Completeness of Eigenstates for Hamiltonians with δ-Interactions

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Outline

- Introduction: Completeness of Eigenfunctions in Quantum Mechanics
- Spectrum of the Hamiltonian modified by δ interactions
- Main Result: Orthonormality and Completeness of Eigenfunctions of the Modified Hamiltonians
- Application: Sudden Pertubation Problem

Introduction

In $D = 2, 3$ dimensions, contact delta interactions in quantum mechanics requires renormalization (coupling becomes scale-dependent).

Question: Suppose we perturb "some" Hamiltonian H_0 having complete set of eigenfunctions with contact delta potentials,

$$\boxed{H = H_0 - \alpha\, \delta(\mathbf{x} - \mathbf{a})} \,, \tag{1}$$

do we still have a complete eigenbasis?

Introduction

Fact: If A is a self-adjoint operator in a Hilbert space $\mathcal{H}$ and it has pure point spectrum (*discrete eigenvalues of finite multiplicity and no accumulation point*), then its eigenvectors form a complete orthonormal (Schauder) basis of $\mathcal{H}$:

- $\langle \psi_m | \psi_n \rangle = \delta_{mn}$ for all integers m, n,
- Every $|\psi\rangle \in \mathcal{H}$ has the expansion

$$\boxed{|\psi\rangle = \sum_{n=1}^{\infty} \langle \psi_n | \psi \rangle \, |\psi_n\rangle} \tag{2}$$

with convergence in norm, and Parseval's identity holds:

$$\|\psi\|^2 = \langle \psi | \psi \rangle = \sum_n |\langle \psi_n | \psi \rangle|^2 .$$

Equivalently, $\sum_n |\psi_n\rangle\langle\psi_n| = 1$ (Resolution of identity), or

$$\boxed{\sum_n \psi_n(x)\psi_n(y) = \delta(x-y) \text{ (Completeness relation).}} \tag{3}$$

Introduction

Some operators have both boud states (discrete) and scattering states (continuous). Then, the resolution of identity is formally given by

$$\sum_{n \in bound} |n\rangle\langle n| + \int_{cont} |E\rangle\langle E| \, d\mu(E) = 1 \ .$$

Introduction

Pedagogical explicit examples:

- K. R. Brownstein, “Calculation of a Bound State Wavefunction Using Free State Wavefunctions Only”, Am. J. Phys. 43, 173–176 (1975).
- N. Mukunda, “Completeness of the Coulomb Wave Functions in Quantum Mechanics”, Am. J. Phys. 46, 910 (1978).
- S. H. Patil, “Completeness of the Energy Eigenfunctions for the One-dimensional δ-Function Potential”, Am. J. Phys. 68, 81 (2000).
- M. A. Dalabeeh, N. Chair, “Completeness and orthonormality of the energy eigenfunctions of the Dirac delta derivative potential”, Eur. J. Phys. 43 2 (2022).
- F. E., O. T. Turgut, Completeness of energy eigenfunctions for the reflectionless potential in quantum mechanics, Am. J. Phys. 92 12 (2024).

The Choice of Initial Hamiltonian H_0

Consider two class of Hamiltonians (initial/unmodified Hamiltonians):

- $\boxed{H_0 = -\frac{\hbar^2}{2m}\Delta + V}$ on $D = 2, 3$ dimensional Euclidean space,

- $\boxed{H_0 = -\frac{\hbar^2}{2m}\nabla_g^2}$ on $D = 2, 3$ dimensional *compact Riemannian manifold*,

where

$$(\nabla_g^2 \psi)(x) = \frac{1}{\sqrt{\det g}} \sum_{i,j=1}^{D} \frac{\partial}{\partial x^i} \left(\sqrt{\det g}\, g^{ij} \frac{\partial \psi(x)}{\partial x^j} \right) ,$$

in some local coordinates, with g^{ij} being the components of inverse of the metric g.

Remark

- *In this approach, we think of the particle intrinsically moving on the manifold.*
- *Units:* $\hbar = 2m = 1$ *for simplicity.*

Restrictions on V

$$H_0 = -\Delta + V \, . \tag{4}$$

- H_0 is self-adjoint on some dense domain $D(H_0) \subseteq L^2(\mathbb{R}^D)$.
- Spectrum $\sigma_d(H_0)$ of H_0 is discrete (set of eigenvalues),
- The discrete spectrum has no accumulation point, except possibly at infinity.
- For stability, we assume H_0 has spectrum bounded below.
- More technical assumption: The heat kernel associated with H_0 has Gaussian upper and lower bounds.

