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# Dynamical capture in quantum mechanics

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**Abstract.** Using simple time-dependent methods, we study the phenomenon of dynamical capture in non-relativistic quantum mechanics. We show that for time-dependent potentials that are asymptotically constant in time, the probability of an incoming particle becoming trapped in the interaction region is in general non-zero. Capture in a stationary beam is also discussed.

A salient feature of scattering theory with time-independent short-range potentials is asymptotic completeness. Let $H_0 = p^2/2m$ be the kinetic energy of a Schrödinger particle, $V(x)$ a short-range potential with total Hamiltonian

$$H = H_0 + V \tag{1}$$

and corresponding evolution groups $\exp(-\mathrm{i}H_0 t)$ and $\exp(-\mathrm{i}Ht)$, acting in the Hilbert space $\mathcal{H}$ of square integrable wavefunctions‡. Consider the associated isometric wave operators $\Omega_\pm = \text{s-lim}_{t\to\pm\infty} \exp(\mathrm{i}Ht)\exp(-\mathrm{i}H_0 t)$ and scattering operator $S = \Omega_+^\dagger \Omega_-$. The ranges $P_\pm^{\rm sc}\mathcal{H}$ of the wave operators, $P_\pm^{\rm sc} = \Omega_\pm \Omega_\pm^\dagger$, are the set of scattering states that move freely as $t \to \pm\infty$. If one has the relation

$$P_+^{\rm sc} P_-^{\rm sc} = P_-^{\rm sc} \qquad \text{or equivalently} \qquad (I - P_+^{\rm sc}) P_-^{\rm sc} = 0 \tag{2}$$

every incoming state has outgoing free asymptotics and $S^\dagger S = I$: no incoming state (or part of it) can remain trapped in the interaction region. Relation (2) is implied by the stronger statement of asymptotic completeness:

$$I - P_-^{\rm sc} = P^{\rm bd} = I - P_+^{\rm sc} \tag{3}$$

where $P^{\rm bd}$ is the projection onto the set of bound states of $H$. This situation is known to hold in great generality for scattering with time-independent interactions [1]§.

The purpose of the present paper is to show that, in contrast to the case of static potentials, trapping can become a common phenomenon when one deals with time-dependent force-fields. This is simply because a non-conservative interaction may lower the energy of an incoming particle so that it can reach a bound-state level of the asymptotic Hamiltonian. We shall call such a phenomenon *dynamical capture*, since it is a consequence of the pure dynamical effect of energy transfer from the particle to the field. A simple case

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‡ The Planck constant is set equal to 1.

§ There are, however, very special potentials, rapidly oscillating near a strong singularity, for which (3) does not hold. They show the phenomenon of local absorption: a part of the incoming (or outgoing) state moves closer and closer to the point of singularity and remains trapped there [2].

 

that we shall discuss later is when the potential is switched on during the scattering process, i.e. replacing (1) by

$$H(t) = H_0 + \lambda(t)V \qquad \lim_{t\to-\infty}\lambda(t) = 0 \qquad \lim_{t\to\infty}\lambda(t) = 1. \tag{4}$$

Let us first define the concept of dynamical capture in a general setting. Consider a quantum mechanical system described by a time-dependent Hamiltonian $H(t) = H_0 + V(t)$ in some Hilbert space $\mathcal{H}$, where $H_0$ is the free reference Hamiltonian and $V(t)$ the time-dependent perturbation. We denote by $U(t, t_0)$ the total evolution operator, with initial condition $U(t_0, t_0) = I$, and we assume the existence on all of $\mathcal{H}$ of the wave operators

$$\Omega_\pm(t_0) = \operatorname*{s-lim}_{t\to\pm\infty} U^\dagger(t, t_0)\, e^{-iH_0(t-t_0)} \tag{5}$$

which are related by the generalized intertwining property

$$\Omega_\pm(t_0) = U(t_0, t_1)\Omega_\pm(t_1)\, e^{iH_0(t_0-t_1)}. \tag{6}$$

As strong limits of unitary operators, $\Omega_\pm(t_0)$ are isometries; as before $P_\pm^{sc}(t_0) = \Omega_\pm(t_0)\Omega_\pm^\dagger(t_0)$ are the projections onto the set of states (with initial condition at time $t = t_0$) propagating freely as $t \to \pm\infty$, and we define the corresponding scattering operator $S(t_0) = \Omega_+^\dagger(t_0)\Omega_-(t_0)$. As a consequence of (6), one has

$$S(t_0) = e^{-iH_0t_0} S(0) e^{iH_0t_0}. \tag{7}$$

Since the system is no longer invariant under time translations, it is now important to distinguish between the different possible initial times $t_0$. The point is that particles entering the interaction region at different times do not experience the same configuration of the interaction, so giving rise to different scattering data. In fact, one can check that the scattering operator $S(t_0)$ with initial condition at time $t = t_0$ coincides with the scattering operator $S^{t_0}(0)$ with initial condition at time $t = 0$, but for the time-translated interaction $V(t + t_0)$ (see the discussion in [3]).

