Introduction to time dependent scattering theory

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Basic Non-Relativistic Quantum Mechanics

A physical system is described by a Hilbert space $\mathcal{H}$ and a collection of self-adjoint operators on $\mathcal{H}$.

Every one dimensional subspace of $\mathcal{H}$ represents a possible *state* of the system. We may represent a state by a unit vector $\psi \in \mathcal{H}$, keeping in mind that ψ and $e^{i\theta}\psi$ represent the same state.

Observables are measurable quantities such as position, momentum or energy. They are represented by (possibly unbounded) self-adjoint operators.

Suppose A is a self-adjoint operator representing, say, potential energy. By the spectral theorem, there is a unitary transformation from $\mathcal{H}$ to $L^2(X, d\mu)$ so that UAU^* is multiplication by $f(x)$. Under this unitary equivalence, every state $\psi \in \mathcal{H}$ corresponds to a function $\psi(x) \in L^2(X, d\mu)$ with

$$\int_X |\psi(x)|^2 d\mu(x) = 1$$

Thus $|\psi(x)|^2 d\mu(x)$ is a probability measure. Let $d\nu_\psi$ denote its push forward, via f, to the real line. Then $d\nu_\psi$ is the probability distribution for the potential energy. In other words, the quantity

$$\int_\Omega d\nu_\psi = \int_{f^{-1}(\Omega)} |\psi(x)|^2 d\mu(x)$$

is the probability that a measurement of potential energy when the system is in the state ψ will lie in the set $\Omega \subset \mathbb{R}$. Notice that $d\nu_\psi$ is supported on the spectrum $\sigma(A)$ of A. To see this recall that the spectrum of A is equal to the range of values taken on by f. Therefore, if Ω has empty intersections with $\sigma(A)$ then $f^{-1}(\Omega) = \emptyset$ and the integral above is equal to zero.

The nature of the spectrum of A is reflected in the possible outcomes when measuring A. For example, if A has discrete spectrum, then a measurement of A will produce one of only a discrete set of values.

The probability distribution $d\nu_\psi$ can be used to compute other quantities of physical interest. For example, the expected value of the potential energy in the state ψ is

$$\int_{\mathbb{R}} \lambda d\nu_\psi(\lambda) = \int_X f(x)|\psi(x)|^2 d\mu(x) = \langle \psi, A\psi \rangle.$$

In fact, for any Borel function g, the expectation of $g(A)$ is

$$\int_{\mathbb{R}} g(\lambda) d\nu_\psi(\lambda) = \int_X g(f(x))|\psi(x)|^2 d\mu(x) = \langle \psi, g(A)\psi \rangle.$$

In particular, if we set g to be the indicator function for an interval, we obtain the probability that the system has its potential energy in that interval when it is in the state ψ.

It is conceptually important to realize that the probabilistic distribution of values of an observable in a given state does not arise from incomplete knowledge of the state, but is inherent in the quantum description. (It is also possible to give a quantum description of a situation where only partial information is known by considering *mixed states*. In this case, probability enters the theory in two distinct ways.)

Time evolution

The total energy of system is a distinguished observable H called the Hamiltonian. It governs the time evolution of states. If the system is in the state ψ_0 at time $t = 0$, then the state $\psi(t)$ at future times is given (formally) by the solution of the time dependent Schrödinger equation

$$i\psi'(t) = H\psi(t)$$

with initial condition $\psi(0) = \psi_0$. Thus formally

$$\psi(t) = e^{-iHt}\psi_0.$$

But this is a meaningful formula, by the spectral theorem. So we define this to be the time evolution generated by the Hamiltonian H. The precise relationship between it and the Schrödinger equation is given by Stone's theorem below.

Actually, there is a second way in which the state of a system may change. This happens whenever a measurement is made. This "collapse of the wave packet" leads to serious philosophical difficulties. These are usually dealt with by ignoring them completely.

