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The Lippmann–Schwinger equations in the rigged Hilbert space

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Abstract
We give a rigorous meaning to the Lippmann–Schwinger equations relating generalized eigenvectors of the free and perturbed Hamiltonians in a scattering process. Some related formulae are also presented. A discussion is made on the context of rigged Hilbert space formulation of quantum mechanics.

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1. Introduction

The Lippmann–Schwinger equations [1] give the Møller wave operators in terms of the Hamiltonian and the potential. When the Møller wave operators are defined as isometries on a Hilbert space a rigorous derivation of these is given in [2, 3]. Rigorous versions of the Lippmann–Schwinger equations on Banach spaces were developed a long time ago by several authors [4–9]. A second version of the Lippmann–Schwinger equations relates the generalized eigenvectors of the total Hamiltonian with the generalized eigenvectors of the free Hamiltonian [10]. As these generalized eigenvectors are functionals on certain test vector spaces, these formulae make sense as identities among functionals on the same vector space, otherwise they have no meaning. The purpose of this paper is to give meaning to the Lippmann–Schwinger equations when they are presented as a relation between functionals. We see that expressions such as

$$|w^{\pm}\rangle = |w\rangle + \frac{1}{w - H_0 \pm \mathrm{i}0} V\, |w^{\pm}\rangle \tag{1}$$

or

$$|w^{\pm}\rangle = |w\rangle + \frac{1}{w - H \pm \mathrm{i}0} V\, |w\rangle \tag{2}$$

acquire meaning when properly interpreted in the context of the rigged Hilbert space formulation of quantum mechanics [10–13].

The functionals $|w^{\pm}\rangle$ and $|w\rangle$ have been discussed in the literature [13–16]. However, it may be necessary to recall briefly their meaning in order to make this presentation self-contained. We start with the spaces of functions given by $S \cap \mathcal{H}^2_{\pm}$, where S is the Schwartz space and $\mathcal{H}^2_{\pm}$ are the spaces of Hardy functions on the upper (+) and lower (−) half planes [17]. The spaces $S \cap \mathcal{H}^2_{\pm}$ are endowed with the topology of S.

Due to a result of van Winter [18], the functions in $S \cap \mathcal{H}^2_{\pm}$ are determined by their restrictions to the positive semi-axis, $\mathbb{R}^+$, and the space of these restrictions is dense in $L^2(\mathbb{R}^+)$. Therefore, there are two bijections (one to one onto mappings)

$$\theta_{\pm} : S \cap \mathcal{H}^2_{\pm} \longmapsto S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+}. \tag{3}$$

The mappings $\theta_{\pm}$ transport the topologies from $S \cap \mathcal{H}^2_{\pm}$ into $S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+}$. As a result the triplets

$$S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+} \subset L^2(\mathbb{R}^+) \subset (S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+})^{\times} \tag{4}$$

are rigged Hilbert spaces (RHS), where the term on the right-hand side of equation (4) is the antidual[1] of $S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+}$.

Under the assumption that the free Hamiltonian H_0 has an absolutely continuous nondegenerate spectrum coinciding with $\mathbb{R}^+ = [0, \infty)$, there is a unitary operator U from the Hilbert space $\mathcal{H}$ onto $L^2(\mathbb{R}^+)$ that transforms H_0 to the multiplication operator on $L^2(\mathbb{R}^+)$.

Let V be a potential and $H = H_0 + V$ the total Hamiltonian. If the Møller operators[2], $\Omega_{\pm}$, exist and are asymptotically complete, the mappings $V_{\pm} := U\,\Omega_{\pm}^{-1}$ are unitary from $\mathcal{H}_{ac}(H)$, the absolutely continuous Hilbert space associated to H [3, 19] onto $L^2(\mathbb{R}^+)$ and $V_{\pm} H V_{\pm}^{-1}$ is the multiplication operator on $L^2(\mathbb{R}^+)$. Let us define the spaces: $\Phi_{\pm} := U^{-1}\,[S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+}]$ and $\Phi^{\pm} := V_{\pm}^{-1}\,[S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+}] = \Omega_{\pm}\,\Phi_{\pm}$ with the topologies transported from $S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+}$. We have two new RHS

$$\Phi_{\pm} \subset \mathcal{H} \subset (\Phi_{\pm})^{\times} \qquad \text{and} \qquad \Phi^{\pm} \subset \mathcal{H} \subset (\Phi^{\pm})^{\times} \tag{5}$$

such that:

(i) H_0 is continuous on $\Phi_{\pm}$ and therefore can be extended to a weakly continuous operator on $(\Phi_{\pm})^{\times}$ that we also call H_0.

