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# THE QUANTUM $n$-BODY PROBLEM AND A THEOREM OF LITTLEWOOD

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**A quantum-mechanical analogue of a theorem of Littlewood on the impossibility of capture or escape is presented.**

**1. Introduction.** About 25 years ago Littlewood **[3]** proved a theorem in classical mechanics which shows that (aside from a set of initial conditions of measure zero) a gravitating system of bodies such as the solar system can never capture an external body, even a "speck". As Littlewood has remarked in his amusing, non-technical account **[4]**, "it is not that the speck promptly goes out again; it may be retained for any number of billion years... The proof in no way shows that it is the speck that goes out, it might be Jupiter." In accordance with the correspondence principle, one expects Littlewood's result to have an analogue in quantum mechanics. Such a theorem is the aim of this paper. Incidentally, Littlewood's argument, though rather general in outline, relies in detail on special properties of inverse square forces; but Littlewood expressed the opinion that this was probably not essential. Our quantum-mechanical theorem is valid for a quite wide class of potentials, including all the usual potentials of nonrelativistic atomic and molecular physics.

Littlewood's argument is roughly as follows. Consider a system of $n$ particles, with phase space $M$. Let $E$ be the subset of $M$ consisting of states $\omega$ of bounded energy such that for all times $t \geqq 0$, the diameter of the system represented by $\omega(t)$ (in physical space) is bounded by a constant $C$; that is, the system remains inside a fixed sphere for all future time. Obviously $E$ is mapped into itself by the dynamical group $\alpha_t\colon \omega \to \omega(t)$ for $t \geqq 0$. Moreover (the stickiest technical point) $E$ has finite Liouville measure. Since $\alpha_t(E) \subseteq E$ and $\alpha_t$ is measure-preserving, it follows that $\alpha_t(E) = E$ except possibly for a subset of measure zero, and hence that $\alpha_t^{-1}(E) = \alpha_{-t}(E)$ is essentially contained in $E$. Thus, with the possible exception of a set of states $\omega$ of measure zero, if $\omega(t)$ lies in a fixed sphere for all future times $t$, then the same is the case for all past times as well. Hence there are essentially no captures (or escapes, by the time-reversal of this argument).

Our quantum mechanical argument is in the same spirit. As Littlewood points out, all such arguments are descended from Poincaré's recurrence theorem. Nevertheless, the details seem of some interest. In particular, quantum mechanics has no direct substitute for

Liouville measure. But the quantum dynamical transformations $\alpha_t$ are isometries. And, amusingly enough, it turns out that one can replace the classical measure-theoretic argument by the well-known fact that an isometry mapping a compact metric space into itself is actually surjective.

**2. The quantum mechanical set-up.** We work on a Hilbert space $\mathcal{H}$ in the usual way. $B_1(\mathcal{H})$ will denote the trace-class operators on $\mathcal{H}$, with the norm $\|\Omega\|_1 = \operatorname{tr}(|\Omega|)$. The space of (mixed) states $\Sigma$ consists of all $\Omega \in B_1(\mathcal{H})$ with $\Omega \geqq 0$ and $\operatorname{tr}(\Omega) = 1$ $(= \|\Omega\|_1)$. The Hamiltonian operator $H$ generates a unitary group $U_t = e^{-itH}$ on $\mathcal{H}$. The dynamical group $\alpha_t : \Sigma \to \Sigma$ is defined by $\alpha_t(\Omega) = U_t \Omega U_t^*$. Note that $\alpha_t$ is an isometry relative to the trace norm $\|\cdot\|_1$.

We will be dealing with a nonrelativistic system of finitely many interacting particles, and we may assume that the coordinates of the center of mass have been separated out. Then $\mathcal{H}$ will be of the form $L^2(\mathbf{R}^d)$; we will not mention "spin" explicitly, but our wave functions may have any fixed finite number of components. We denote the usual position and momentum operators by $Q_i$, $P_j$ for $i, j = 1, 2, \cdots, d$.

We record here some technical results which will be used in the proof of the main theorem.

LEMMA 2.1. *Suppose $A$ and $B$ are compact operators on $\mathcal{H}$. Define $T$ on $B_1(\mathcal{H})$ by $T\Omega = A\Omega B$. Then $T$ is compact.*

*Proof.* Let $A_n, B_n$ be two sequences of finite-rank operators on $\mathcal{H}$ converging in norm to $A, B$ respectively. Define $T_n$ on $B_1(\mathcal{H})$ by $T_n\Omega = A_n \Omega B_n$. Then $T_n$ is a finite-rank operator. We shall show that $T_n \to T$ in operator norm.

