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Non-orthogonality of Lippmann-Schwinger-Low states

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For the general short-ranged potential the Lippmann-Schwinger-Low (LSL) scattering formalism by taking the limit $\varepsilon \to +0$ at the end of the analysis, with ε being an infinitesimal adiabatic parameter has been re-examined. It is found that the LSL state $|\psi_k^L\rangle$ does not strictly satisfy the Schrodinger eigen equation, and the pair $|\psi_n^L\rangle$, $|\psi_k^L\rangle$ is mutually non-orthogonal if $E_n = E_k$, $n \neq k$. For this purpose a new type of projection operator η_k^0, a non-linear relation among transition amplitudes, and a separable interaction as illustration have been used.

[**Keywords:** Scattering theory, Hamiltonian, Schrodinger, Resolvent, Lippmann-Schwinger-Low, Orthogonality]

1 Introduction

Quantum formal scattering theory dealing with the continuum spectrum has been developed both in terms of the Schrödinger differential equation in position-space and the Lipmann-Schwinger-Low (LSL) integral equations in momentum space. The LSL equation[1] for state vectors/transition matrices provide the basis for deriving the Born series in wave mechanics[2], reaction amplitudes in re-arrangement collisions[3], Dyson's perturbation expansion in Dirac picture[4], and various cross-sections in old-fashioned quantum electrodynamics[5]. The aim of the present paper is to examine some features of the LSL equations which have not been treated adequately in the existing literature[1-8]. These features are intimately linked with the manner in which an infinitesimally small adiabatic parameter ε tends to zero.

To be more precise, Lemmas A, B, C, D, E and F below answer the following six questions: (i) Are the LSL representations strictly equivalent to the underlying Schrödinger equation? (ii) What is the action of the full resolvent operator on the LSL state vector? (iii) What is a general off/on energy-shell unitarity-like relation obeyed by the LSL transition matrix elements? (iv) Do the LSL state vectors accurately satisfy the standard Schrödinger orthonormality relations? (v) What happens when the limit $\varepsilon \to +0$ is ultimately taken in various complex functions/distributions? (vi) Can we confirm the results explicitly in the case of a separable potential[7] for which the LSL solutions are obtainable in closed form? Finally, the paper ends by pointing out some implications of our findings.

2 Preliminaries

2.1 Free system

The free Hamiltonian is denoted by H^0 whose continuum eigenket belonging to real positive energy E_k satisfies

$$\left(E_k - H^0\right)|k\rangle = 0, \quad E_k > 0 \qquad \ldots(1)$$

For later convenience the *c*-number functions are introduecd

$$g_{nk} = \frac{1}{E_k - E_n + i\varepsilon},$$

$$\mu_{nk} = i\varepsilon g_{nk}, \; d_{nk} = \varepsilon |g_{nk}|^2 \qquad \ldots(2)$$

with ε general positive at the moment. We shall also need the free resolvent G_k^0, singular operator η_k^0, and distribution D_k^0 is given by;

$$G_k^0 = \frac{1}{E_k - H^0 + i\varepsilon},$$

$$\eta_k^0 = i\varepsilon G_k^0, \; D_k^0 = i\varepsilon G_k^{0\dagger} G_k^0 \qquad \ldots(3)$$

whose eigenbra equations read

$$\langle n|G_k^0 = \langle n|g_{nk}\ , \langle n|\eta_k^0 = \langle n|\mu_{nk}\ ,$$

$$\langle n|D_k^0 = \langle n|d_{nk} \qquad \ldots(4)$$

The free resolvents fulfill a very useful identity:

$$g_{nk}\left(G_n^{0\dagger} - G_k^0\right) = \left(\frac{E_k - E_n + 2i\varepsilon}{E_k - E_n + i\varepsilon}\right)$$

$$G_n^{0\dagger} G_k^0 = \left(1 + \mu_{nk}\right) G_n^{0\dagger} G_k^0 \qquad \ldots(5)$$