(ii) H is continuous on $\Phi^{\pm}$ and therefore can be extended to a weakly continuous operator on $(\Phi_{\pm})^{\times}$ that we also call H.

(iii) The nuclear spectral theorem [20, 21] is fulfilled so that there exist functionals $|w_{\pm}\rangle \in \Phi_{\pm}$ and $|w^{\pm}\rangle \in \Phi^{\pm}$ such that $H_0\,|w_{\pm}\rangle = w\,|w_{\pm}\rangle$ and $H\,|w^{\pm}\rangle = w\,|w^{\pm}\rangle$, for each $w \in \mathbb{R}^+$. For any $\varphi^{\pm} \in \Phi^{\pm}$, we have that the functions

$$(V_{\pm}\,\varphi^{\pm})(w) = \phi_{\pm}(w) := \langle w^{\pm}|\varphi^{\pm}\rangle := \langle \varphi^{\pm}|w^{\pm}\rangle^{*} \in S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+} \tag{6}$$

where $\langle \varphi^{\pm}|w^{\pm}\rangle$ represents the action of $|w^{\pm}\rangle \in (\Phi^{\pm})^{\times}$ on $\varphi^{\pm} \in \Phi^{\pm}$.

For any $\xi_{\pm} \in \Phi_{\pm}$, we have that

$$(U\xi_{\pm})(w) = \eta_{\pm}(w) := \langle w_{\pm}|\xi_{\pm}\rangle := \langle \xi_{\pm}|w_{\pm}\rangle^{*} \in S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+}. \tag{7}$$

Thus, $|w^{\pm}\rangle$ ($|w_{\pm}\rangle$) is the mapping which maps any $\varphi^{\pm} \in \Phi^{\pm}$ ($\xi_{\pm} \in \Phi_{\pm}$) into the complex conjugate of the value of the function $(V_{\pm}\,\varphi^{\pm})(w)$ ($(U\xi_{\pm})(w)$) at the point $w \in \mathbb{R}^+$.

We recall [13] that $\Omega_{\pm}\,|w_{\pm}\rangle = |w^{\pm}\rangle$. This shows that if $\phi^{\pm} = \Omega_{\pm}\,\phi_{\pm}$, then, $(V_{\pm}\,\varphi^{\pm})(w) = (U\,\phi_{\pm})(w)$, i.e., $\langle \varphi^{\pm}|w^{\pm}\rangle = \langle \varphi_{\pm}|w_{\pm}\rangle$, see [13].

It has been proven [15] that $|w_{\pm}\rangle$ are the restrictions to $\Phi_{\pm}$ of a continuous antilinear functional on $\Phi_{+} + \Phi_{-}$ (endowed with an appropriate topology which is described in [15]). This functional carries any $\phi \in \Phi_{+} + \Phi_{-}$ to the complex conjugate of its value at $w \in \mathbb{R}^+$:

[1] The space of continuous antilinear functionals on $S \cap \mathcal{H}^2_{\pm}|_{\mathbb{R}^+}$.

[2] Here we follow the notation $\Omega_{+} = \Omega_{\mathrm{OUT}}$ and $\Omega_{-} = \Omega_{\mathrm{IN}}$, which is the notation used in [3].

$\phi \longmapsto \phi^*(w)$. In the Dirac notation, we represent it as $|w\rangle$ and $\langle\phi|w\rangle = \phi^*(w)$. Then, if $\phi_\pm$ is in $\Phi_\pm$ we have that $\langle\phi_\pm|w\rangle = \langle\phi_\pm|w_\pm\rangle$. For this reason we always omit in this paper the signs in $|w_\pm\rangle$ and write $|w\rangle$. Thus, we have, for instance, $|w^\pm\rangle = \Omega_\pm\,|w\rangle$, etc.

