TIME-ENERGY COHERENT STATES AND ADIABATIC SCATTERING

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Abstract. Coherent states in the time-energy plane provide a natural basis to study adiabatic scattering. We relate the (diagonal) matrix elements of the scattering matrix in this basis with the frozen on-shell scattering data. We describe an exactly solvable model, and show that the error in the frozen data cannot be estimated by the Wigner time delay alone. We introduce the notion of energy shift, a conjugate of Wigner time delay, and show that for incoming state $\rho(H_0)$ the energy shift determines the outgoing state.

1. Introduction

Scattering from a slowly changing scatterer is described, to leading order, by a *time independent* scatterer frozen at the scattering time [11]. Although this seems like stating the obvious, it turns out that in trying to make precise how accurate this approximation is, one encounters both conceptual and technical difficulties. Our aim is to describe these difficulties and explain how they are resolved.

One conceptual difficulty is to understand what the frozen S matrix—a function of energy and scattering time—means. Strictly speaking, a function of both time and energy is in conflict with the uncertainty principle. A wave that is sharp in energy will have an ill-defined scattering time and conversely, a wave with a well-defined scattering time is ill-defined in energy. What, then, is the meaning of the frozen S matrix?

The resolution of this problem is related to the fact that the adiabatic limit naturally leads to different parameterizations of time, and the right parameterization has small uncertainty. Specifically, the physical time t will parameterize the intrinsic "fast" dynamics and has the usual time-energy uncertainty $\hbar$. The slow variation in the external conditions will be parameterized by s. We refer to the latter as *epoch*. Since the epoch often plays a role of a parameter it is convenient to choose s dimensionless. The two parameterizations are related by $s = \omega t$, with ω a slow frequency—the adiabaticity parameter. The epoch-energy uncertainty then takes the form $\delta s\, \delta e \sim \hbar\omega$ and so arbitrarily small in the adiabatic limit.

Coherent states provide a convenient basis to analyze the semi-classical limit [12, 6]. Semi-classical analysis is traditionally about the $\hbar \to 0$ limit, but is equally valid when $\hbar$ is fixed (and henceforth set equal to one) and $\omega \to 0$. Here we introduce coherent states labelled by points in the time-energy plane, with time being the scattering time. As we shall see, the frozen S matrix approximates the diagonal matrix elements of the dynamical scattering matrix in such coherent states.

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This reconciles the time-energy uncertainty with the frozen scattering data. In a further step, matrix elements of the frozen S matrix can be approximated by the on-shell data.

Another thorny issue that we address is when a description in terms of frozen data is meaningful and how accurate it is. The question can also be rephrased as a question about the intrinsic time scale relevant to scattering. If τ denotes this time scale, then $\omega\tau$ is the error in the frozen data and $\omega\tau \ll 1$ characterizes the adiabatic regime.

The Wigner time delay $\tau_w(E,s)$ conveys information about the time the particle spends near the scatterer. It is a function of the energy E and scattering epoch s. It is tempting to hope that τ might be estimated by $\tau_w(E,s)$, but there is no compelling argument for doing so. One cannot argue on the basis of dimensional analysis alone, since $\dot{\tau}_w$ and $\sqrt{\tau_w'}$, with dot a derivative with respect to the epoch and prime with respect to the energy, give additional and independent time scales. In fact, since Wigner time delay is a *comparison* of the arrival time at a faraway point, relative to the time of arrival in the free dynamics, it is not even positive-definite. This suggests that it cannot quite capture τ, which is more closely related to the "dwell time" near the scatterer.

The way to determine τ is to consider the error in approximating the scattering data by the frozen data. The error is, to leading order, proportional to the adiabaticity parameter ω. Since the error is, in general, complex, we identify τ with the absolute value of the error divided by ω. Calculating the error, to leading order in ω, is no harder, and reminiscent of, calculating the scattering in the lowest order of the Born approximation.

We shall see that, to leading order, the adiabatic time scale τ can be estimated from the scattering data and the derivative of the Hamiltonian H with respect to the epoch, Eq. (7.3) below, but not from the Wigner time delay alone. We show this by considering an exactly soluble model where the dynamical S matrix can be computed explicitly.