2.2 Interacting system

The total Hamiltonian operator is called $H = H^0 + V$ with V being a short-range hermitian interaction. The scattering eigenstates of H obey the Schrödinger (superscript S) equation:

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

The boundary condition on the position-space wave function is

$$\left\langle \vec{r}\,\middle|\psi_k^S\right\rangle \xrightarrow{a<<r} \text{plane+outgoing spherical waves} \quad \ldots(7)$$

where $\langle \vec{r}\,|$ is a generic position eigenbra and a is some measure of the potential range. The full resolvent G_k, singular operator η_k, and distribution D_k are given by:

$$G_k = \frac{1}{E_k - H + i\varepsilon},$$

$$\eta_k = i\varepsilon G_k\ , D_k = \varepsilon G_k^\dagger G_k \qquad \ldots(8)$$

Since the η_k operator is unfamiliar in standard scattering theory, its salient properties are summarized in the Appendix for the sake of convenience.

It is customary to replace Eqs (1, 6) by the LSL (superscript L) representations

$$\left|\psi_k^L\right\rangle = |k\rangle + |\chi_k\rangle \qquad \ldots(9)$$

$$|\chi_k\rangle = G_k^0 V \left|\psi_k^L\right\rangle = G_k V|k\rangle \qquad \ldots(10)$$

with ε finite at the moment. Our objective below is to propose a few Lemmas on some interesting algebraic properties of $\left|\psi_k^L\right\rangle$ by paying careful attention to the ε factors as well as the operators η_k^0 , η_k .

3 Theory

3.1 Lemma A (Comparison with Schrödinger)

"In sharp contrast to the underlying Eq. (6) the LSL states satisfy a non-eigenvalue condition

$$\left(E_k - H + i\varepsilon\right)\left|\psi_k^L\right\rangle = i\varepsilon|k\rangle \qquad \ldots(11)$$

or equivalently

$$\left(E_k - H\right)\left|\psi_k^L\right\rangle = -|\Lambda_k\rangle \qquad \ldots(12)$$

$$|\Lambda_k\rangle = i\varepsilon|\chi_k\rangle = \eta_k^0 V\left|\psi_k^L\right\rangle = \eta_k V|k\rangle'' \qquad \ldots(13)$$

Corollary — It is also possible to view the LSL states as obeying a peculiar type of eigenvalue condition

$$\left(E_k - H_k\right)\left|\psi_k^L\right\rangle = 0 \qquad \ldots(14)$$

containing an effective, energy-dependent, non-hermitian Hamiltonian

$$H_k = H - \eta_k^0 V'' \qquad \ldots(15)$$

Proof — Eq. (11) follows from the application of the operator (E_k–H^0+$i\varepsilon$) or (E_k–H+$i\varepsilon$) on the LSL representation in Eqs (9 and 10). Eq. (12) is a consequence of the fact that $i\varepsilon\left(\left|\psi_k^L\right\rangle - |k\rangle\right)$ equals $|\Lambda_k\rangle$ by definition. Finally Eq. (15) is obtained upon transferring $|\Lambda_k\rangle = \eta_k^0 V\left|\psi_k^L\right\rangle$ to the left.

Discussion — It may be stressed that the objects η_k^0 , η_k and $|\Lambda_k\rangle$ have been used by us for the first time in the context of scattering theory. In order to extract physical results it is now essential to impose the scattering boundary condition given in Eq. (7) on the LSL framework by taking the limit as ε tends to zero. Unfortunately, this limit is not uniform because ε can be made to vanish either at the very beginning or at the very end of the calculation and these two routes are different as elucidated below.