Although there is in general no notion of bound states for non-conservative Hamiltonians, it is still meaningful to consider the subspaces $P_+^{bd}(t_0)\mathcal{H}$ ($P_-^{bd}(t_0)\mathcal{H}$) of states $\varphi$ that remain localized in bounded regions for $t > t_0$ ($t < t_0$). In potential scattering, such states may be characterized by the property

$$\lim_{R\to\infty} \sup_{t>t_0\ (t<t_0)} \|(I - Q_R)U(t, t_0)\varphi\| = 0 \tag{8}$$

where $Q_R$ is the projection onto the set of states localized in a ball of radius $R$ in configuration space (for a discussion of this concept, see [4]). In what follows, we make the (non-trivial) assumption that for the dynamics under consideration one has†

$$I - P_+^{sc}(t_0) = P_+^{bd}(t_0) \tag{9}$$

i.e. for $t > t_0$, either states have free asymptotics or remain in bounded regions.

Let $\psi(t) = U(t, t_0)\Omega_-(t_0)\varphi$ be the state of a particle (with initial time $t_0$) corresponding to an incoming state $\varphi$ having free asymptotics as $t \to -\infty$. We define the probability of capture $\mathcal{P}_{cap}(\varphi, t_0)$ as the probability that this particle remains trapped in bounded regions for all times $t \geqslant t_0$:

$$\begin{aligned}\mathcal{P}_{cap}(\varphi, t_0) &= \langle\psi(t)|P_+^{bd}(t)\psi(t)\rangle \\ &= \langle\varphi|\Omega_-^\dagger(t_0)U^\dagger(t, t_0)P_+^{bd}(t)U(t, t_0)\Omega_-(t_0)\varphi\rangle \\ &= \langle\varphi|\Omega_-^\dagger(t_0)P_+^{bd}(t_0)\Omega_-(t_0)\varphi\rangle \\ &= 1 - \langle\varphi|S^\dagger(t_0)S(t_0)\varphi\rangle.\end{aligned} \tag{10}$$

† This is the equivalent for time-dependent interactions of the second equality in (3).

Thus, the probability of capture is measured by the average of the *unitary deficiency* $I - S^\dagger(t_0)S(t_0)$ of the scattering operator with respect to the incoming state $\varphi$. It is clear that as soon as

$$P_+^{\rm bd}(t_0)P_-^{\rm sc}(t_0) \neq 0 \tag{11}$$

there exists at least one incoming state such that $\mathcal{P}_{\rm cap}(\varphi, t_0) \neq 0$. Indeed there exists $\varphi'$, normalized to 1, in $P_-^{\rm sc}(t_0)\mathcal{H}$ such that $P_+^{\rm bd}(t_0)\varphi' \neq 0$. Then, setting $\varphi = \Omega_-^\dagger(t_0)\varphi'$, one has $\langle\varphi|\varphi\rangle = 1$ and

$$\begin{aligned}\mathcal{P}_{\rm cap}(\varphi, t_0) &= \langle\varphi|\Omega_-^\dagger(t_0)P_+^{\rm bd}(t_0)\Omega_-(t_0)\varphi\rangle \\ &= \langle\varphi'|P_-^{\rm sc}(t_0)P_+^{\rm bd}(t_0)P_-^{\rm sc}(t_0)\varphi'\rangle \\ &= \langle\varphi'|P_+^{\rm bd}(t_0)\varphi'\rangle \neq 0.\end{aligned} \tag{12}$$

Moreover, if in addition $\varphi'$ is a common eigenvector of $P_+^{\rm bd}(t_0)$ and $P_-^{\rm sc}(t_0)$, $\mathcal{P}_{\rm cap}(\varphi, t_0) = 1$.

In the following proposition, we show that the existence of a non-vanishing probability of capture is typical for a situation where one has different asymptotic Hamiltonians as $t \to \pm\infty$, as in the example (4).

*Proposition 1.* Let $H(t) = H_0 + V(t)$, where $H_0 = p^2/2m$ is the kinetic energy and $V(t)$ a bounded time-dependent potential. We assume that $V(t)$ converges in norm to $V_\pm$ as $t \to \pm\infty$ with

(i) $\pm\int_{t_0}^{\pm\infty} {\rm d}t\, \|V(t) - V_\pm\| < \infty$,
(ii) the time-independent asymptotic Hamiltonians $H_\pm = H_0 + V_\pm$ together with $H_0$ form complete scattering systems in the sense of (3),
(iii) $H_-$ has a purely absolutely continuous spectrum, whereas $H_+$ has bound states.

