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Time dependence of Lippmann-Schwinger states

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Due to the presence of an infinitesimal parameter ε in the resolvent, the Lippmann-Schwinger states cannot be strict eigenstates of the Hamiltonian, and their time evolution is very non-trivial (in agreement with Fermi's golden rule). In sharp contrast, strict Schrödinger eigenstates cannot make transitions into free channels. Artefacts such as adiabatic switching, wave packets, or infinite time span are not needed in our analysis.

[**Keywords:** Schrödinger, Lippmann-Schwinger, Epsilon, Non-eigenstate, Time evolution, Fermi's golden rule]

Quantum formal scattering theory dealing with the continuum spectrum has been developed both in terms of the Schrödinger differential equation[1] in position space and the Lippmann-Schwinger (LS) integral equation[2] in momentum space. It is believed that both these descriptions are equivalent if the limit ε = +0 is taken at the outset where ε is an infinitesimal parameter appearing in the free resolvent operator G_k^0 of the theory. But the existing literature[1-5] has never pointed out the fact that the Schrödinger and LS formalisms become different if the limit ε → +0 is taken at the end of the analysis owing to the appearance of a new type of projection operator $\eta_k^0 = i\varepsilon G_k^0$. This important feature has been established by us very recently[6] in the context of time-independent scattering theory. The aim of the present note is to apply this idea to deal with time-dependent transitions assuming that the total Hamiltonian H still does not contain t explicitly.

We prove that the LS state $\left|\psi_k^L\right\rangle$ at time t=0 cannot strictly satisfy the Schrödinger eigenequation in the full Hilbert space because of a peculiar ket $\left|\Lambda_k\right\rangle$. Next, Sec. 3 demonstrates that whereas the Schrödinger eigenket $\left|\psi_k^S(t)\right\rangle$ at general time t cannot scatter into free states $\left|n\right\rangle$ yet over LS non-eigenket does make such transitions in nice agreement with Fermi's golden rule. Finally, some concluding remarks are given in Sec. 4 emphasizing how our treatment differs from known approaches like wave packets[4], adiabatic switching[5], etc. in the context of time evolution.

Time-Independent Quantities—The free system —We denote the free Hamiltonian by H° whose continuum eigenket $\left|k\right\rangle$ belonging to real positive energy E_k satisfies:

$$\left(E_k - H^\circ\right)\left|k\right\rangle = 0\,,\; E_k > 0 \qquad \dots (1)$$

For later convenience we introduce the c-number functions:

$$g_{nk} = \frac{1}{E_k - E_n + i\varepsilon}\;,\; \mu_{nk} = i\varepsilon g_{nk}\;,\; d_{nk} = \varepsilon\left|g_{nk}\right|^2 \quad \dots (2)$$

with ε general positive at this stage. Note that even in the limit ε → +0 our μ_{nk} cannot vanish everywhere because its on-shell value is always unity:

$$\mu_{nk}\left(E_n = E_k\right) = i\varepsilon / i\varepsilon = 1 \qquad \dots (3)$$

We shall also need the free resolvent G_k^0, singular operator η_k^0, and distribution D_k^0 given by:

$$G_k^0 = \frac{1}{E_k - H^\circ + i\varepsilon}\,,\; \eta_k^0 = i\varepsilon G_k^0\,,\; D_k^0 = \varepsilon\left|G_k^0\right|^2 \qquad \dots (4)$$

whose eigenbra equations read

$$\left\langle n\right|G_k^0 = \left\langle n\right|g_{nk}\,,\; \left\langle n\right|\eta_k^0 = \left\langle n\right|\mu_{nk}\,,\; \left\langle n\right|D_k^0 = \left\langle n\right|d_{nk} \dots (5)$$

Clearly, even in the limit ε → +0 our η_k^0 will not reduce to the null operator because $\left\langle n\right|\eta_k^0 = \left\langle n\right|$ if $E_n = E_k$. All these information will be utilized in the sequel.