Conventional route — Previous literature[1-8] takes $\varepsilon = +0$ at the outset in the LSL Eqs (9 and 10) and examines the position-space wave function $\left\langle \vec{r}\,\middle|\psi_k^{LC}\right\rangle$ where C stands for conventional. In suitable units, the poles of the free Green function produce factors like exp (- εr) which are set equal to unity. Also, operators like η_k^0 and η_k having $i\varepsilon$ in the numerator are supposed to disappear identically. Finally, the extra ket $|\Lambda_k\rangle$ is also dropped in the whole Hilbert space, forcing Eq. (12) to coincide with Eq. (6). Thereby, the conventional LSL states have the same orthogonality properties as Schrodinger's. Hence this viewpoint (superscript *C*) may be summarized as:

$$\varepsilon \xrightarrow{outset} = +0,\ exp(-\varepsilon r) = 1, \eta_k^0 = 0$$

$$|\Lambda_k\rangle = ,|\psi_k^{LC}\rangle = |\psi_k^S\rangle, \langle\psi_n^{LC}|\psi_k^{LC}\rangle = \langle n|k\rangle \qquad \dots(16)$$

Our route — In sharp contrast, we adopt the view that, although ε is an infinitesimal parameter, yet the limit $\varepsilon \rightarrow +0$ should be taken at the end of the analysis. Then, in the position-space, factors such as exp ($-\varepsilon r$) arising from the Green function poles cannot be replaced by unity at all *r*. Also, in the eigenbra relation given in Eq. (4) our η_k^0 becomes a projection operator onto free states of energy E_k since μ_{nk} in Eq. (4) equals unity if $E_n = E_k$ and tends to vanish otherwise. By the same token the distribution D_k^0 goes into $\pi\delta$ ($E_k - H^0$). Next, retainment of iε in Eq. (5) will be essential for the rigorous derivation of a general unitarity-like relation in Eq. (26) later. Finally, the ket $|\Lambda_k\rangle$ cannot disappear in the whole Hilbert space because the overlap $\langle n|\Lambda_k\rangle = \mu_{nk}\langle n|V|\psi_k^L\rangle$ reduces to the on-shell transition matrix element for $E_n = E_k$. Thus our route may be summarized via

$$\varepsilon \xrightarrow{end} = +0, exp(-\varepsilon r) \neq 1, \eta_k^0 \neq 0$$

$$|\Lambda_k\rangle \neq 0,\ |\psi_k^L\rangle \neq |\psi_k^S\rangle,\ \langle\psi_n^L|\psi_k^L\rangle = ? \qquad \dots(17)$$

where the state's inner product has been left as a question (?) mark. The route in Eq. (17) clearly shows that Eq. (12) cannot coincide with Schrodinger Eq. (6) even as $\varepsilon \rightarrow +0$. However, for $\varepsilon r \ll 1$ (in suitable units) the two wave functions nearly agree, i.e.,

$$\langle\vec{r}|\psi_k^L\rangle \approx \langle\vec{r}|\psi_k^S\rangle,\ r \ll \varepsilon^{-1} \qquad \dots(18)$$

so that the physical boundary condition in Eq. (7) is obeyed also in our route over the domain $a \ll r \ll \varepsilon^{-1} \rightarrow +\infty$. We shall continue with further development of our viewpoint given in Eq. (17) through more Lemmas, reverting back to general ε once again.

3.2 Lemma B (Action by full resolvent)

"The Schrödinger state $|\psi_n^S\rangle$ is known to be an eigenbra of G_k with eigenvalue g_{nk} such that:

$$\langle\psi_n^S|G_k = \langle\psi_n^S|g_{nk} \qquad \dots(19)$$

In sharp contrast, the operation on our LSL state is expressed by:

$$\langle\psi_n^L|G_k\langle\psi_n^L|g_{nk}\langle F_{nk}|\mu_{nk} \qquad \dots(20)$$

$$\langle F_{nk}| = \langle\chi_n|G_k = \langle n|VG_n^\dagger G_k\text{"} \qquad \dots(21)$$