Then there exists $\varphi \in \mathcal{H}$ for which the probability of capture is 1.

*Proof.* By the chain rule, we have $\Omega_\pm = \tilde\Omega_\pm\Omega_\pm^0$, where $\tilde\Omega_\pm$ are the wave operators belonging to the pair $(H(t), H_\pm)$, and $\Omega_\pm^0$ those for $(H_\pm, H_0)$ (for brevity, we omit the argument $t_0$). Therefore, $P_\pm^{\rm sc} = \Omega_\pm\Omega_\pm^\dagger = \tilde\Omega_\pm P_\pm^{0,{\rm sc}}\tilde\Omega_\pm^\dagger$, where $P_\pm^{0,{\rm sc}} = \Omega_\pm^0\Omega_\pm^{0\dagger}$ are the projections onto the continuous subspaces of $H_\pm$. Note that $\tilde\Omega_\pm$ are unitary since by (i) the Cook estimate holds in norm for both $\tilde\Omega_\pm$ and $\tilde\Omega_\pm^\dagger$, for instance

$$\begin{aligned}\left\|{\rm e}^{{\rm i}H_+(t-t_0)}U(t,t_0) - \tilde\Omega_+^\dagger(t_0)\right\| &\leqslant \int_t^\infty {\rm d}s\ \left\|\partial_s\left({\rm e}^{{\rm i}H_\pm(s-t_0)}U(t,t_0)\right)\right\| \\ &\leqslant \int_t^\infty {\rm d}s\ \|V(s) - V_+\|\end{aligned} \tag{13}$$

so that $\tilde\Omega_+^\dagger$ exists as uniform limit of unitary operators. Hence, since by assumptions (ii) and (iii) $P_-^{0,{\rm sc}} = I$, one has also $P_-^{\rm sc} = I$, implying $P_+^{\rm bd}P_-^{\rm sc} = P_+^{\rm bd}$. But $P_+^{\rm bd} = \tilde\Omega_+P_+^{0,{\rm bd}}\tilde\Omega_+^\dagger \neq 0$, since $\tilde\Omega_+$ is unitary and $P_+^{0,{\rm bd}} \neq 0$ by (iii). Thus, equation (11) holds and the probability of capture equals 1 for incoming states of the form $\varphi = \tilde\Omega_+^\dagger\varphi'$ with $\varphi'$ in $P_+^{0,{\rm bd}}\mathcal{H}$. □

The potential was assumed to be bounded for the sake of simplicity, but local singularities can be allowed using the methods of [6]. In particular, the characterization (8) of localization together with the relation (9) hold as shown in lemma 4.1 of [6].

As an illustration, consider the special case (4) with sudden switching on of the coupling constant, $\lambda(t) = 0$ for $t < 0$, $\lambda(t) = 1$ for $t > 0$, and $H_+$ has $N$ bound states

$H_+\phi_n = E_n\phi_n$, $\langle\phi_n|\phi_m\rangle = \delta_{n,m}$, $n, m = 0, \ldots, N-1$. In this case, we have $\Omega_-(0) = I$ and $\Omega_+(0)\Omega_+^\dagger(0) = I - \sum_{n=0}^{N-1} |\phi_n\rangle\langle\phi_n|$. Thus, also using equation (7)

$$I - S^\dagger(t_0)S(t_0) = \sum_{n=0}^{N-1} \exp(-\mathrm{i}H_0t_0)|\phi_n\rangle\langle\phi_n| \exp(\mathrm{i}H_0t_0)$$

and by (3) we get

$$\mathcal{P}_{\mathrm{cap}}(\varphi, t_0) = \sum_{n=0}^{N-1} \left|\langle\phi_n|\mathrm{e}^{\mathrm{i}H_0t_0}\varphi\rangle\right|^2 . \tag{14}$$

Since free states leave any bounded region, $\langle\phi_n|\mathrm{e}^{\mathrm{i}H_0t_0}\varphi\rangle$ and hence $\mathcal{P}_{\mathrm{cap}}(\varphi, t_0)$ tend to zero as $t_0 \to \pm\infty$. This reflects the fact that energy transfer will not be possible if the wave packet enters the interaction region long before or long after the switching on of the potential. More generally, as $t_0 \to \pm\infty$, $S(t_0)$ will converge (strongly) to the unitary scattering operators $S_\pm$ associated with the conservative Hamiltonians $H_\pm$ (see the comment after (7)) and capture will not occur in this limit.