Indeed, for any $\Omega \in B_1(\mathcal{H})$, we have

$$\begin{aligned}
\| T\Omega - T_n\Omega \|_1 &= \| A\Omega B - A_n\Omega B + A_n\Omega B - A_n\Omega B_n \|_1 \\
&\leqq \| (A - A_n)\Omega B \|_1 + \| A_n\Omega(B - B_n) \|_1 \\
&\leqq \| A - A_n \| \, \| B \| \, \| \Omega \|_1 + \| A_n \| \, \| B - B_n \| \, \| \Omega \|_1
\end{aligned}$$

so that

$$\| T - T_n \| \leqq \| A - A_n \| \, \| B \| + \| A_n \| \, \| B - B_n \|.$$

This tends to 0 as $n$ approaches $\infty$.

PROPOSITION 2.2. *Let $A$ be a positive compact operator on $\mathcal{H}$. Define*

$$\mathcal{S} = \{\Omega \in B_1(\mathcal{H}) : \Omega \geqq 0, \ \operatorname{tr}(\Omega) = 1, \quad \textit{and} \quad \operatorname{tr}(\Omega A^{-1}) \leqq 1\}.$$

*Then $\mathcal{S}$ is a compact subset of $B_1(\mathcal{H})$.*

NOTE. The condition $\operatorname{tr}(\Omega A^{-1}) \leqq 1$ means that $A^{-1/2}\Omega A^{-1/2}$ is trace class with $\operatorname{tr}(A^{-1/2}\Omega A^{-1/2}) \leqq 1$. Note that the operators $A^{-1}$ and $A^{-1/2}$ are unbounded in general.

*Proof.* Consider the operator $T$ on $B_1(\mathcal{H})$ defined by $T\Omega = A^{1/2}\Omega A^{1/2}$. By the lemma, $T$ is compact. Moreover, $\mathcal{S}$ consists of those $\Omega$ such that $\Omega \geqq 0$, $\operatorname{tr}(\Omega) = 1$, and $\Omega = T\Omega'$ for some $\Omega'$ (namely $A^{-1/2}\Omega A^{-1/2}$) with $\|\Omega'\|_1 \leqq 1$. Hence $\mathcal{S}$ is a subset of the $T$-image of the unit ball of $B_1(\mathcal{H})$. Since $T$ is compact, $\mathcal{S}$ has compact closure.

The proof will be finished if we show that $\mathcal{S}$ is closed in norm. Suppose $\Omega_n \in \mathcal{S}$ converges to $\Omega$ in trace norm. Then clearly $\Omega \geqq 0$ and $\operatorname{tr}(\Omega) = 1$. We have to show that $\operatorname{tr}(\Omega A^{-1})$ is finite and $\leqq 1$. To see this let $\{e_k\}_1^\infty$ be a basis of eigenvectors for $A$: $Ae_k = \lambda_k e_k$. Then (Fatou's lemma):

$$\begin{aligned}
\sum_k (\Omega A^{-1} e_k, e_k) &= \sum_k \lambda_k^{-1}(\Omega e_k, e_k) \\
&\leqq \limsup_{n\to\infty} \sum_k \lambda_k^{-1}(\Omega_n e_k, e_k) \\
&= \limsup_{n\to\infty} \operatorname{tr}(\Omega_n A^{-1}) \leqq 1.
\end{aligned}$$

The quantum-mechanical applications rely upon the following corollary, which is a sort of "noncommutative" version of the Rellich–Sobolev embedding theorem.

COROLLARY 2.3. *Let $\mathcal{H} = L^2(\mathbf{R}^d)$, $P^2 = \sum_{i=1}^d P_i^2$, $Q^2 = \sum_{i=1}^d Q_i^2$, where $P_i$, $Q_i$ are the usual momentum and position operators. Let $C > 0$. Define*

$$\mathcal{S}_C = \{\Omega \in B_1(\mathcal{H}) : \Omega \geqq 0, \ \operatorname{tr}(\Omega) = 1, \ \operatorname{tr}(\Omega P^2) \leqq C, \ \operatorname{tr}(\Omega Q^2) \leqq C\}.$$

*Then $\mathcal{S}_C$ is compact.*

*Physical interpretation.* The set of quantum mechanical states with bounded expectation of position and momentum is compact. (Obviously the corresponding region of classical phase space has finite measure.)

*Proof.* Let $H_0 = P^2 + Q^2$, the usual harmonic oscillator Hamiltonian. It is well known that $A = H_0^{-1}$ is compact. And clearly $\mathscr{S}_C$ is a closed subset of

$$\mathscr{S} = \{\Omega: \Omega \geqq 0, \operatorname{tr}(\Omega) = 1, \operatorname{tr}(\Omega A^{-1}) \leqq 2C\}.$$

By the proposition, $\mathscr{S}$ is compact. Hence so is $\mathscr{S}_C$.