Proof — We start from the dual version of the corollary given in Eqs (14 and 15) viz:

$$\langle\psi_n^L|H_n^\dagger = \langle\psi_n^L|E_n,\ H_n^\dagger = H = H - V\eta_n^{0\dagger} \qquad \dots(22)$$

The total resolvent can be cast into the form

$$G_k = \frac{1}{(E_k - H_n^\dagger + i\varepsilon) - V\eta_n^{0\dagger}} \qquad \dots(23)$$

$$= \frac{1}{(E_k - H_n^\dagger + i\varepsilon)}(1 + V\eta_n^{0\dagger}G_k) \qquad \dots(24)$$

We operate by Eq. (24) on $\langle\psi_n^L|$, factor out a *c*-number coefficient g_{nk}, and use the information $\langle\psi_n^L|V\eta_n^{0\dagger} = \langle\Lambda_n|$. Then we get:

$$\langle\psi_n^L|G_k = g_{nk}\left[|\psi_n^L\rangle + \langle\Lambda_n|G_k\right] \qquad \dots(25)$$

But the term $\langle\Lambda_n|g_{nk}G_k = \langle\chi_n|\mu_{nk}G_k = -\langle F_{nk}|\mu_{nk}$ so that Eq. (25) coincides with the stated Lemma.

Discussion — Books such as Goldberger-Watson[6] do mention the result given in Eq. (19) by adopting the conventional LSL route given in Eq. (16). We have demonstrated specifically how this result is altered due to the modified LSL eigenvalue condition given in Eq. (14). The present Lemma will be applied later to the orthogonality problem.

3.3 Lemma C (Non-linear relation for T-matrix)

The LSL transition amplitudes $T_{nk} = \langle n|V|\psi_k^L\rangle$ fulfill a non-linear relation

$$g_{nk}(T_{nk} - T_{kn}^*) = -(1 + \mu_{nk})C_{nk} \qquad \dots(26)$$

$$C_{nk} = \langle \chi_n | \chi_k \rangle = \langle \psi_n^L | VG_n^{0\dagger} G_k^0 V | \psi_k^L \rangle \\ = \langle n | VG_n^\dagger G_k V | k \rangle'' \qquad \ldots(27)$$

Proof — From Eqs (9 and 10) we first obtain $\langle n|$ and thereby write:

$$T_{nk} = \langle \psi_n^L | V | \psi_k^L \rangle - \langle \psi_n^L | VG_n^{0\dagger} V | \psi_k^L \rangle \qquad \ldots(28)$$

Interchanging n, k and complex-conjugating:

$$T_{kn}^* = \langle \psi_n^L | V | \psi_k^L \rangle - \langle \psi_n^L | VG_k^0 V | \psi_k^L \rangle \qquad \ldots(29)$$

Subtracting these two relations and employing the useful identity given in Eq. (5) the desired Lemma follows.

Corollary — Multiplication by ($E_k - E_n + i\varepsilon$) on both sides of Eq. (27) yields a general off-shell formula:

$$T_{nk} - T_{kn}^* = -(E_k - E_n + 2i\varepsilon)C_{nk} \text{ for all } n, k \qquad \ldots(30)$$

Its on-shell special case is also of interest viz.

$$[T_{nk} - T_{kn}^*]_{E_n = E_k} = -2iA_{nk} \qquad \ldots(31)$$

$$A_{nk} = [\varepsilon C_{nk}]_{E_n = E_k} = \langle \psi_n^L | VD_k^0 V | \psi_k^L \rangle \\ = \langle n | VD_k V | k \rangle, \quad E_n = E_k \qquad \ldots(32)$$

Discussion — The occurrence of μ_{nk} and $2i\varepsilon$ has played a crucial role in the above derivation, lending support to our route given in Eq. (17). Incidentally, if the $\varepsilon \to +0$ limit was now taken then Eq. (31) would agree with the standard on-shell unitarity relation. Also, for $n = k$ with $\varepsilon \to +0$ our Eq. (31) would reduce to the optical theorem because $-A_{nk}$ would become the imaginary (absorptive) part of the forward scattering amplitude. Let us revert back to finite ε again.