Stone's theorem

A strongly continuous, one-parameter group of unitary transformations is a map $U(t)$ from $\mathbb{R}$ into the unitary operators on a Hilbert $\mathcal{H}$ space satisfying

(i) $t \mapsto U(t)\psi$ is continuous in $\mathcal{H}$ for every $\psi \in \mathcal{H}$

(ii) $U(t+s) = U(t)U(s)$

Every self-adjoint operator A defines a strongly continuous, one-parameter group of unitary transformations given by e^{-itA}. To see this, use the spectral theorem to diagonalize A. Then e^{-itA} becomes multiplication by $e^{-itf(x)}$ on $L^2(X, d\mu)$. This is clearly unitary and satisfies (ii). To prove strong continuity, notice that $|e^{-i\epsilon f(x)} - 1|^2$ tends to zero pointwise as $\epsilon \to 0$, and $|e^{-i\epsilon f(x)} - 1|^2 \leq 4$. Thus,

$$\begin{aligned}\lim_{\epsilon\to 0} \|e^{-i(t+\epsilon)A}\psi - e^{-itA}\psi\|^2 &= \lim_{\epsilon\to 0} \int_X |\left(e^{-i(t+\epsilon)f(x)} - e^{-itf(x)}\right)\psi(x)|^2 d\mu(x) \\ &= \lim_{\epsilon\to 0} \int_X |e^{-i\epsilon f(x)} - 1|^2 |\psi(x)|^2 d\mu(x) \\ &= 0\end{aligned}$$

by the dominated convergence theorem.

Even though $e^{-itA}\psi$ is defined and continuous as a function of t for every $\psi \in \mathcal{H}$, it may not be differentiable in t.

Lemma 1.1 *Let A be a selfadjoint operator with domain $D(A)$. Then $e^{-itA}\psi$ is differentiable in t if and only if $\psi \in D(A)$. In this case*

$$\frac{d}{dt} e^{-itA}\psi = -iAe^{-itA}\psi$$

So even though the equation only makes sense if $\psi \in D(A)$, the solution $e^{-itA}\psi$ makes sense for all initial conditions ψ. To illustrate this point, consider $A = -id/dx$ acting in $L^2(\mathbb{R})$. Then the equation

$$i\frac{d\psi}{dt} = A\psi = -i\frac{d\psi}{dx}$$

with initial condition some differentiable function ψ_0 has solution $\psi_0(x-t)$ since

$$\frac{d\psi}{dt} = -\psi_0'(x-t) = -\frac{d\psi}{dx}$$

So, the equation only makes sense for suitably differentiable initial conditions, for which ψ_0' has a meaning. However the solution $(e^{-itA}\psi_0)(x) = \psi_0(x-t)$ makes sense for any $\psi_0 \in L^2(\mathbb{R})$ and defines a strongly continuous unitary group of transformations.

Stone's theorem asserts that all one-parameter groups of unitary transformations are given by self-adjoint operators.

Theorem 1.2 (Stone's theorem) *Every strongly continuous, one-parameter group of unitary transformations is given by e^{-itA} for some self-adjoint operator A.*

This theorem shows that if a symmetric operator has different self-adjoint extensions, then these extensions will generate different dynamics.

This can be illustrated by the symmetric operator $A = -id/dx$ acting in $L^2([0,1], dx)$ with domain C_0^∞. Different self-adjoint extensions A_α correspond to the boundary conditions $\psi(0) = e^{i\alpha}\psi(1)$. The group $e^{-iA_\alpha}t$ acts by shifting functions to the right, just like the example on the whole line. But when the left endpoint is reached, the function gets fed in again from the right—multiplied by the phase $e^{i\alpha}$.

The wave operators

The goal of time dependent scattering theory is to give a detailed description of the evolution of $e^{-itH}\psi$ as $t \to \pm\infty$.