2. The formal solution

The Lippmann–Schwinger equations are derived rigorously in [3] where the Møller operators are isometries on Hilbert space. The formal expression for the Lippmann–Schwinger equations are then

$$\Omega_\pm = I - \int_{-\infty}^{\infty} \frac{1}{H - w' \pm \mathrm{i}0}\, V\, \mathrm{d}E^0_{w'} \tag{8}$$

where I is the identity on[3] $\mathcal{H}$, $H = H_0 + V$ and $E^0_{w'}$ is the spectral measure of H_0. Another expression [3] for $\Omega_\pm$ is the following

$$\Omega_\pm = I - \int_{-\infty}^{\infty} \frac{1}{H_0 - w' \pm \mathrm{i}0}\, V\, \Omega_\pm\, \mathrm{d}E^0_{w'}. \tag{9}$$

To obtain formally equations (1) and (2), we recall our hypothesis that H_0 has a continuous nondegenerate spectrum supported on $\mathbb{R}^+$. In this case, it has been shown [22] that

$$\mathrm{d}E^0_{w'} = |w'\rangle\langle w'|\,\mathrm{d}w' \tag{10}$$

where $|w'\rangle\langle w'| \in \mathcal{L}(\Phi_\pm, (\Phi_\pm)^\times)$ and[4] $w' \in \mathbb{R}^+$. Thus, to arrive to (1) we write

$$\begin{aligned} |w^\pm\rangle = \Omega_\pm\,|w\rangle &= \left(I - \int_0^\infty \frac{1}{H_0 - w' \pm \mathrm{i}0}\, V\,\Omega_\pm\,|w'\rangle\langle w'|\,\mathrm{d}w'\right)|w\rangle \\ &= |w\rangle - \int_0^\infty \frac{1}{H_0 - w' \pm \mathrm{i}0}\, V\,\Omega_\pm\,|w'\rangle\langle w'|w\rangle\,\mathrm{d}w' \\ &= |w\rangle - \int_0^\infty \frac{1}{H_0 - w' \pm \mathrm{i}0}\, V\,\Omega_\pm\,|w'\rangle\,\delta(w - w')\,\mathrm{d}w' \\ &= |w\rangle - \frac{1}{H_0 - w \pm \mathrm{i}0}\, V\,\Omega_\pm\,|w\rangle = |w\rangle - \frac{1}{H_0 - w \pm \mathrm{i}0}\, V\,|w^\pm\rangle \end{aligned} \tag{11}$$

where we have made use of (9) and (10). Analogously, making use of (8) and (10), we get (2).

When we extend $\Omega_\pm$ as bicontinuous operators[5] from $(\Phi_\pm)^\times$ onto $(\Phi^\pm)^\times$, they are no longer isometries between Hilbert spaces and the meaning of the above manipulations is not clear. We intend to clarify all this in the next section.

3. The meaning of Lippmann–Schwinger formulae (1) and (2)

Formulae (1) and (2) acquire meaning because $|w_\pm\rangle$ (or simply $|w\rangle$) are *also* functionals on $\Phi^\pm$ and $|w^\pm\rangle$ are *also* functionals on $\Phi_\pm$. The proof needs formulae (8) and (9). Let us first show that $|w\rangle$, $w \in \mathbb{R}^+$, is a continuous antilinear functional on $\Phi^\pm$. In order to do this, we have to define first the action of $|w\rangle$ on each $\varphi^\pm \in \Phi^\pm$ as follows[6]:

$$\langle w|\varphi^\pm\rangle = \langle w|\Omega_\pm\,\varphi_\pm\rangle := \langle w|\varphi_\pm\rangle - \langle w| \int_0^\infty \frac{1}{H - w' \pm \mathrm{i}0}\, V\,|w'\rangle\langle w'|\varphi_\pm\rangle\,\mathrm{d}w'. \tag{12}$$