**3. Main theorem.** On $\mathscr{H} = L^2(\mathbf{R}^d)$ define $K = -\Sigma_{j=1}^{d}(1/2m_j)P_j^2$, the kinetic energy operator. Here $m_1, m_2, \cdots, m_d > 0$ are the masses of the particles (more properly, the reduced masses, since we have separated out the center of mass). Then the Hamiltonian $H = K + V$, where $V$ is a suitable potential function on $\mathbf{R}^d$.

We will restrict our attention to potentials $V$ satisfying the following technical hypotheses. (For background, including the proof that the usual potentials in atomic and molecular physics satisfy these conditions, see Kato's book **[2]**.) First of all, $K + V$ should be (essentially) self-adjoint. Moreover, $V$ should have a decomposition $V = V_1 + V_2$ where $V_1$ is relatively bounded with respect to $K$ with relative bound $< 1$, while $V_2$ satisfies an inequality of the form $V_2 \geqq -\lambda Q^2$; that is, $V_2$ does not decrease too rapidly at infinity. The condition on $V_1$ implies in particular that there are constants $\epsilon > 0$ and $a < \infty$ such that

$$K + V_1 \geqq \epsilon K - aI.$$

Because $K \geqq$ constant $P^2$, it follows (for smaller $\epsilon$ possibly) that

$$K + V_1 \geqq \epsilon P^2 - aI.$$

Hence $H = K + V_1 + V_2$ satisfies

$$H \geqq \epsilon P^2 - \lambda Q^2 - aI. \tag{1}$$

A potential $V$ satisfying the above conditions will be called *regular.*

Now consider the state space $\Sigma \subseteq B_1(\mathscr{H})$. A state $\Omega \in \Sigma$ will be called *quasi-bounded*, provided:

(i) $\operatorname{tr}(\Omega H) < \infty$, i.e., the energy has expected value $< \infty$ in the state $\Omega$;

(ii) there exists a constant $C < \infty$ so that, for all $t \geqq 0$,

$$\operatorname{tr}(\Omega(t)Q^2) < C. \tag{2}$$

Here $\Omega(t) = \alpha(t)\Omega$ where $\alpha(t)$ is the dynamical group.

(Thus, for each $j$, $\mathrm{tr}(\Omega(t)Q_j^2) < C$, and therefore the probability distributions for all the position vectors are largely concentrated in a fixed sphere in space for all times $t \geqq 0$.)

THEOREM. 3.1. *Let $V$ be a regular potential on $\mathbf{R}^d$. Let $\mathcal{H} = L^2(\mathbf{R}^d)$, $H = K + V$. Suppose that $\Omega \in B_1(\mathcal{H})$ is a quasi-bounded state, i.e.,* (2) *holds for some $C$ and all $t \geqq 0$. Then* (2) *holds also for all $t < 0$.*

(Thus, a state which is quasi-bounded for all future time must have been quasi-bounded in the past as well. This is the point of Littlewood's theorem.)

*Proof.* Since $V$ is regular, it follows from (1) that

$$H + (\lambda + \epsilon)Q^2 + aI \geqq \epsilon(P^2 + Q^2) = \epsilon H_0, \tag{3}$$

a key inequality. (Incidentally, no such inequality is valid on the classical level; the quantum case is thus "easier" than the classical case.)

If $C$ is a fixed constant, define

$$\mathcal{S} = \{\Omega \in \Sigma \colon \mathrm{tr}(\Omega H) \leqq C \quad \text{and} \quad \mathrm{tr}(\Omega Q^2) \leqq C\}.$$

Then let $\mathcal{S}' = \bigcap_{t \geqq 0} \alpha_t^{-1}(\mathcal{S}) = \{\Omega \colon \alpha_t(\Omega) \in \mathcal{S} \text{ for all } t \geqq 0\}$. We claim that if $\Omega \in \mathcal{S}'$ then $\alpha_t(\Omega) \in \mathcal{S}$ for all $t < 0$ as well.

If $\Omega \in \mathcal{S}$, it follows from (3) that

$$\mathrm{tr}(\Omega H_0) \leqq \epsilon^{-1}\mathrm{tr}(\Omega(H + (\lambda + \epsilon)Q^2 + aI)) \leqq C',$$
$$\text{where} \quad C' = \epsilon^{-1}(C + (\lambda + \epsilon)C + a).$$

It follows from Proposition 2.3 that $\mathcal{S}$ is compact in $B_1(\mathcal{H})$, hence so is $\mathcal{S}'$. Moreover, it is obvious that if $t \geqq 0$ then $\alpha_t(\mathcal{S}') \subseteq \mathcal{S}'$. But $\alpha_t$ is an isometry. Hence, by the fact about compact metric spaces which we recalled in §1, it follows that $\alpha_t(\mathcal{S}') = \mathcal{S}'$.