3.4 Lemma D (Non-orthonormality)

Schrödinger scattering states with plane plus outgoing boundary conditions are known to have the overlap:

$$I_{nk}^S \equiv \langle \psi_n^S | \psi_k^S \rangle = \langle n | k \rangle \qquad \ldots(33)$$

In sharp contrast, our LSL states have the inner product:

$$I_{nk}^L \equiv \langle \psi_n^L | \psi_k^L \rangle = \langle n | k \rangle - \mu_{nk} C_{nk}" \qquad \ldots(34)$$

1st Proof (based on resolvent action)

Using the Low form given in Eqs (9 and 10) from $|\psi_k^L\rangle$ we have:

$$I_{nk}^L = \langle \psi_n^L | k \rangle + \langle \psi_n^L | G_k V | k \rangle \qquad \ldots(35)$$

The first term here can be handled via LS equation as:

$$\langle \psi_n^L | k \rangle = \langle n | k \rangle + \langle \psi_n^L | V G_n^{0\dagger} | k \rangle \qquad \ldots(36)$$

Also, with the help of Eq. (20) the second term becomes:

$$\langle \psi_n^L | G_k V | k \rangle = g_{nk} \langle \psi_n^L | V | k \rangle - \mu_{nk} \langle F_{nk} | V | k \rangle \qquad \ldots(37)$$

Inserting these informations back into Eq. (35) the desired Lemma follows.

2nd Proof (based on product breakage)

We start from the definition, breaking the product into 4 pieces viz.

$$I_{nk}^L = \langle n + \chi_n | k + \chi_k \rangle \qquad \ldots(38)$$

$$= \langle n | k \rangle + \langle n | \chi_k \rangle + \langle \chi_n | k \rangle + \langle \chi_n | \chi_k \rangle \qquad \ldots(39)$$

Recalling the definitions given in Eq. (10) of $|\chi_k\rangle$ and Eq. (27) of C_{nk} we obtain:

$$I_{nk}^L = \langle n | k \rangle + g_{nk}(T_{nk} - T_{kn}^*) + C_{nk} \qquad \ldots(40)$$

which agrees with the desired Lemma in view of the non-linear relation given in Eq. (26).

Discussion — Books[6] have exploited the eigenvalue condition given in Eq. (19) to establish the orthogonality of conventional LSL states characterized by $\varepsilon = +0$. Our 1st proof based on Eq. (35) runs on similar lines except for the use of the crucial input given in Eq. (20) along with finite ε. Of course, our 2nd proof based on Eq. (39) is entirely new in the sense that its analogy does not exist in the conventional literature[1-8]. It is now pertinent to ask what happens to the extra term $\mu_{nk}C_{nk}$ when ε tends to zero.

3.5 Lemma E (Ultimate $\varepsilon \to +0$ limit)

When $\varepsilon \to +0$ various distributions in our Eqs (2, 3, 8) tend to:

$$d_{nk} \to \pi\delta\left(E_k - E_n\right), D_k^0 \to \pi\delta\left(E_k - H^0\right) \quad \ldots(41)$$

$$D_k \to \pi\delta\left(E_k - H\right), g_{nk} \to P\frac{1}{E_k - E_n} - id_{nk} \quad \ldots(42)$$

Also, the overlap of our LSL states tends to

$$I_{nk}^L \equiv \left\langle \psi_n^L \middle| \psi_k^L \right\rangle \to \left\langle n \middle| k \right\rangle - d_{nk}\, A_{nk} \quad \ldots(43)$$

where δ stands for Dirac delta, P denotes Cauchy principal part, and the well-defined amplitude A_{nk} is read-off from Eq. (32).