[3] We assume that H_0 has an absolutely continuous spectrum only. If this is not the case, I has to be replaced by the projection onto the absolutely continuous subspace of $\mathcal{H}$ with respect to H_0.
[4] Here, $\mathcal{L}(\Phi_\pm, (\Phi_\pm)^\times)$ is the space of continuous linear operators from $\Phi_\pm$ into $(\Phi_\pm)^\times$.
[5] Continuous, bijective (one to one and onto) and with continuous inverse.
[6] Recall that $\langle w|\varphi^\pm\rangle = \langle\varphi^\pm|w\rangle^*$, where the star denotes complex conjugation.

From now on, we make the assumption that the operators $(H - w' \pm \mathrm{i}0)^{-1}\, V$ are bounded[7], so that the integral term in (12) is well defined as an integral operator on $L^2(\mathbb{R}^+)$. The kernel of this integral operator is given by

$$B(w, w', \pm\mathrm{i}0) := \langle w|\, \frac{1}{H - w' \pm \mathrm{i}0}\, V\, |w'\rangle \tag{13}$$

so that both terms in the right-hand side of (12) are well defined. Thus, for almost all $w \in \mathbb{R}^+$, the functions $\psi_\pm(w) := \langle w|\varphi^\pm\rangle$ are well defined. For each $w \in \mathbb{R}^+$ the mappings $\Phi^\pm \longmapsto \mathbb{C}$ given by $\varphi^\pm \longmapsto \psi_\pm(w)$ are well defined and even linear. We have to show that they are continuous for which we have to show that, for each $w \in \mathbb{R}^+$, the mappings $F_w^\pm$ from $\Phi^\pm$ into $\mathbb{C}$ given by

$$F_w^\pm(\varphi^\pm) := \int_0^\infty B(w, w', \pm\mathrm{i}0)\, \langle w'|\varphi_\pm\rangle\, \mathrm{d}w \tag{14}$$

are continuous. The continuity of the operator $(H - w' \pm \mathrm{i}0)^{-1}\, V$ shows that

$$|F_w^\pm(\varphi^\pm)| \leqslant K\, \|\langle w'|\varphi_\pm\rangle\|_{L^2(\mathbb{R}^+)} \tag{15}$$

with $K > 0$. As $\langle w'|\varphi_\pm\rangle$ is the restriction to $\mathbb{R}^+$ of a function $\varphi_\pm(w') \in S \cap \mathcal{H}^2_\pm$, we have

$$|F_w^\pm(\varphi^\pm)| \leqslant K \left\{ \int_0^\infty |\varphi_\pm(w')|^2\, \mathrm{d}w' \right\}^{1/2} \leqslant K \left\{ \int_{-\infty}^\infty |\varphi_\pm(w')|^2\, \mathrm{d}w' \right\}^{1/2} \leqslant K \|\varphi_\pm(w')\|_{L^2(\mathbb{R})}. \tag{16}$$

Since the Hilbert space norm on $L^2(\mathbb{R})$ is a continuous seminorm on S, we conclude the continuity of the functional $F_w^\pm$, [19]. This proves the continuity of the mapping $\varphi^\pm \longmapsto \psi_\pm(w)$ for each $w \in \mathbb{R}^+$ and hence, the continuity of the antilinear mapping $\varphi^\pm \longmapsto \psi_\pm^*(w) = \langle\varphi^\pm|w\rangle$.

To prove that $|w^\pm\rangle$ can be defined as continuous antilinear functionals on $\Phi_\pm$, we use (9) in

$$\begin{aligned} \langle w^\pm|\varphi^\pm\rangle = \langle w^\pm|\Omega_\pm\, \varphi_\pm\rangle &= \langle w^\pm|\varphi_\pm\rangle - \langle w^\pm|\, \int_0^\infty \frac{1}{H_0 - w' \pm \mathrm{i}0}\, V\, \Omega_\pm\, |w'\rangle\langle w'|\varphi_\pm\rangle\, \mathrm{d}w' \\ &= \langle w^\pm|\varphi_\pm\rangle - \int_0^\infty \langle w^\pm|\, \frac{1}{H_0 - w' \pm \mathrm{i}0}\, V\, |w'^\pm\rangle\, \langle w'|\varphi_\pm\rangle\, \mathrm{d}w. \end{aligned} \tag{17}$$