If ψ is an eigenfunction of H with $H\psi = \lambda\psi$ then the time evolution of ψ is given by

$$\psi_t = e^{-itH}\psi = e^{it\lambda}\psi.$$

Theses are just different unit vector representations for the same state. The the probability measures $d\nu_{\psi_t}$ (for any observable) do not change with time. These states are called *bound states*.

We therefore restrict our attention to $\psi \in \mathcal{H}_c(H)$ and study $e^{-itH}P_c$, where P_c is the projection onto the continuous spectral subspace $\mathcal{H}_c(H)$.

One way to describe the long time behaviour of $e^{-itH}\psi$ is to find a simpler operator H_0 (called the *free Hamiltonian*) that describes the large time behaviour. We will assume that H_0 has purely absolutely continuous spectrum. The pair (H, H_0) are said to be *asymptotically complete* if

> *(1) For large positive and negative times, every orbit $e^{-itH}\psi$ with $\psi \in \mathcal{H}_c(H)$ is approximated by a free orbit. In other words, for every $\psi \in \mathcal{H}_c(H)$ there exists two vectors $\varphi_\pm$ such that*
>
> $$\lim_{t\to\pm\infty} \|e^{-itH}\psi - e^{-itH_0}\varphi_\pm\| = 0$$
>
> *(2) For large positive and negative times, every free orbit $e^{-itH_0}\varphi$ is the asymptotic description of some orbit under H. In other words, for every $\varphi \in \mathcal{H}$ there exists two vectors $\psi_\pm \in \mathcal{H}_c(H)$ such that*
>
> $$\lim_{t\to\pm\infty} \|e^{-itH_0}\varphi - e^{-itH}\psi_\pm\| = 0$$

Since

$$\|e^{-itH}\psi - e^{-itH_0}\psi_\pm\| = \|e^{-itH_0}\left((e^{itH_0}e^{-itH}\psi - \psi_\pm\right)\| = \|(e^{itH_0}e^{-itH}\psi - \psi_\pm\|$$

condition (1) is equivalent to the existence of the strong limit

$$\Omega_\pm(H_0, H) = \operatorname*{s-lim}_{t\to\mp\infty} e^{itH_0}e^{-itH}P_c$$

while condition (2) is equivalent to the existence of the strong limit

$$\Omega_\pm(H, H_0) = \operatorname*{s-lim}_{t\to\mp\infty} e^{itH}e^{-itH_0}$$

It is usually much easier to establish the existence of the wave operators $\Omega_\pm(H, H_0)$.

Proposition 1.3 *Suppose that $\Omega_{\pm}(H, H_0)$ exist. Then*

$$\mathrm{Ran}\Omega_{\pm}(H, H_0) \subseteq \mathcal{H}_{ac}(H)$$

Proof: To begin, we note that if $d\nu_{\psi,H}$ is the probability measure associated with the observable H and the state ψ, then

$$\langle \psi, e^{-itH}\psi \rangle = \int_{\mathbb{R}} e^{-it\lambda} d\nu_{\psi,H}(\lambda)$$

is the Fourier transform of the measure.

Secondly, we note the intertwining property

$$\begin{aligned} e^{-itH}\Omega_{\pm}(H, H_0) &= \operatorname*{s-lim}_{s\to\mp\infty} e^{-itH} e^{isH} e^{-isH_0} \\ &= \operatorname*{s-lim}_{s\to\mp\infty} e^{i(s-t)H} e^{-i(s-t)H_0} e^{-itH_0} \\ &= \Omega_{\pm}(H, H_0) e^{-itH_0} \end{aligned}$$