Proof — The limiting forms given in Eqs (41 and 42) arise from the usual Dirac-Cauchy prescriptions in elementary calculus. The important result given in Eq. (43) will be proved below by paying attention to the Green-like function g_{nk} and the projection-like function μ_{nk} respectively.

1st method using g_{nk}

For general values of E_n, E_k and ε we recall the definition given in Eq. (27) of the matrix element C_{nk}. Then the product:

$$\begin{aligned}\mu_{nk}\, C_{nk} &= ig_{nk}\varepsilon C_{nk} \\ &= i\left(P\frac{1}{E_k - E_n} - i\pi\delta\left(E_k - E_n\right)\right)\left[\left\langle n \middle| V\varepsilon G_n^{\dagger} G_k V \middle| k \right\rangle\right]\end{aligned} \quad \ldots(44)$$

where

$$\varepsilon G_n^{\dagger} G_k = \frac{\varepsilon}{\left[\left(E_n - H - i\varepsilon\right)\left(E_k - H + i\varepsilon\right)\right]} \quad \ldots(45)$$

As it stands, Eq. (45) involves the confluence of two simple poles at $E_n - i\varepsilon$ and $E_k + i\varepsilon$ in the H plane. Now let us ask what happens as $\varepsilon \to +0$. In the *Cauchy principal part* ($En \neq E_k$) the two poles cannot pinch the real H axis as $\varepsilon \to 0$, forcing $\varepsilon G_n^{\dagger} G_k \to 0$. But in the *Dirac delta part* ($E_n = E_k$) the two poles do pinch the real H axis from opposite directions, forcing $\varepsilon G_n^{\dagger} G_k \to D_k$. Hence the limiting value of Eq. (44) becomes:

$$\mu_{nk} C_{nk} \to 0 + i\left(-id_{nk}\right)\left[A_{nk}\right] \to d_{nk} A_{nk} \quad \ldots(46)$$

in agreement with Eq. (43).

2nd method employing μ_{nk}

For general values of E_n, E_k and ε let us rationalize:

$$\begin{aligned}\mu_{nk} = i\varepsilon g_{nk} &= i\varepsilon\left[\left(E_k - E_n\right) - i\varepsilon\right] \left|g_{nk}\right|^2 \\ &= i\left[\left(E_k - E_n\right) - i\varepsilon\right] d_{nk}\end{aligned} \quad \ldots(47)$$

where the exact definition given in Eq. (2) of d_{nk} has been recalled. Now let us ask what happens when $\varepsilon \to +0$. By Dirac delta properties ($E_k - E_n$) $d_{nk} \to 0$ so that $\mu_{nk} \to \varepsilon\, d_{nk}$ at a formal level [Incidentally, this very simple limt of μ_{nk} still preserves the projection property viz. becoming unity if $E_n = E_k$ and vanishing if $E_n \neq E_k$]. Therefore the product

$$\mu_{nk}\, C_{nk} \to d_{nk}\left[\varepsilon C_{nk}\right] \to d_{nk}\, A_{nk} \quad \ldots(48)$$

in view of the definition given in Eq. (32) of A_{nk}. Eq. (48) again proves the desired Lemma.

Discussion — Eq. (43) is the central result of the present work. It shows that I_{nk}^L reduces to $\langle n|k\rangle$ if $En \neq E_k$ but fails to do so if $En = E_k$. In other words, the set of our LSL states which are degenerate at a given collision energy E_k are mutually non-orthogonal. Of course, no explicit model of the interaction V has been assumed so far.