If $(H_0 - w' \pm \mathrm{i}0)^{-1}\, V$ are bounded operators, the kernels

$$B_\pm(w, w', \pm\mathrm{i}0) := \langle w^\pm|\, \frac{1}{H_0 - w' \pm \mathrm{i}0}\, V\, |w'^\pm\rangle \tag{18}$$

are well defined and therefore, (17) defines $\langle w^\pm|\varphi_\pm\rangle$, for each $w \in \mathbb{R}^+$. The same arguments as before show that $\langle\varphi_\pm|w^\pm\rangle := \langle w^\pm|\varphi_\pm\rangle^*$ defines for each $w \in \mathbb{R}^+$ a continuous antilinear functional on $\Phi_\pm$. Let us write the complex conjugate of (12) as

$$\langle\varphi_\pm|w\rangle = \langle\Omega_\pm\varphi_\pm|\Omega_\pm\, |w\rangle = \langle\varphi^\pm|w^\pm\rangle = \langle\varphi^\pm|w\rangle + \int_0^\infty B^*(w, w', \pm\mathrm{i}0)\, \langle\varphi^\pm|w'^\pm\rangle\, \mathrm{d}w'. \tag{19}$$

Omitting the arbitrary $\varphi^\pm \in \Phi^\pm$, we have

$$|w^\pm\rangle = |w\rangle + \int_0^\infty B^*(w, w', \pm\mathrm{i}0)\, |w'^\pm\rangle\, \mathrm{d}w'. \tag{20}$$

[7] We need some conditions on the potential V in order to ensure this continuity; for instance, that V be a continuous operator. This situation arises if, for instance, the potential vanishes at a certain distance of the origin in coordinate representation.

If we compare (20) with (11), we conclude that, if we want these two formulae to be identical, we must have that

$$\int_0^\infty B^*(w, w', \pm i0)\,|w'^\pm\rangle\,dw' = -\frac{1}{H_0 - w \pm i0}\,V\,|w^\pm\rangle. \tag{21}$$

Both sides of (21) are functionals on $\Phi^\pm$. Thus, if we choose $\varphi^\pm \in \Phi^\pm$, equation (21) gives

$$\begin{aligned}\int_0^\infty B^*(w, w', \pm i0)\,\langle\varphi^\pm|w'^\pm\rangle\,dw' &= -\langle\varphi^\pm|\frac{1}{H_0 - w \pm i0}\,V\,|w^\pm\rangle\\ &= -\int_0^\infty \langle\varphi^\pm|w'^\pm\rangle\langle w'^\pm|\frac{1}{H_0 - w \pm i0}\,V\,|w^\pm\rangle.\end{aligned} \tag{22}$$

Therefore, we arrive at

$$B^*(w, w', \pm i0) = -\langle w'^\pm|\frac{1}{H_0 - w \pm i0}\,V\,|w^\pm\rangle. \tag{23}$$

We now take the complex conjugate of (17) as

$$\langle\varphi_\pm|w^\pm\rangle = \langle\varphi_\pm|w\rangle + \int_0^\infty B_\pm^*(w, w', \pm i0)\langle\varphi_\pm|w'\rangle\,dw'. \tag{24}$$

Then, if we omit the arbitrary $\varphi_\pm \in \Phi_\pm$, we have

$$|w^\pm\rangle = |w\rangle + \int_0^\infty B_\pm^*(w, w', \pm i0)\,|w'\rangle\,dw'. \tag{25}$$

If we compare (25) with (2), we get

$$B_\pm^*(w, w', \pm i0) = \langle w'|\frac{1}{w - H \pm i0}\,V|w\rangle. \tag{26}$$