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Interacting system—The total Hamiltonian operator is called $H = H^{\circ} + V$ with V being a sort-range hermitian interaction. The scattering eigen states of H obey the Schrödinger (superscript S) equation:

$$\left(E_k - H\right)\left|\psi_k^S\right\rangle = 0 \ , E_k > 0 \qquad \ldots (6)$$

subject to plane + outgoing wave boundary condition. It is customary to replace Eq. (6) by the LS (superscript L) state vector:

$$\left|\psi_k^L\right\rangle = \left|k\right\rangle + G_k^0 V\left|\psi_k^L\right\rangle \qquad \ldots (7)$$

and to compute transition matrix elements from:

$$T_{nk} = \left\langle n\right|V\left|\psi_k^L\right\rangle \qquad \ldots (8)$$

If the setting ε = 0 is made at the very start then $\left|\psi_k^S\right\rangle$ and $\left|\psi_k^L\right\rangle$ indeed coincide in position space. But if ε is kept general positive (with the limit ε→+0 postponed till end) then such a coincidence will not happen in the full Hilbert space. Our objective below is to discuss this strange feature given in Eq. (7) by proposing several lemmas along with their consequences.

1st Lemma (Comparison with Schrödinger)—In sharp contrast to the Schrödinger eigenequation (6) our LS state Eq. (7) satisfies a non-eigenequation:

$$\left(E_k - H\right)\left|\psi_k^L\right\rangle = -\left|\Lambda_k\right\rangle \qquad \ldots (9a)$$

where the extra ket $\left|\Lambda_k\right\rangle$ is defined by:

$$\left|\Lambda_k\right\rangle = \eta_k^0 V\left|\psi_k^L\right\rangle, \ \left\langle n\middle|\Lambda_k\right\rangle = \mu_{nk} T_{nk} \qquad \ldots (9b)$$

Proof—Application of the operator $(E_k - H^{\circ} + i\varepsilon)$ on Eq. (7) yields:

$$\left(E_k - H^{\circ} + i\varepsilon\right)\left|\psi_k^L\right\rangle = i\varepsilon\left|k\right\rangle + V\left|\psi_k^L\right\rangle \qquad \ldots (10)$$

Upon rearranging terms and remembering that $i\varepsilon\left(\left|\psi_k^L\right\rangle - \left|k\right\rangle\right) = i\varepsilon G_k^0 V\left|\psi_k^L\right\rangle = \left|\Lambda_k\right\rangle$ we arrive at the stated result.

Discussion—It may be stressed that the objects μ_{nk}, η_k^0 and $\left|\Lambda_k\right\rangle$ have been used by us for the first time in formal scattering theory. Even as ε → 0 our $\left|\Lambda_k\right\rangle$ cannot become the null ket. This is because, in view of the property given in Eq. (3), the on-shell value of the inner product $\left\langle n\middle|\Lambda_k\right\rangle$ become the physical scattering amplitude:

$$\left\langle n\middle|\Lambda_k\right\rangle = T_{nk} \quad \text{if } E_n = E_k \qquad \ldots (11)$$

Time-dependent aspects (ħ = 1 units)

A free state n evolves with the time t according to:

$$\left|\phi_n(t)\right\rangle \equiv e^{-iH^{\circ}t}\left|n\right\rangle = e^{-iE_n t}\left|n\right\rangle \qquad \ldots (12)$$

However, for the interacting system the action of the evolution operator e^{-iHt} is different on the Schrödinger and LS states as described below.

2nd Lemma (Schrödinger Evolution)

At any finite t the Schrödinger state $\left|\psi_k^S(t)\right\rangle$, the probability amplitude $a_{nk}^S(t)$, and transition rate $W_{nk}^S(t)$ are given by:

$$\left|\psi_k^S(t)\right\rangle \equiv \exp(-iHt)\left|\psi_k^S\right\rangle = \exp(-iE_k t)\left|\psi_k^S\right\rangle \qquad \ldots (13a)$$

$$a_{nk}^S(t) \equiv \left\langle\phi_n(t)\middle|\psi_k^S(t)\right\rangle = \exp\left[i(E_n - E_k)t\right]\left\langle n\middle|\psi_k^S\right\rangle \qquad \ldots (13b)$$

$$W_{nk}^S(t) \equiv \frac{d}{dt}\left|a_{nk}^S(t)\right|^2 = 0 \qquad \ldots (13c)$$

Proof—Eq. (13a) is a consequence of the fact that $\left|\psi_k^S\right\rangle$ is strict eigenstate of H belonging to energy E_k. Next, Eq. (13b) follows from the definition given in Eq. (12) of freely evolving bra $\left\langle\phi_n(t)\right|$. Finally, Eq. (13c) holds because the modulus square:

$$\left|e^{i(E_n - E_k)t}\right|^2 \equiv 1 \qquad \ldots (14)$$

has zero time derivative.