Since $\Omega_{\pm}$ are limits of unitary operators $\|\Omega_{\pm}\psi\| = \|\psi\|$ for any $\psi \in \mathcal{H}$. This implies $\langle \Omega_{\pm}\psi, \Omega_{\pm}\phi \rangle = \langle \psi, \phi \rangle$. Now suppose that $\psi \in \mathrm{Ran}\Omega_{\pm}$. Then $\psi = \Omega_{\pm}\phi_{\pm}$. Therefore

$$\begin{aligned} \widehat{d\nu_{\psi,H}}(t) &= \langle \psi, e^{-itH}\psi \rangle \\ &= \langle \Omega_{\pm}\phi_{\pm}, e^{-itH}\Omega_{\pm}\phi_{\pm} \rangle \\ &= \langle \Omega_{\pm}\phi_{\pm}, \Omega_{\pm} e^{-itH_0}\phi_{\pm} \rangle \\ &= \langle \phi_{\pm}, e^{-itH_0}\phi_{\pm} \rangle \\ &= \widehat{d\nu_{\phi_{\pm},H_0}}(t) \end{aligned}$$

This implies $d\nu_{\phi,H_0} = d\nu_{\psi,H}$. But $d\nu_{\phi_{\pm},H_0}$ is purely absolutely continuous, since H_0 has purely absolutely continuous spectrum. Thus $\psi \in H_{ac}(\mathcal{H})$. $\square$

Proposition 1.4 *Suppose that $\Omega_{\pm}(H, H_0)$ exist. Then $\Omega_{\pm}(H_0, H)$ exist (and asymptotic completeness holds) if and only if $\mathcal{H}_c(H) \subseteq \mathrm{Ran}\Omega_{\pm}(H, H_0)$*

Proof: $\Omega_{\pm}(H_0, H)$ exists if and only if for every $\psi \in \mathcal{H}_c(H)$, there exists $\psi_{\pm}$ with

$$\lim_{t\to\pm\infty} \|e^{-itH}\psi - e^{-itH_0}\varphi_{\pm}\| = 0.$$

This happens if and only if for every $\psi \in \mathcal{H}_c(H)$, there exists $\psi_{\pm}$ with

$$\lim_{t\to\pm\infty} \|\psi - e^{itH} e^{-itH_0}\varphi_{\pm}\| = 0,$$

i.e., with $\psi = \Omega_{\pm}(H, H_0)\varphi_{\pm}$. $\square$

These two propositions show that asymptotic completeness is equivalent to the existence of the wave operators $\Omega_{\pm}(H, H_0)$ and the equalities $\mathrm{Ran}\Omega_{\pm}(H, H_0) = \mathcal{H}_c(H) = \mathcal{H}_{ac}(H)$. In particular, if asymptotic completeness holds, H has no singular continuous spectrum.

If asymptotic completeness holds, the scattering operator, defined by

$$S = \Omega_-(H_0, H)\Omega_+(H, H_0)$$

is an isometry. The scattering operator has the following physical interpretation. Consider an orbit $\psi_t = e^{-itH}\psi$. If in the distant past $\psi_t \sim e^{-itH_0}\phi$, then in the far future $\psi_t \sim e^{-itH_0}S\phi$.

Trace class scattering

There are two main methods in time dependent scattering theory. They are trace class methods and positive commutator methods. Positive commutator methods have led to great advances in the last fifteen years. They give the strongest results in situations where H_0 is known explicitly. A good reference is *Scattering Theory of Classical and Quantum N-particle Systems,* by Dereziński and Gérard.

In this lecture I will present a sketch of the proof of the existence of wave operator under a trace condition. This theorem is due to Pearson and taken from Barry Simon's book on trace ideals. Omitted details can be found there.

Notice that to show that a strong limit of operators of the form $W_t = e^{itA}Je^{-itB}P_c(B)$ exists, it suffices to show that the limit exists on a dense set $\mathcal{D}$. Here J is assumed to be a bounded operator. To see this notice

$$\|W_t\| \le \|J\|$$

and so is bounded independently of t. Thus to show that $W_t\psi$ has a limit we let $\epsilon > 0$ and choose $\phi \in \mathcal{D}$ such that $\|\psi - \phi\| < \epsilon$. Then

$$\limsup_{s,t\to\infty} \|W_t\psi - W_s\psi\| \le \limsup_{s,t\to\infty} \|W_t\phi - W_s\phi\| + 2\|J\|\epsilon = 2\|J\|\epsilon$$

This implies that $W_t\psi$ is Cauchy and thus converges.