Since $\alpha_{-t} = \alpha_t^{-1}$, it follows that $\alpha_{-t}(\mathcal{S}') = \mathcal{S}'$ for all $t \geqq 0$, and so $\alpha_t(\mathcal{S}') = \mathcal{S}'$ for all $t$, positive or negative.

But this implies that if $\Omega \in \mathcal{S}'$ then $\alpha_t(\Omega) \in \mathcal{S}$ for all real $t$, as we wanted to show.

From the proof, we draw the following conclusion about "recurrence": If $\Omega$ is a quasi-bounded state then $\alpha_t(\Omega)$ returns arbitrarily close to $\Omega$ for arbitrarily large values of $t$. To see this, consider any $p > 0$. We have a sequence $\Omega_n = \alpha_{np}(\Omega)$ in the compact metric space $\mathcal{S}'$. Then, given $\epsilon > 0$, we can find $m < n$ with $\|\Omega_n - \Omega_m\|_1 < \epsilon$. Hence $\|\alpha_{(n-m)p}(\Omega) - \Omega\|_1 < \epsilon$; since $(n - m)p \geqq p$ we have $\|\alpha_t(\Omega) - \Omega\|_1 < \epsilon$ for some $t \geqq p$.

The theorem has some connections with the question of unitarity and completeness of the scattering operator. We briefly recall the definitions [2]: If $\phi \in \mathcal{H}$ and $e^{-itK}\phi \sim e^{-itH}\psi$ as $t \to +\infty$ we write $\psi = W_+\phi$. Similarly for $W_-$; thus we have the wave operators

$$W_\pm \phi = \lim_{t \to \pm\infty} e^{itH} e^{-itK} \phi$$

if the limits exist. The scattering operator $S = W_+^* W_-$. One hopes that under suitable hypotheses $S$ is unitary, and this means in particular that $R(W_-) \subseteq R(W_+)$. More precisely, it would be desirable to show that $R(W_+) = R(W_-)$ and that the orthogonal complement $R(W_+)^\perp$ is just the closed linear subspace spanned by the bound states of $H$ ("completeness" of the wave operators). This is in general a very difficult problem. Nevertheless, Theorem 3.1 has something (not a great deal) to say about it.

LEMMA 3.2. *Under the hypotheses of Theorem* 3.1, *suppose that* $\psi \in \mathcal{H}$ *is a quasi-bounded state.* (This means that the corresponding operator $\Omega_\psi = |\psi\rangle\langle\psi|$ is a quasi-bounded state.)
*Then* $\psi \in R(W_+)^\perp$.

*Proof.* Suppose $\phi \in \mathcal{D}(W_+)$. Then

$$\begin{aligned}(\psi, W_+\phi) &= \lim_{t \to +\infty} (\psi, e^{itH} e^{-itK}\phi) \\ &= \lim_{t \to +\infty} (e^{-itH}\psi, e^{-itK}\phi).\end{aligned}$$

We must show this limit equals zero.

First of all, for any fixed $\theta \in \mathcal{H}$, we have $(\theta, e^{-itK}\phi) \to 0$ as $t \to \infty$. (This may be seen by writing the inner product in terms of the Fourier transforms of $\theta$ and $\phi$ and applying the Riemann–Lebesgue lemma.) It then follows that $(\theta, e^{-itK}\phi) \to 0$ as $t \to +\infty$, uniformly as $\theta$ varies over any compact subset of $\mathcal{H}$.

But since $\psi$ is quasi-bounded, our earlier arguments may be adapted to show that $\{e^{-itH}\psi\}_{t \geq 0}$ has compact closure in $\mathcal{H}$. Hence $(e^{-itH}\psi, e^{-itK}\phi)$ tends to 0 as $t \to +\infty$.

We thus have the following interpretation of Theorem 3.1. If $\psi \in \mathcal{H}$ is quasi-bounded, Lemma 3.2 shows that $\psi \in R(W_+)^\perp$. But the conclusion of Theorem 3.1 enables us to argue similarly that $\psi \in R(W_-)^\perp$. Thus Theorem 3.1 tends to support the equality of $R(W_+)$ and $R(W_-)$; of course the latter equality would be a vastly stronger conclusion.

NOTE. It has been pointed out to us that our results are related to the contents of refs. **[1]**, **[5]**.

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