3.6 Lemma F (Illustration)

Consider a rank 1 separable[7] potential $V = \lambda \left| f \right\rangle\left\langle f \right|$ with λ being a real coupling and $\left| f \right\rangle$ some normalizable ket. Then, the inner product I_{nk}^L can be independently shown to be:

$$I_{nk}^L \xrightarrow{\varepsilon \to 0} \left\langle n \middle| k \right\rangle - d_{nk}\lambda^2 f_n f_k^* \frac{\left\langle f \middle| D_k^0 \middle| f \right\rangle}{\Delta_n^* \Delta_k} \quad \ldots(49)$$

where the form factor f_k and Fredholm determinant Δ_k are defined by:

$$f_k = \left\langle k \middle| f \right\rangle,\ \Delta_k = 1 - \lambda\left\langle f \middle| G_k^0 \middle| f \right\rangle" \quad \ldots(50)$$

Proof — For general E_n, E_k, ε and with $V = \lambda \left| f \right\rangle\left\langle f \right|$, the LSL Eqs (9 and 10) can be solved in closed form as:

$$\left|\psi_k^L\right\rangle = \left|k\right\rangle + G_k^0 \left| f\right\rangle \left(\lambda g_k^* / \Delta_k\right) \quad \ldots(51)$$

$$\left\langle \psi_n^L \right| = \left\langle n\right| + \left(\lambda f_n / \Delta_n^*\right)\left\langle f\right| G_n^{0\dagger} \quad \ldots(52)$$

Then, it is straightforward to compute:

$$I_{nk}^L = \left\langle n | k\right\rangle -$$

$$- \frac{\lambda^2 f_n f_k^*}{\Delta_n^* \Delta_k}\left[\frac{g_{nk}}{\lambda}\left(\Delta_k - \Delta_n^*\right) - \left\langle f\left|G_n^{0\dagger} G_k^0\right| f\right\rangle\right] \ldots(53)$$

By employing the definition given in Eq. (50) of *Δ's* and the useful identity given in Eq. (5) we obtain the compact, exact expression:

$$I_{nk}^L = \left\langle n | k\right\rangle - - \mu_{nk}\left(\frac{\lambda^2 f_n f_k^*}{\Delta_n^* \Delta_k}\right)\left\langle f\left|G_n^{0\dagger} G_k^0\right| f\right\rangle \ldots(54)$$

which is completely equivalent to the general result given in Eq. (34). Now, the limit $\varepsilon \to +0$ may be taken on the same lines as Eqs. (44) or (47) yielding the desired Lemma, in full agreement with the general formula given in Eq. (43).

4 Conclusion

A standard result of time-independent formal scattering theory is that if the adiabatic parameter ε is made zero at the outset (cf. Eq. (16)) then the conventional LSL state vector in position-space reduces to the Schrodinger one with the specified boundary condition given in Eq. (7). In the present paper we have demonstrated that the said reduction cannot happen in the whole Hilbert space if the limit $\varepsilon \to +0$ is taken at the end of the analysis (cf. Eq. (17)) although the boundary condition can still be retrieved over a wide domain viz. potential range $a << r << \varepsilon^{-1} \to +\infty$. Our main findings are contained in Lemmas *A-F* along with their corollaries/discussions. The non-orthogonality of our LSL states (for $E_n = E_k$, $n \neq k$) implies that, even in the absence of bound states, our Moller operator connecting $|k\rangle$ to $\left|\psi_k^L\right\rangle$ may become non-unitary and $\sum_k \left|\psi_k^L\right\rangle\left\langle\psi_k^L\right|$ may lose its significance as the unit matrix.

Our viewpoint may also have interesting consequences in time-dependent quantum phenomena. This is because in the case of Schrodinger eigenstates $\left|\psi_k^S(t)\right\rangle = \exp\left(-iE_k t/\hbar\right) \left|\psi_k^S\right\rangle$ the overlap probability $\left|\left\langle n\right|\left|\psi_k^S(t)\right\rangle\right|^2$ becomes time-independent for any free bra $\langle n|$. However, since our LSL states are not eigenstates of H the overlap probability $\left|\left\langle n\right|\psi_k^L(t)\right\rangle\right|^2$ will have non-trivial time-dependence. Before ending it may be added that the present work is not concerned with another peculiarity of the LSL equation — the Feddeev ambiguity — arising from the non-compactness of the kernel[8].