We introduce the *energy shift* operator $\mathcal{E}$. This is a measure of the energy change in time dependent scattering and is a natural dual of the Wigner time delay. As we shall see, in the case that the incoming state is $\rho(H_0)$, the outgoing state is $\rho(H_0 - \omega\mathcal{E})$. In the adiabatic limit, the energy shift can be approximated by the frozen energy shift, which is related to the logarithmic derivative of the on-shell scattering matrix with respect to the epoch, Eq. (4.2). The energy shift then gives a handle on the exchange of energy [2, 9] and the pumping of charge in adiabatic scattering [3].

2. Elements of scattering theory

Scattering theory is a comparison of dynamics: One is the actual dynamics generated by the time dependent $H(t) = H_s$, $(s = \omega t)$, the other is a fiducial dynamics generated by a *time independent* Hamiltonian H_0. The Hamiltonian H_0 is the generator of dynamics for which there is trivial scattering and the S matrix is the identity.

The results of this section are true in general, without taking the adiabatic limit $\omega \to 0$. We shall assume that H and H_0 admit good scattering. Namely, we assume the existence of wave operators and the unitarity of the S matrix. For explicit conditions on H_0 and $H(t)$ that guarantee this see e.g. [14, 15].

2.1. **The wave operator.** Let $U(t'',t')$ and $U_0(t'',t') = U_0(t''-t')$ denote the evolution from time t' to t'', generated by $H(t)$ and the time-independent H_0 respectively.

Definition 2.1. *The wave operators, based at epoch s, are defined by the (strong) limit*

$$\Omega_\pm(s;H,H_0) = \lim_{t'\to\pm\infty} U(t,t')U_0(t'-t), \quad (s=\omega t). \tag{2.1}$$

The existence of the limit, and the equation of motion imply

Proposition 2.2. *The dependence of the wave operator on the base point s satisfy the differential equation*

$$-i\omega\dot{\Omega}_\pm(s) = H_s\Omega_\pm(s,H,H_0) - \Omega_\pm(s,H,H_0)H_0. \tag{2.2}$$

As we shall presently see, the notion of wave operator based at epoch s is only interesting in the case of a time dependent $H(t)$.

2.2. **The frozen wave operators.** The frozen Hamiltonian H_s is *time independent* so $U(t'',t') = e^{iH_s(t''-t')}$, in this case and $\Omega_\pm(s_0,H_s,H_0)$ is independent of the base point $s_0=\omega t_0$. This follows from the existence of the limit in Eq. (2.1) since $t'\to\pm\infty$ is the same as $t'-t_0\to\pm\infty$. To stress this we write $\Omega_\pm(H_s,H_0)$. From Eq. (2.2) then follows the standard intertwining relation of time-independent scattering theory:

Corollary 2.3. *The wave operators $\Omega_\pm(H_s,H_0)$ relating the frozen Hamiltonian at epoch s and H_0 are independent of the base point, and intertwine the two dynamics:*

$$H_s\Omega_\pm(H_s,H_0) = \Omega_\pm(H_s,H_0)H_0. \tag{2.3}$$

2.3. **The dynamical S matrix.** The (dynamical) scattering matrix based at epoch s is defined by

$$\mathcal{S}_d(s;H,H_0) = \Omega_+^\dagger(s;H,H_0)\Omega_-(s;H,H_0). \tag{2.4}$$

The S matrices based on different points in time are all related by conjugation generated by the free evolution. Namely:

Proposition 2.4. *Suppose that the wave operators exist. Then*

$$\mathcal{S}_d(s;H,H_0) = e^{-iH_0t}\mathcal{S}_d(0;H,H_0)e^{iH_0t}, \quad (s=\omega t). \tag{2.5}$$

