the *free* evolution $\langle g, |\mathbf{x}(t)|^5 g\rangle = \infty$ for most t's since roughly $\langle g, |\mathbf{x}(t)|^5 g\rangle \sim \langle g, |\mathbf{x}(0) + 2t\mathbf{p}(0)|^5 g\rangle$. One might certainly expect that for a *repulsive* force the corresponding $\mathbf{x}(t)$ will have moments strictly larger than under free evolution. This intuition is also wrong, however, as we shall see in detail in the next section; we give a simple example here illustrating this phenomenon.

EXAMPLE. Consider the normalized wavefunction $f(x) = 2^{1/2}|x| \exp(-|x|)$ in $L^2(\mathbb{R})$. Its Fourier transform is

$$\hat{f}(k) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} e^{-ikx} f(x)\, dx = 2\pi^{-1/2}(1 - k^2)(1 + k^2)^{-2}.$$

Under the free evolution (which we denote by a superscript (0)) we have

$$\hat{f}_t^{(0)}(k) = \widehat{e^{-iH_0 t} f}(k) = e^{-ik^2 t} \hat{f}(k)$$

and using $\widehat{x^n f} = (id/dk)^n \hat{f}$ one sees easily that

$$\langle f_t^{(0)}, x^4 f_t^{(0)} \rangle = <\infty \qquad \text{for} \quad t = 0$$
$$= +\infty \qquad \text{for} \quad t \neq 0.$$

since $(d^2/dk^2) \exp(-ik^2t) \hat{f}(k)$ is not in L^2 if $t \neq 0$.

Now let $H = H_0 + \infty\delta(x)$, i.e. let H be the operator $-d^2/dx^2$ with Dirichlet boundary condition at $x = 0$. Let $g(x) = 2^{1/2} x \exp(-|x|)$. Then

$$\exp(-iHt)g = \exp(-iH_0 t)g$$

since $H = H_0$ on odd functions. But

$$f_t(x) = (e^{-iHt}f)(x) = (\operatorname{sgn} x)(e^{-iHt}g)(x)$$
$$= (\operatorname{sgn} x)(e^{-iH_0 t}g)(x)$$
$$= (\operatorname{sgn} x)\, g_t^{(0)}(x)$$

since H decouples the positive and negative halves of the real axis and $f(x) = (\operatorname{sgn} x)\, g(x)$. Thus $\langle f_t, x^4 f_t \rangle = \langle g_t^{(0)}, x^4 g_t^{(0)} \rangle$ and since

$$\hat{g}_t^{(0)}(k) = e^{-ik^2 t} \pi^{-1/2} (1 + k^2)^{-2} (-4ik)$$

one sees that $(d^2/dk^2)\hat{g}_t^{(0)} \in L^2$ and so $\langle f_t, x^4 f_t \rangle < \infty$ for all t.

Thus in this example f remains, in time, "better localized" about $x = 0$ under an evolution with a repulsive force centered at $x = 0$ than it would under a free evolution.

4. Decoupling of Local Singularities

In this final section we want to sketch a proof that local singularities in the potential energy V will not cause moments in position to diverge in time even though they can, of course, cause moments in momentum to diverge (see Theorem 3.1).

Theorem 4.1. *Suppose V obeys* (1) *and that outside some ball in $\mathbb{R}^m$, V is C^∞ with uniformly bounded derivatives (e.g., $V(\mathbf{x}) = \lambda |\mathbf{x}|^{-1}$). Let $f \in C^\infty(H)$ with $|\mathbf{x}|^n f \in L^2$ for all $n \in \mathbb{N}$. Then $|\mathbf{x}|^n f_t \in L^2$ for all $t \in \mathbb{R}$ and all $n \in \mathbb{N}$.*

Proof. Let the ball in the theorem be contained in $\{\mathbf{x} \mid |\mathbf{x}| \leqslant R\}$ and choose a function $q(\mathbf{x})$ with $1 - q \in C_0^\infty$, and $q(\mathbf{x}) = 0$ for $|\mathbf{x}| \leqslant R$ and $q(\mathbf{x}) = 1$ for $|\mathbf{x}| \geqslant 2R$. Clearly it suffices to show that $\langle f, q(\mathbf{x}(t)) |\mathbf{x}(t)|^{2^n} f \rangle < \infty$ for all t and n. Since all derivatives of q are bounded functions of compact support, if

$\langle f, q(\mathbf{x}(t)) \mid \mathbf{p}(t)|^{2^n} f\rangle < \infty$ for all n and t then by mimicking the proof of Theorem 2.2 we see that $\langle f, q(\mathbf{x}(t)) \mid \mathbf{x}(t)|^{2^n} f\rangle < \infty$. But $\mathbf{p}(t)^2 = H - V(\mathbf{x}(t))$ so that $q(\mathbf{x}(t)) \mid \mathbf{p}(t)|^{2^n}$ is a sum of terms of the form $q(\mathbf{x}(t))\, w(\mathbf{x}(t)) H^r$ and $p_j(t)\, q(\mathbf{x}(t))\, w(\mathbf{x}(t)) H^r$ with $q(y)\, w(y)$ uniformly bounded. Since

$$\begin{aligned}&|\langle f, p_j(t)\, q(\mathbf{x}(t))\, w(\mathbf{x}(t)) H^r f\rangle| \\ &\quad = |\langle f_t\,, p_j q(\mathbf{x})\, w(\mathbf{x})\, H^r f_t\rangle| \leqslant \| p_j f_t \| \, \| qw \|_\infty \, \| H^r f \|\end{aligned}$$

we see that $\langle f_t\,, q(\mathbf{x})\, w(\mathbf{x})\, H^r f_t\rangle$ is finite, which completes the proof.

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