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Appendix

Formal Properties of the η Operator

Algebraic relations

Consider the operator $\eta_k = i\varepsilon G_k$ for general positive ε using the notation of Eq. (8). It has the following special value and modulus-square:

$$\eta_k\left(H = E_k\right) = \frac{i\varepsilon}{0 + i\varepsilon} = 1 \quad \ldots(A1)$$

$$\left|\eta_k\right|^2 = \eta_k^{\dagger}\eta_k = \varepsilon^2 G_k^{\dagger} G_k = \varepsilon D_k \qquad \ldots(\text{A2})$$

Clearly the on-shell value of η_k in Eq. (A1) is unity and never zero for any ε howsoever small.

Action on states

Recall the Schrodinger eigenket of Eq. (6) and LSL non-eigenket of Eq. (11). Then it is straightforward to verify:

$$\left|\psi_k^S\right\rangle = G_k\left(E_k - H + i\varepsilon\right)\left|\psi_k^S\right\rangle = \eta_k\left|\psi_k^S\right\rangle \qquad \ldots(\text{A3})$$

$$\left|\psi_k^L\right\rangle = G_k\left(E_k - H + i\varepsilon\right)\left|\psi_k^L\right\rangle = \eta_k\left|k\right\rangle \qquad \ldots(\text{A4})$$

These important representation (viewed in the full Hilbert space) guarantee that η_k cannot become the null operator, the states $\left|\psi_k^S\right\rangle$ and $\left|\psi_k^L\right\rangle$ in Eqs (A3 and A4) cannot coincide, and the extra term $\left|\Lambda_k\right\rangle = \eta_k V\left|k\right\rangle$ present in Eq. (12) cannot reduce to the zero ket.

Integral condition

Since η_k is a generalized function/distribution it is necessary to examine its convolution with any good test function f(H) which is smooth around the point E_k and is damped at remote points of the H axis. For sufficiently small ε the partial-fractioned integral

$$\int_0^{\infty} dH\, \eta_k\, f\left(H\right) = \pi\varepsilon f\left(E_k\right) + 0\left(\varepsilon\right) \qquad \ldots(\text{A5})$$

where the first piece in Eq. (A5) arises from the pole of η_k, and the second piece of order ε is contributed by far-off singularities of f(H) if any:

The $\varepsilon \to 0$ limit

It is now easy to verify that the leading behaviour of η for $\varepsilon \to +0$ must be

$$\eta_k \to \varepsilon D_k \to \varepsilon\pi\delta\left(E_k - H\right) \to$$

projection operator …(A6)

Indeed, this prescription preserves the relations in (A1 – A4) while the integral criterion (A5) becomes very simple viz.

$$\int_0^{\infty} dH\ \eta_k\ f\left(H\right) \to 0 \ as\ \varepsilon \to 0 \qquad \ldots(\text{A7})$$

We emphasizes that a **naive** recipe $\eta_k^{naive} = 0$ will spoil the special value in (A1) and also destroy the important representations in (A3, A4).

Measure theory implications

Since the integral in (A7) vanishes for all good test functions f(H) hence by a well known theorem of Lebesgue calculus the integrand η_k needs to vanish almost everywhere viz. over the off-shell subspace specified by $H \neq E_k$. But the same theorem permits η_k to survive over an exceptional set of null measure viz. over the on-shell subspace characterized by $H = E_k$. This is the precise meaning of our refined prescription $\eta_k \to \varepsilon D_k$ in sharp contrast to the naive recipe $\eta_k^{naive} = 0$.

Generalized function μ_{nk}

In Eqs (2 and 47) exactly similar arguments can be applied to the object $\mu_{nk} = i\varepsilon g_{nk} \to \varepsilon d_{nk}$, which cannot vanish identically in spite of the occurrence of iε in the numerator.