This follows from $U(s,t)\Omega_\pm(s;H,H_0) = \Omega_\pm(s;H,H_0)e^{-iH_0(s-t)}$. Under a change of the reference Hamiltonian, say to the frozen Hamiltonian H_s,

$$\mathcal{S}_d(s;H,H_0) = \Omega_+^\dagger(H_s,H_0)\mathcal{S}_d(s;H,H_s)\Omega_-(H_s,H_0). \tag{2.6}$$

2.4. **The frozen S matrix.** In the frozen S data the epoch is decoupled from time. As such it can also be studied using time independent methods, which are normally quite powerful [15]. Its basic properties are in marked contrast with that of the dynamical S matrix, namely:

Corollary 2.5. *The frozen S matrix*

$$\mathcal{S}_f(H_s,H_0) = \Omega_+^\dagger(H_s,H_0)\Omega_-(H_s,H_0) \tag{2.7}$$

is independent of the base point. It depends on the freezing time parametrically through H_s.

2.5. **The on-shell S matrix.** H_0 provides a basis that spans the Hilbert space of scattering states. Let $|E,j)$ denote the generalized eigenvectors of H_0:

$$H_0|E,j) = E\,|E,j), \quad (E,j|E',j') = \delta(E-E')\delta_{j,j'}. \tag{2.8}$$

E is the energy and j labels the scattering channels. $\mathcal{S}_f$ commutes with H_0, by Eq. (2.3), hence

$$(E,j|\mathcal{S}_f\big(H_s,H_0\big)|E',j') = \delta(E-E')\,S_{jj'}(s,E). \tag{2.9}$$

$S_{jj'}(s,E)$ is the *on-shell* scattering matrix. Note that in the frozen Hamiltonian the physical time is decoupled from the epoch, which now has been relegated to the role of a parameter. The on-shell scattering matrix therefore is not in conflict with the uncertainty principle.

3. The energy shift

By taking the s-derivatives of Eq. (2.5) one gets

$$i\,\omega\dot{\mathcal{S}}_d(s)\mathcal{S}_d(s)^\dagger = H_0 - \mathcal{S}_d(s)\,H_0\,\mathcal{S}_d(s)^\dagger = [H_0,\mathcal{S}_d]\mathcal{S}_d^\dagger. \tag{3.1}$$

This equation may interpreted as follows. If we think of H_0 as the asymptotic observable associated with the outgoing energy, then $H_{0,in} = \mathcal{S}_d(s)\,H_0\,\mathcal{S}_d(s)^\dagger$ represents the asymptotic observable [5] corresponding to the incoming energy. This motivates calling

$$\mathcal{E}_d(s) = i\dot{\mathcal{S}}_d(s)\mathcal{S}_d^\dagger(s). \tag{3.2}$$

the operator of energy shift.

The energy shift vanishes for time independent scattering, as it must. It gives a handle on changes in (certain) quantum states. By the functional calculus applied to Eq. (3.1), for any function ρ:

$$\mathcal{S}_d(s)\,\rho(H_0)\,\mathcal{S}_d(s)^\dagger = \rho\big(H_0 - \omega\mathcal{E}_s(s)\big). \tag{3.3}$$

This is interpreted as follows: If $\rho(H_0)$ is the incoming state, then the corresponding outgoing state is $\rho\big(H_0 - \omega\mathcal{E}_s(s)\big)$. The energy shift is a first order quantity in the adiabaticity parameter and, as we shall see, it can be approximated, to leading order by the frozen data. This then gives a handle on the outgoing state ρ to first order in the adiabaticity parameter.

Proposition 3.1. *The energy shift based on time s is conjugate to the energy shift based on time zero*

$$\mathcal{E}_d(s) = e^{iH_0t}\mathcal{E}_d(0)\,e^{-iH_0t}, \quad (s=\omega t). \tag{3.4}$$

This follows directly from Eq. (2.5) and Eq. (3.1).

4. The problem of adiabatic scattering

The dynamical S matrix has qualitatively different properties from the frozen S matrix: The dynamical S matrix has no freezing time—It does not "know" when the incoming wave is going to hit the scatterer. It does depend however, by conjugation, on a choice of a base point. In contrast, the frozen S matrix is independent of the choice of a base point and depends non-trivially on the freezing time—The frozen scattering data for one epoch know nothing a-priori about the corresponding data at any other epoch.