Discussion —The physical significance of Eq. (13c) is that a pure Schrödinger scattering eigenket cannot make transitions into free channels as the time progresses. To overcome this difficulty, i.e., to derive Fermi's golden rule the following recipes/artefacts have been suggested in the literature:

(a) Use of harmonic or constant perturbation[3] with $\left|k\right\rangle$ as the initial state at zero time; (b) Use of a wave packet[4] (i.e., superposition of free kets) as the initial state in the remote past; (c) Use of adiabatically switched Hamiltonian[5] of the form $H^0 + \exp(-\varepsilon|t|)V$ with $|k\rangle$, being the initial state in the remote past. Of course, such Hamiltonians cannot possess stationary states like Eq. (13a).

The main drawback of all these recipes/artefacts is that an infinitely long time span t_∞ is considered to calculate an average transition rate. We shall now demonstrate how this trouble gets automatically resolved by employing our LS non-eigenstates given in Eq.(7).

3rd Lemma (LS Evolution)—"For any tiny ε we consider a wide temporal range $-\varepsilon^{-1} \ll t \ll \varepsilon^{-1}$ and remember the extra ket $|\Lambda_k\rangle$ of Eq. (9a). Then the time-dependent LS state $|\psi_k^L(t)\rangle$, the probability amplitude $a_{nk}^L(t)$, and transition rate $W_{nk}^L(t)$ are given up to terms of order O(εt) by:

$$|\psi_k^L(t)\rangle \equiv \exp(-iHt)|\psi_k^L\rangle = \exp(-iE_k t)\left[|\psi_k^L\rangle - it|\Lambda_k\rangle + O(\varepsilon t)^2\right] \quad \dots (15a)$$

$$a_{nk}^L(t) \equiv \langle\phi_n(t)|\psi_k^L(t)\rangle = \exp\left[i(E_n - E_k)t\right]\left[\langle n|\psi_k^L\rangle - it\mu_{nk}T_{nk} + O(\varepsilon t)^2\right] \quad \dots (15b)$$

$$W_{nk}^L(t) \equiv \frac{d}{dt}\left|a_{nk}^L(t)\right|^2 = \left[-2\langle k|n\rangle \operatorname{Im} T_{kk} + 2d_{nk}\left|T_{nk}\right|^2 + O(\varepsilon t)\right] \text{"} \quad \dots (15c)$$

Proof —To prove Eq. (15a) we do a linear Taylor expansion of:

$$|\psi_k^L(t)\rangle \equiv \exp\left[-iE_k t + i(E_k - H)t\right]|\psi_k^L\rangle = e^{iE_k t}\left[1 + i(E_k - H)t + ...\right]|\psi_k^L\rangle \quad \dots (16a)$$

and recall the property Eq. (9a). Next, upon taking the overlap with $\langle\phi_n(t)|$ and writing $\langle n|\Lambda_k\rangle = \mu_{nk}T_{nk}$ our (15b) follows. Finally, we simplify the overlap probability:

$$\left|a_{nk}^L(t)\right|^2 = \left|\langle n|\psi_k^L\rangle\right|^2 + 2\operatorname{Im}\left[\langle\psi_k^L|n\rangle\mu_{nk}T_{nk}\right] t + O(\varepsilon t)^2 \quad \dots (16b)$$

where Im stands for the imaginary part. Differentiating Eq. (16b) with respect to t and employing the relation:

$$\langle\psi_k^L|n\rangle = \langle k|n\rangle^* + g_{nk}^* T_{nk}^* \quad \dots (16c)$$

we arrive at desired Eq. (15c).