4. Other related formulae

In this section, we discuss the meaning of the formula

$$|w^+\rangle = S(w - i0)\,|w^-\rangle \tag{27}$$

which is, in principle, not valid because $|w^+\rangle$ and $|w^-\rangle$ are functionals on different spaces. One possible solution is to define $|w^\pm\rangle$ on the same space and then prove the identity (27) on this space, which will be either Φ^+ or Φ^-. Take an arbitrary $\varphi^- \in \Phi^-$ and define[8]

$$\langle\varphi^-|w^+\rangle := \langle\varphi^-|w^-\rangle\,S(w - i0). \tag{28}$$

This definition would be completely consistent if $\Phi^+ \cap \Phi^- = \{\mathbf{0}\}$. However, this may not be the case, and then we have to make sure that (28) does not lead to inconsistencies. As a matter of fact, the sole inconsistency may arise if there exists a nonzero vector φ^- such that $\varphi^- \in \Phi^+ \cap \Phi^-$. In this case, we have two definitions of $\langle\varphi^-|w^+\rangle$. One is (28) and the other comes from the fact that $|w^+\rangle$ has already been defined on Φ^+. Both must be identical. To show this, let $\varphi \in \Phi^+ \cap \Phi^-$ and let

$$V_+\varphi = \langle w^+|\varphi\rangle \in S \cap \mathcal{H}_+^2|_{\mathbb{R}^+}; \qquad V_-\varphi = \langle w^-|\varphi\rangle \in S \cap \mathcal{H}_-^2|_{\mathbb{R}^+}. \tag{29}$$

From here, we get

$$\langle w^+|\varphi\rangle = U\,\Omega_+^{-1}\,\Omega_-\,U^{-1}\,\langle w^-|\varphi\rangle = U\,S\,U^{-1}\,\langle w^-|\varphi\rangle \tag{30}$$

[8] This definition was suggested by A Bohm. Note that Bohm has the signs interchanged in $|w^\pm\rangle$ because he uses the notation $\varphi^\mp \in \Phi^\pm$, $\Omega_- = \Omega_{OUT}$ and $\Omega_+ = \Omega_{IN}$ [10].

where S is the S-operator. On the other hand, we have that[9] $U\,S\,U^{-1} = S(w + \mathrm{i}0)$. Then, for any $\varphi \in \Phi^+ \cap \Phi^-$, we have that

$$\langle w^+|\varphi\rangle = S(w + \mathrm{i}0)\,\langle w^-|\varphi\rangle \tag{31}$$

so that in the intersection $\Phi^+ \cap \Phi^-$, we have

$$|w^+\rangle = S(w - \mathrm{i}0)\,|w^-\rangle \tag{32}$$

and the definition given by formula (28) is consistent. Note that $|w^+\rangle$ is obviously antilinear and continuous on Φ^- and that on this space

$$|w^-\rangle = S(w + \mathrm{i}0)\,|w^+\rangle. \tag{33}$$

Finally, note also that $|w^-\rangle$ can be defined as a continuous antilinear functional on Φ^+ as

$$\langle\varphi^+|w^-\rangle = S(w + \mathrm{i}0)\,\langle\varphi^+|w^+\rangle, \qquad \forall\,\varphi^+ \in \Phi^+. \tag{34}$$

This definition gives again formulae (27) and (28), as $S(w+\mathrm{i}0) = S^*(w-\mathrm{i}0) = S^{-1}(w-\mathrm{i}0)$.

We can also define the following kernels valid for $[0, \infty)$

$$\begin{aligned}\langle w'|w^\pm\rangle &= \langle w'|w\rangle + \langle w'|\frac{1}{w - H \pm \mathrm{i}0}\,V|w\rangle \\ &= \delta(w - w') + B^*_\pm(w, w', \pm\mathrm{i}0)\end{aligned} \tag{35}$$

where $\delta(w - w')$ is the Dirac delta for the integration between 0 and ∞. This Dirac delta is also defined for $z \in \mathbb{C}^\pm$, where $\mathbb{C}^+$ and $\mathbb{C}^-$ are, respectively, the upper and lower open half planes [23]. In this case $\delta(z - w')$ is defined by series of distributions converging in $(S \cap \mathcal{H}^2_\pm|_{\mathbb{R}^+})^\times$.

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