Matrix elements of the scattering matrix carry information about the time that the wave is near the scatterer. For such matrix elements, the adiabatic limit can be expressed in terms of the corresponding frozen matrix elements. However, the introduction of wave packets promotes the epoch from playing the role of a parameter, to that of real, albeit slow, time. One then needs to confront the uncertainty principle. We do that by considering matrix elements between coherent states labelled by points in the energy time plane.

4.1. **The Wigner time delay.** The Wigner time delay is defined in terms of the on-shell scattering matrix. When this definition is transcribed to the frozen, on-shell, S matrix it reads

$$\tau_w(s,E) = -i\, S'(s,E)S^\dagger(s,E). \tag{4.1}$$

Prime denotes partial derivative with respect to the energy. With this definition, the Wigner time-delay is a Hermitian matrix.

4.2. **The frozen energy shift.** For the frozen, on-shell, Hamiltonian one can associate a matrix of energy shift which is a natural conjugate of the Wigner time delay:

$$\mathcal{E}(s,E) = i\, \dot{S}(s,E)S^\dagger(s,E), \tag{4.2}$$

where dot denotes derivative with respect to the epoch.

4.3. **Time scales.** The frozen on-shell S matrix defines several time scales. Among them: τ_w and the (dimensionless) time scale $\mathcal{E}^{-1}$. The coherent states provide us with yet another time scale related to the time-width of the coherent states. One of the problems of adiabatic scattering is to study the relation between these time scales and the time scale τ such that $\omega\tau \ll 1$ characterizes the adiabatic regime.

5. Time-Energy Coherent states

5.1. **The role of dispersion.** For a particle moving on the line, its energy and the time that it crosses the origin are canonical coordinates. One can therefore construct energy-time coherent states in analogy with the usual phase space coherent states. The explicit construction, however, depends on the dispersion law. For linear dispersion the construction is particularly simple.

Consider a classical particle with dispersion law $e(p)$ moving freely on the line. The velocity of the particle is $e'(p)$ so the time of passage through the origin is $t = \frac{-q}{e'(p)}$. Time-energy are (local) canonical coordinates since

$$de \wedge dt = dq \wedge dp. \tag{5.1}$$

The global aspects of the energy-time phase space can be complicated. For example, for a free (massive) particle, with quadratic dispersion $e(p) = p^2$ the energy-time phase space is made of two copies of the half plane $e \geq 0$ depending on the direction of crossing of the origin.

A simpler situation is obtained in the case of linear dispersion, $e(p) = p$. There is now no ambiguity in the direction of crossing and the energy-time phase space is again the plane. The map $(q,p) \leftrightarrow (e,t)$ is, in fact, the identity

$$e = p, \quad t = -q. \tag{5.2}$$

The usual coherent states are then also the coherent states on the energy-time plane.

5.2. **Coherent states for linear dispersion.** The time-energy coherent states are

$$|t,e;\varepsilon\rangle = e^{i(tP+eX)}\,|g_\varepsilon\rangle\,,\quad [P,X]=-i, \tag{5.3}$$

with g_ε Gaussian:

$$\langle p|g_\varepsilon\rangle = \frac{1}{\sqrt[4]{\pi\varepsilon^2}}\,e^{-\frac{p^2}{2\varepsilon^2}}. \tag{5.4}$$

They have the following properties [12]:

A The states $|t,e;\varepsilon\rangle$ are normalized.

B $|t,e;\varepsilon\rangle$ have Gaussian localization in time and energy near the point (t,e) with width

$$\delta e\sim\varepsilon,\quad \delta t\sim\frac{1}{\varepsilon},\quad \delta s\sim\frac{\omega}{\varepsilon}.$$

Hence ω plays the role of $\hbar$ in the epoch-energy plane.