Discussion —Eqs. (15a,b,c) hold for any tiny ε and are new in formal scattering theory. Our Eq. (15a) clearly brings out the important role played by the ket $|\Lambda_k\rangle$ in computing the time-dependent state vector. Next, the on-shell ($E_n = E_k$) value of $\langle n|\Lambda_k\rangle = T_{nk}$ gives crucial contribution to the overlap probability Eq. (16b). Finally, Eq. (15c) has nice physical interpretation to be clarified below by letting ε tend to zero.

4th Lemma (Ultimate ε → +0 Limit) —As ε → +0 the generalized functions μ_{nk} and d_{nk} tend to:

$$\mu_{nk} \to \varepsilon d_{nk}\,;\ d_{nk} \to \pi\delta(E_k - E_n) \quad \dots (17)$$

where δ is the Dirac delta. Also, the second term of Eq. (15c) precisely coincides with Fermi's (superscript F) golden rule rate:

$$\Gamma_{nk}^F \equiv 2\pi\delta(E_k - E_n)\left|T_{nk}\right|^2 \quad \dots (18)$$

Proof —The properties $\mu_{nk}(E_n \neq E_k) = 0$ and $\mu_{nk}(E_n = E_k) = 1$ are consistent with the product εd_{nk} in Eq. (17). Next, the product $d_{nk} \equiv \varepsilon\left|g_{nk}\right|^2$ agrees with a well-known representation of π times Dirac delta. Hence the term $2d_{nk}\left|T_{nk}\right|^2$ merges with Fermi's rate Eq. (18).

Discussion —As ε → +0 the $O(\varepsilon t)^2$ and $O(\varepsilon t)$ terms drop out in Eqs[15 (a,b,c)] at any finite t. Our Eq. (15c) now becomes a master rate equation not available in the existing literature[3-5] since it receives contribution from the forward formation of state n and its backward decay into all other channels. Next, Eq. (15c) is consistent with the requirement of total probability conservation viz.:

$$\frac{d}{dt}\langle\psi_k^L(t)|\psi_k^L(t)\rangle = \sum_n W_{nk}^L(t) = 0 \quad \dots (19)$$

Finally, Eq.(15c) has the merit that holds locally at every finite t so that an average over infinite time span t_∞ need not be considered.

Conclusions—The main findings of the present note may be summarized as follows under the provision that $\varepsilon \to +0$ at the end:

(i) At time t = 0 and in sharp contrast to the Schrödinger continuum eigenket $\left|\psi_k^S\right\rangle$ our Lippmann-Schwinger state $\left|\psi_k^L\right\rangle$ cannot be a strict eigenstate of H due to appearance of a peculiar ket $\left|\Lambda_k\right\rangle$ in Eq. (9a,b). The inner product $\left\langle n\middle|\Lambda_k\right\rangle$ vanishes in the off-shell ($E_n \neq E_k$) subspace but survives in the on-shell ($E_n = E_k$) subspace. This feature has not been mentioned in the existing literature[1-5] but was reported recently by us[6].

(ii) At times t ≠ 0 the Scrödinger eigenstate $\left|\psi_k^S(t)\right\rangle$ cannot make transition into free channels but our LS non-eigenstate $\left|\psi_k^L(t)\right\rangle$ can do so as shown explicitly by Eq. [15(a,b,c)]. For non-forward/non-elastic case (n ≠ k) our Eq. (15c) coincides with Fermi's golden rule. For elastic, forward case (n = k) two terms appear naturally in Eq. (15c) corresponding to formation as well as decay of a given state k. Such treatment of time-dependence is not available in the literature.

(iii) Our derivation in Eq. (15c) does not require use of artefacts like averaging over infinite time span[3], wave packets[4], adiabatically-switched Hamiltonian[5], etc. However, we have consistently employed a time-independent H because, then the difference between the Schrödinger evolution in Eq. (13) and LS prediction Eq. (15) stands out in the most prominent manner.

Before ending it may be added that the present note is not concerned with other technicalities such as non-compactness of the LS kernel $G_k^0 V$ and construction of asymptotic states at t = $\mp\infty$.

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