We will need the following lemma

Lemma 1.5 *Suppose that A is self-adjoint, C is bounded with $C(A+i)^{-n}$ compact for some n. Then*

$$\operatorname*{s-lim}_{t\to\pm\infty} Ce^{-itA}P_{ac} = 0$$

Theorem 1.6 *Let A and B be self-adjoint operators. Suppose there exists a bounded operator J so that $AJ - JB$ is trace class. Then*

$$\Omega_\pm(A, B; J) = \operatorname*{s-lim}_{t\to\mp\infty} e^{itA}Je^{-itB}P_c(B)$$

exist.

If $J = I$ we obtain the so-called Kato-Rosenblum theorem. However, for $H = -\Delta + V$ and $H_0 = -\Delta$ this would require V to be trace class. This never happens for a multiplication operator. The power of including the operator J is demonstrated by the following corollary.

Corollary 1.7 *(***Kuroda-Birman theorem***) If $(A+i)^{-1} - (B+i)^{-1}$ is trace class then the pair (A, B) then $\Omega_{\pm}(A, B)$ exists.*

Since the hypotheses are symmetric in A and B we automatically get asymptotic completeness.

Proof: Take $J = (A+i)^{-1}(B+i)^{-1}$. Then $AJ - JB = (A+i)^{-1} - (B+i)^{-1}$ and is compact, so we may apply Theorem 1.6 to conclude that $\Omega_{\pm}(A, B; (A+i)^{-1}(B+i)^{-1})$ exist.

Now we have

$$\Omega_{\pm}(A, B; (A+i)^{-1}(B+i)^{-1})(B+i)\psi = \Omega_{\pm}(A, B; (A+i)^{-1})\psi$$

so $\Omega_{\pm}(A, B; (A+i)^{-1})$ exists on the dense set $D(B)$ and hence exists.

Since $(A+i)^{-1} - (B+i)^{-1}$ is compact $\Omega_{\pm}(A, B; (A+i)^{-1} - (B+i)^{-1})$ and equals zero by the lemma. Thus

$$\Omega_{\pm}(A, B; (B+i)^{-1}) = \Omega_{\pm}(A, B; (A+i)^{-1}) - \Omega_{\pm}(A, B; (A+i)^{-1} - (B+i)^{-1})$$

exists. But $\Omega_{\pm}(A, B; (B+i)^{-1})(B+i)\psi = \Omega_{\pm}(A, B)\psi$ so $\Omega_{\pm}(A, B)$ exists on the dense set $D(B)$ and hence everywhere. $\square$

When $H = -\Delta + V$ and $H_0 = -\Delta$ this theorem applies when $(-\Delta + V + i)^{-1}V(-\Delta + i)^{-1}$ is trace class. This can be proved for sufficiently rapidly decaying V ($V \sim |x|^{-n-\epsilon}$ in $\mathbb{R}^n$).

We need the following lemma

Lemma 1.8 *There is a dense subset $\mathcal{M}$ of $\mathcal{H}_{ac}(A)$ such that for $\phi \in \mathcal{M}$*

$$\int_{-\infty}^{\infty} |\langle \psi, e^{-itA}\phi \rangle|^2 dt \le C_\phi \|\psi\|$$

Proof of Theorem 1.6: Let $W_t = e^{itA}Je^{-itB}P_c(B)$. We will show that $\lim W_t\phi$ exists for $\phi \in \mathcal{M}$.