C H_0 is the generator of shifts of the coherent states:

$$e^{-iH_0t'}\,|t,e;\varepsilon\rangle = e^{-it'e/2}\,|t-t',e;\varepsilon\rangle\,.$$

D The overlap of coherent states is:

$$\langle t,e,\varepsilon|t',e',\varepsilon\rangle = e^{-\frac{(e-e')^2}{4\varepsilon^2}}\,e^{-\frac{\varepsilon^2(t-t')^2}{4}}\,e^{-i\frac{et'-e't}{2}}.$$

E The coherent states give a resolution of the identity

$$\int\frac{dt\,de}{2\pi}\,|t,e;\varepsilon\rangle\,\langle t,e;\varepsilon| = 1.$$

F The scalar product between coherent states and the eigenstates of $H_0 = P$ is

$$(E\,|t,e;\varepsilon\rangle = e^{-ite/2}e^{-itE}\,\frac{e^{-(E-e)^2/2\varepsilon^2}}{\sqrt[4]{\pi\varepsilon^2}}.$$

6. Scattering between channels with linear dispersion

Linear dispersion approximates the low energy physics of electrons in one dimensional channels provided the Fermi energy is large. The price one pays is that the "ultraviolet" properties are pathological. In particular, the spectrum is unbounded below and this then leads to certain anomalies which must be correctly interpreted. With linear dispersion one can also solve certain models with interacting electrons [10].

In the following we shall study adiabatic scattering for *non interacting* particles with linear dispersion. The particles move on a collection of lines and are allowed to "hop" from one line to the other and scatter. Each line serves as an incoming and outgoing channel since the flow on it is uni-directional. An example with two channels is shown in Fig. 1. (Such models bear some resemblance to Schrödinger operators on graphs [1].) The Hilbert space is $\oplus_{j=1}^n L^2(\mathbb{R})$, a finite direct sum. j labels the scattering channels. H_0 is then

$$\big(H_0\psi\big)\,(x,j) = -i\,\psi'(x,j),\quad x\in\mathbb{R},\ 1\le j\le n.$$

For the interaction one may take, for example,

$$\Big(\big(H(s)-H_0\big)\psi\Big)(x,j) = \sum_{j'} v_{j,j'}(x,s)\psi(x,j')$$

with $v_{jj'}$ hermitian, and compactly supported. Alternatively, one may consider finite rank perturbations.

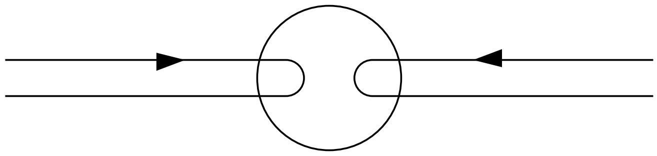

FIGURE 1. A network of two channels. Each channel is chiral and lets particles propagate to and from infinity, according to the arrows. The circle denotes the region where the channels are coupled.

6.1. **A soluble model.** Here we describe a simple, time dependent, model for which the calculation of both the dynamical and frozen scattering matrices is reduced to quadrature.

Consider scattering on the line with

$$H_0 = P = -i\nabla, \quad H_s = P + f(s)\,V, \quad s = \omega t$$

with $\big(V\psi\big)(x) = v(x)\psi(x)$ a potential (multiplication operator) which is sufficiently regular and short range so that $\int |v(x)|\,dx,\ \int |xv(x)|\,dx < \infty$. The model has one channel and should not be confused with the 2-channel example pictured in Figure 1.

To calculate the dynamical S matrix note that

$$\Omega(t,t') := U(t,t')U_0(t'-t), \tag{6.1}$$

satisfies the Volterra type equation:

$$\frac{\partial\Omega(t,t')}{\partial t'} = i f(\omega t')\Omega(t,t')V(t-t'), \quad \Omega(t',t') = 1, \tag{6.2}$$

with $V(t)$ the (backward) free Heisenberg evolution of the potential, i.e.

$$V(t) := U_0(t)\ V\ U_0(-t). \tag{6.3}$$

Since $H_0 = P$ is the generator of shifts, $V(t)$ is the shifted potential:

$$\big(V(t)\psi\big)(x) = v(x-t)\psi(x). \tag{6.4}$$

In particular, $V(t)$ at different times commute, and the solution of the Volterra type problem is given simply by

$$\Omega(t,t') = e^{-i\int_0^{t-t'} f(s-\omega t'')V(t'')dt''}, \quad s = \omega t. \tag{6.5}$$