So far, we have treated individual scattering events with specified incoming states $\varphi$ and initial times $t_0$. However, in experiments, it is more realistic to consider the scattering of a stationary beam of particles at a given incoming energy $E$. One may think to the incoming beam as consisting of a succession of incoming wave packets $\mathrm{e}^{\mathrm{i}H_0t_j}\varphi$ prepared with small time lags $t_{j+1} - t_j \simeq \Delta t$, which are scattered independently. We denote by $\mathcal{N}_0 = 1/\Delta t$ the (average) number of incoming particles per unit time. Let $\mathcal{N}_{\mathrm{cap}}$ be the total (average) number of particles captured by the interaction in a time interval much larger than the time scale of variation of the external potential: $\mathcal{N}_{\mathrm{cap}}$ measures the depletion of the beam when the potential has varied from $t = -\infty$ to $t = \infty$. Then, we define the (average) *capture time* $\tau_{\mathrm{cap}}$ by the proportionality relation

$$\mathcal{N}_{\mathrm{cap}} = \tau_{\mathrm{cap}}\mathcal{N}_0. \tag{15}$$

If the particles are scattered independently we may add the individual probabilities

$$\mathcal{N}_{\mathrm{cap}} = \sum_j \mathcal{P}_{\mathrm{cap}}(\varphi, t_j) \tag{16}$$

and it follows from these definitions that for $\Delta t$ small compared to the rate of variation of the potential, $\tau_{\mathrm{cap}}(\varphi) = \mathcal{N}_0^{-1}\mathcal{N}_{\mathrm{cap}}$ is well approximated by

$$\begin{aligned} \tau_{\mathrm{cap}}(\varphi) &= \lim_{\Delta t\to 0} \sum_j \mathcal{P}_{\mathrm{cap}}(\varphi, t_j)\Delta t \\ &= \int \mathrm{d}t\ \mathcal{P}_{\mathrm{cap}}(\varphi, t) \\ &= \langle\varphi|\tau_{\mathrm{cap}}\varphi\rangle \end{aligned} \tag{17}$$

where

$$\tau_{\mathrm{cap}} = \int \mathrm{d}t\ \mathrm{e}^{-\mathrm{i}H_0t}\ \Omega_-^\dagger(0)\ P_+^{\mathrm{bd}}(0)\ \Omega_-(0)\ \mathrm{e}^{\mathrm{i}H_0t}. \tag{18}$$

This last expression may be called the capture time operator and results from the definition of the probability of capture (10) (again using equation (6)). It is positive and it commutes with the free evolution. Hence, it has energy shell components

$$\tau_{\mathrm{cap}}(E) = 2\pi\ \langle E|\ \Omega_-^\dagger(0)\ P_+^{\mathrm{bd}}(0)\ \Omega_-(0)\ |E\rangle \tag{19}$$

in the direct integral $\mathcal{H} = \int^{\oplus} \mathrm{d}E \, \mathcal{H}_E$ that diagonalizes $H_0$. In the limit of incident packets that are sharply peaked in energy, $\tau_{\mathrm{cap}}(E)$ gives the total capture when the potential has varied in a beam having incident energy $E$. This quantity is now independent of the origin of the time and of the details of the preparation of the beam. The procedure followed here is analogous the averaging over incoming impact parameters in the definition of the scattering cross-section: the capture time may be seen as the average of capture probabilities over incoming 'impact times'.

For illustration, we apply equation (19) to the special case (14), limiting ourselves to the s-wave of a spherically symmetric potential having a single bound state $\phi_0$†. Then, in the $\ell = 0$ subspace, one has $|\phi_0\rangle\langle\phi_0| = P_+^{\mathrm{bd}}(0)$, and with $\Omega_-^\dagger(0) = I$, equation (19) reduces to $\tau_{\mathrm{cap}}(E) = 2\pi \, |\phi_0(E)|^2$. So, by pure scattering experiments at various incident energies $E$ one can in principle probe the spectral density of this bound state of $H$.

In conclusion, we recall that there are other important classes of time-dependent potentials for which asymptotic completeness is known to hold. Such classes are potentials that are switched on and off sufficiently rapidly [5, 6]‡ and potentials periodic in time [8]. We have shown that for the type of potentials considered here (with different limits for negative and positive times) the violation of asymptotic completeness is not a pathology, but leads to the effect of dynamical capture discussed in this paper.

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† This is an idealization: strictly speaking, the potential is switched on rapidly, but it is supposed that its time variation can still be resolved by the time intervals $\Delta t$.

‡ However, asymptotic completeness may also be broken in the case of [6] if the switching is too slow [7].