Since

$$\|(W_t - W_s)\phi\|^2 = \langle \phi, W_t^*(W_t - W_s)\phi \rangle - \langle \phi, W_s^*(W_t - W_s)\phi \rangle$$

it suffices to show $\lim_{s,t\to\infty} \langle \phi, W_t^*(W_t - W_s)\phi \rangle = 0$. For convenience we consider the case $s \le t$.

Now

$$\begin{aligned}
&\langle \phi, W_t^*(W_t - W_s)\phi \rangle \\
&\quad = \langle \phi, e^{iaB}e^{-iaB}W_t^*(W_t - W_s)e^{iaB}e^{-iaB}\phi \rangle \\
&\quad = \langle \phi, e^{iaB}\left(W_t^*(W_t - W_s) + \int_0^a \frac{d}{dw}\Big(e^{-iwB}W_t^*(W_t - W_s)e^{iwB} \Big) dw \right) e^{-iaB}\phi \rangle \\
&\quad = \langle \phi, e^{iaB}W_t^*(W_t - W_s)e^{-iaB}\phi \rangle + \int_0^a \langle \phi, e^{iaB}e^{-iwB}[W_t^*(W_t - W_s), iB]e^{iwB}e^{-iaB}\phi \rangle \\
&\quad = \langle \phi, e^{iaB}W_t^*(W_t - W_s)e^{-iaB}\phi \rangle + \int_0^a \langle \phi, e^{iuB}[W_t^*(W_t - W_s), iB]e^{-iuB}\phi \rangle
\end{aligned}$$

Here we made the change of variable $u = a - w$.

Now we let $a \to \infty$.

$$W_t - W_s = i \int_s^t e^{iuA}(AJ - JB)e^{-iuB} P_c(B) du$$

is compact. So as $a \to \infty$ the first term above tends to zero.

To estimate the second term, we use that the quantity $[W_t^*(W_t - W_s), iB]$ is a sum of terms of the form $Y(s,t)Ce^{-isB}$ or its adjoint, where $Y(s,t)$ is uniformly bounded in s and t and C is trace class. Let

$$C = \sum \mu_n \langle \psi_n, \cdot \rangle \eta_n$$

with $\sum \mu_n < \infty$. Then we must estimate terms like

$$\begin{aligned}
&\int_0^\infty \langle \phi, e^{iuB} Y(s,t) C e^{-isB} e^{-iuB} \phi \rangle du \\
&\qquad \le \int_0^\infty \sum \mu_n \langle \phi, e^{iuB} Y(s,t) \eta_n \rangle \langle \psi_n, e^{-isB} e^{-iuB} \phi \rangle du \\
&\qquad \le \int_0^\infty \sum \mu_n |\langle e^{-iuB} \phi, Y(s,t) \eta_n \rangle| |\langle \psi_n, e^{-i(s+u)B} \phi \rangle| du \\
&\qquad \le \left\{ \int_0^\infty \sum \mu_n |\langle e^{-iuB} \phi, Y(s,t) \eta_n \rangle|^2 du \right\}^{1/2} \left\{ \int_s^\infty \sum \mu_n |\langle \psi_n, e^{iuB} \phi \rangle|^2 du \right\}^{1/2}
\end{aligned}$$

Since $\phi \in \mathcal{M}$ we have

$$\begin{aligned}
\int_0^\infty \sum \mu_n |\langle e^{-iuB} \phi, Y(s,t) \eta_n \rangle|^2 du &\le \sum \mu_n \int_{-\infty}^\infty |\langle e^{-iuB} \phi, Y(s,t) \eta_n \rangle|^2 du \\
&\le \sum \mu_n \|Y_{s,t}\|^2 C_\phi \\
&\le C'_\phi
\end{aligned}$$

Similary we find that $\sum \mu_n |\langle \psi_n, e^{iuB} \phi \rangle|^2 \in L^1(du)$ Hence

$$\lim_{s \to \infty} \int_s^\infty \sum \mu_n |\langle \psi_n, e^{i(u)B} \phi \rangle|^2 = 0$$

$\square$