From the definition of the wave operators based on time s, Eq. (2.1), we obtain for the dynamical wave operators:

$$\Omega_-(s;H,H_0) = e^{-i\int_0^\infty f(s-\omega t')V(t')dt'}, \quad \Omega_+(s;H,H_0) = e^{i\int_{-\infty}^0 f(s-\omega t')V(t')dt'}.$$

From this we obtain for the dynamical scattering matrix

$$S_d(s,H,H_0) = e^{-i\int_{-\infty}^\infty f(s-\omega t')V(t')\,dt'}. \tag{6.6}$$

The dynamical scattering matrix, as well as the wave operators, are local gauge transformations, i.e. multiplication by a *function* of position, of modulus one.

The wave operators and the S matrix reduce to the frozen ones upon replacing the function $f(s-\omega t')$ by its frozen value $f(s)$, hence:

$$S_f(H_s,H_0) = e^{-if(s)\int_{-\infty}^\infty V(t)\,dt} = e^{-if(s)\int_{-\infty}^\infty V_+(t)\,dt}, \tag{6.7}$$

where $2V_+(t) = V(t) + V(-t)$. S_f is just a number, not a function of position.

The frozen scattering matrix provide very little information on the potential $v(x)$, for it depends one just one number—the total weight of the potential[1]. The dynamical S matrix, in contrast, provides independent information about the potential for each value of s.

Since the frozen S matrix is independent of the incident energy, the Wigner time delay vanishes identically in this model: $\tau_w = 0$. The (frozen) energy shift is just a real number (a multiple of the identity)

$$\mathcal{E}_f = \dot f(s)\int_{-\infty}^\infty v(x)dx.$$

In contrast, the dynamical energy shift, is the multiplication operator:

$$\mathcal{E}_d = \int_{-\infty}^\infty \dot f(s-\omega t')V(t')\,dt'. \tag{6.8}$$

6.2. **The on-shell matrix and coherent states.** For later purposes we shall need the matrix elements of the frozen S matrix. Since $\mathcal{S}_f$ commutes with H_0, the matrix elements are independent of t and are related to the on-shell matrix by

$$\begin{aligned}\langle t,e,j;\varepsilon|\,\mathcal{S}_f\big(H_s,H_0\big)\,|t,e,j';\varepsilon\rangle &= \frac{1}{\sqrt{\pi}\varepsilon}\int dE\, S_{jj'}(s,E)e^{-\frac{(E-e)^2}{\varepsilon^2}}\\ &= S_{jj'}(s,e) + O(\varepsilon^2\partial_{EE}S).\end{aligned} \tag{6.9}$$

The estimate is obtained by observing that $S_{jj'}(s,E)-S_{jj'}(s,e)$ does not contribute to the integral to first order in $E-e$. Since

$$(\partial_{EE}S)\,S^\dagger = -\tau_w^2 + i\tau_w',$$

(with prime denoting the derivative with respect to the energy) we see that the on-shell S matrix approximates the diagonal entries of the frozen S matrix, provided the Wigner time delay and its energy dependence are both small:

$$\varepsilon^2(\tau_w^2 + |\tau_w'|) \ll 1. \tag{6.10}$$

[1]This is in sharp contrast with scattering problems where H_0 is the Laplacian [4].

7. The adiabatic time scale τ

In this section we compute, to leading order, the time scale τ relevant to adiabatic scattering. This time scale is defined so that $\omega\tau \ll 1$ characterizes the adiabatic regime in the sense that the frozen scattering data approximate the dynamical scattering data.

There are two results in this section, one positive and one negative. The positive result says that, at least to leading order, τ can be computed from time independent quantities alone, Eq. (7.3) below. The negative result is that τ cannot be computed from the on-shell scattering matrix and its derivatives. In particular, the Wigner time delay alone does not determine τ.

Using Eqs. (2.5,2.6,2.7) and property 5.2.C one finds

$$\begin{aligned}\langle t,e,j;\varepsilon|\left(\mathcal{S}_d(0;H,H_0)-\mathcal{S}_f(H_s,H_0)\right)|t,e,j';\varepsilon\rangle = \\ \langle 0,e,j;\varepsilon|\,\Omega_+^\dagger(H_s,H_0)\big(\mathcal{S}_d(s;H,H_s)-1\big)\Omega_-(H_s,H_0)\,|0,e,j;\varepsilon\rangle\,.\end{aligned}\tag{7.1}$$

We expand the S matrix into the formal asymptotic series in adiabatic parameter ω [15]:

$$\mathcal{S}_d\big(s;H,H_s\big)-1 \;=\; -i\omega\int_{-\infty}^{\infty} e^{iH_st'}\,\dot H_s\,e^{-iH_st'}\,t'dt' \;+\; O(\omega^2).\tag{7.2}$$

The matrix element of $\langle t,e,j;\varepsilon|\left(\mathcal{S}_d(0;H,H_0)-\mathcal{S}_f(H_s,H_0)\right)|t,e,j';\varepsilon\rangle$ is then controlled by

$$\omega\tau(e,s;\varepsilon):=\omega\int_{-\infty}^{\infty}\langle t',e,j;\varepsilon|\,\Omega_+^\dagger(H_s,H_0)\dot H_s\Omega_-(H_s,H_0)\,|t',e,j;\varepsilon\rangle\;t'\,dt',\tag{7.3}$$

where we have used

$$e^{-iH_st}\Omega_-(H_s,H_0)\,|0,e,j;\varepsilon\rangle = e^{-iet/2}\,\Omega_-(H_s,H_0)\,|t,e,j;\varepsilon\rangle\,.$$

The last identity follows from property 5.2.C.

Notice that $\tau(e,s;\varepsilon)$ involves the frozen wave operators and the rate of change of the Hamiltonian at the epoch s. Since $\dot H_s$ is supported near the origin, only small t' contribute to the matrix elements in Eq. (7.3). More precisely, this depends only on the time localization property of either the bra or the ket. One can use methods of time-independent scattering theory to compute it. It is in general complex. The adiabatic time scale, $\tau = |\tau(e,s;\varepsilon)|$ is a measure of the error, and $\omega\tau \ll 1$ then clearly characterizes the adiabatic regime.

Propagation estimates can, and have been, used [13] to bound the error in the frozen data. These estimates yield bounds on τ.

7.1. Example: the soluble model.

For the case of one channel scattering with $H(s) = P + f(s)V$, by Eq. (6.6,6.7)

$$\begin{aligned}S_d(s;H,H_0)-S_f(H_s,H_0) \;&=\; \left(e^{-i\int_{-\infty}^{\infty}\left(f(s-\omega t)-f(s)\right)V(t)\,dt}-1\right)\;S_f(H_s,H_0)\\ &\approx\; i\omega\dot f(s)\left(\int_{-\infty}^{\infty}tV(t)\,dt\right)\;S_f(H_s,H_0).\end{aligned}\tag{7.4}$$

The adiabatic time scale τ is, in analogy with Eq. (7.3), the multiplication operator:

$$\tau\approx-\dot f(s)\left(\int_{-\infty}^{\infty}tV(t)\,dt\right)\;S_f(H_s,H_0)=-\dot f(s)\left(\int_{-\infty}^{\infty}tV_-(t)\,dt\right)\;S_f(H_s,H_0);\tag{7.5}$$

$$2V_-(t)=V(t)-V(-t).$$

By Eq. (6.7) the frozen S matrix only depends on V_+, while the error only depends on V_-. Since V_- and V_+ are independent this shows that the error term in the adiabatic expansion cannot be estimated in terms on the frozen scattering data alone.

Combining Eqs. (6.9) and (7.3) we obtain a relation between matrix elements of the dynamical S matrix and the on-shell S matrix:

(7.6)
$$\langle t,e,j;\varepsilon|\,\mathcal{S}_d(0;H,H_0)\,|t,e,j';\varepsilon\rangle = S_{jj'}(s,e) + O\big(\varepsilon^2(\tau_w^2+|\tau_w'|)+\omega\tau(e,s;\varepsilon)\big),$$

8. The energy shift

The energy shift is a first order quantity, nevertheless, it is determined, to leading order in ω, by the frozen data:

$$\langle t,e,j;\varepsilon|\,\mathcal{E}_d(0)\,|t,e,j';\varepsilon\rangle \;=\; i\,\omega\big(\dot S(s,e)S^\dagger(s,e)\big)_{jj'} \;+\; O(\omega^2), \quad (s=\omega t). \tag{8.1}$$

Here is one of the possible ways to see it: As in previous section, we first expand $\mathcal{E}_d(0)$ in the formal power series in ω, using Eq. 3.1.

$$\begin{aligned}\mathcal{E}_d(0) &= i\,\omega\dot{\mathcal{S}}_d(0)\mathcal{S}_d(0)^\dagger = [\;H_0,\mathcal{S}_d\;]\;\mathcal{S}_d^\dagger \\ &= [\;H_0,\mathcal{S}_f(s)\;]\;\mathcal{S}_d^\dagger(0) \;+\; [\;H_0,\mathcal{S}_d(0)-\mathcal{S}_f(s)\;]\;\mathcal{S}_d^\dagger(0)\\ &= -i\omega\Omega_+^\dagger(H_s,H_0)\left[\,H_s,\int_{-\infty}^{\infty} e^{iH_st'}\,\dot H_s\,e^{-iH_st'}\,t'dt'\,\right]\Omega_-(H_s,H_0)\mathcal{S}_f^\dagger(s)+O(\omega^2).\end{aligned} \tag{8.2}$$

where we have used $[H_0,\mathcal{S}_f(s)]=0$ and Eq. 7.2. We integrate by parts the commutator in the last equation:

$$[H_s,\int_{-\infty}^{\infty} e^{iH_st'}\,\dot H_s\,e^{-iH_st'}\,t'dt'] \;=\; -i\int_{-\infty}^{\infty} e^{iH_st'}\,\dot H_s\,e^{-iH_st'}\,dt' \;+\; \text{boundary terms}. \tag{8.3}$$

We can ignore the boundary contributions, which vanish when we consider the matrix element of the spectral shift. Expanding the derivative of the frozen S matrix into the asymptotic series, we obtain

$$\dot{\mathcal{S}}_f(s) \;=\; \Omega_+^\dagger(H_s,H_0)\;\int_{-\infty}^{\infty} e^{iH_st'}\,\dot H_s\,e^{-iH_st'}\,dt'\;\Omega_-(H_s,H_0) \;+\; O(\omega), \tag{8.4}$$

and combining last three equations, we get the power expansion for a spectral shift:

$$\mathcal{E}_d(0) \;=\; i\,\omega\dot{\mathcal{S}}_f(s)\mathcal{S}_f^\dagger(s) \;+\; O(\omega^2). \tag{8.5}$$

Once again, this is a *formal* asymptotic expansion, but one can make sense out of it, considering the fixed matrix element of $\mathcal{E}_d$. The result follows now from the relation $\dot{\mathcal{S}}_f(s)\mathcal{S}_f^\dagger(s)$

$$\langle t,e,j;\varepsilon|\,\dot{\mathcal{S}}_f(s)\mathcal{S}_f^\dagger(s)\,|t,e,j';\varepsilon\rangle \;=\; i\,\big(\dot S(s,e)S^\dagger(s,e)\big)_{jj'} \;+\; O(\omega), \quad (s=\omega t). \tag{8.6}$$

The energy shift plays a role in the theory of adiabatic quantum pumps. In particular, the pumped charge, the entropy production and noise generation in quantum pumps can all be expressed in terms of the energy shift [3]. It is remarkable that basic properties of adiabatic quantum pumps can be understood, to leading order, in terms of the frozen scattering data alone.

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