Restrictions on the geometry of $\mathcal{M}$

- $\mathcal{M}$ is a two/three dimensional compact, connected Riemannian manifold without boundary.
- Often, it is essential to assume some regularity on the geometry, experience has shown that a lower bound on the Ricci curvature satisfies most of the technical requirements:
$$Ric_g(\cdot,\cdot) \geq (D-1)\kappa g(\cdot,\cdot)\ . \tag{5}$$
- For two dimensional compact manifolds, this does not impose any restriction, as Ricci curvature is exactly given by
$$Ric_g(\cdot,\cdot) = \frac{R}{2} g(\cdot,\cdot),$$
where R is the scalar curvature, and R has a minimum (and a maximum) value on a *compact* manifold.

Hamiltonian modified by δ interaction

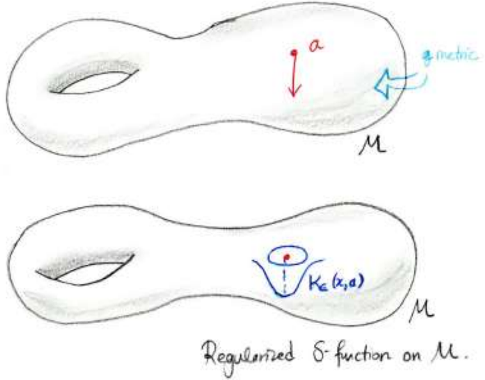
Hamiltonian at the operator level:

$$\boxed{H = H_0 - \alpha |a\rangle\langle a|} \, . \tag{6}$$

Notice that

$$\begin{aligned} \langle \mathbf{x}|H|\psi\rangle &= -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}) - \alpha\delta(\mathbf{x}-\mathbf{a})\psi(\mathbf{x}) \, , \\ \langle x|H|\psi\rangle &= -\frac{\hbar^2}{2m}\nabla_g^2\psi(x) - \alpha\delta(x,a)\psi(x) \end{aligned}$$

Hamiltonian modified by δ interaction



$$\boxed{H_\epsilon = H_0 - \alpha(\epsilon)|a_\epsilon\rangle\langle a_\epsilon|}\ , \tag{7}$$

where $|a_\epsilon\rangle = e^{-\epsilon H_0}|a\rangle$ and $\langle x|a_\epsilon\rangle = K_\epsilon(x,a) \to \delta(x,a)$ as $\epsilon \to 0^+$.

Hamiltonian modified by δ interaction

$K_t(x,y)$ is the heat the kernel associated with the operator H_0:

$$K_t(x,y) := \langle x | e^{-tH_0} | y \rangle \ .$$

It solves the heat equation

$$H_0 K_t(x,y) = \frac{\partial K_t(x,y)}{\partial t} \qquad \lim_{t \to 0^+} K_t(x,y) = \delta(x-y)$$

• Resolvent (energy Green's function) $G_0 = (H_0 - E)^{-1}$ is the Laplace transform of the heat kernel:

$$\boxed{G_0(x,y|E) = \int_0^\infty K_t(x,y) e^{tE} dt} \ , \tag{8}$$

where $\mathrm{Re}(E) < 0$.

• Fact: For any self-adjoint elliptic second-order differential operator H_0 in D dimensions

$$\boxed{K_t(x,x) \sim t^{-D/2} \qquad as \qquad t \to 0^+} \ .$$

Hamiltonian modified by δ interaction

Formal derivation of Green's function:

Solve the inhomogenous equation to find the resolvent (energy Green's function) $G^{\epsilon}(E) := (H_{\epsilon} - E)^{-1}$

$$\Big[(H_0 - E) - \alpha(\epsilon)|a_{\epsilon}\rangle\langle a_{\epsilon}|\Big]|\psi\rangle = |\rho\rangle \ .$$

From this, it is not hard to see

$$\boxed{G^{\epsilon}(E) = G_0(E) + \frac{1}{\Phi_{\epsilon}(E)} G_0(E)|a_{\epsilon}\rangle\langle a_{\epsilon}|G_0(E)} \ , \tag{9}$$

where

$$\boxed{\Phi_{\epsilon}(E) = \frac{1}{\alpha(\epsilon)} - \langle a_{\epsilon}|G_0(E)|a_{\epsilon}\rangle = \frac{1}{\alpha(\epsilon)} - \int_{\epsilon}^{\infty} K_t(a,a) e^{tE} dt} \tag{10}$$

The diagonal part of G_0 is divergent around $t = 0$:

$$\int_0^{\infty} \frac{e^{-t|E|}}{t^{D/2}} \, dt \ .$$

Hamiltonian modified by δ interaction

• A natural choice for absorbing the divergent part in a *redefinition of the coupling constant* is given by

$$\boxed{\frac{1}{\alpha(\epsilon)} = \frac{1}{\alpha_R} + \int_{\epsilon}^{\infty} K_t(a,a) e^{-t\mu^2} dt}\,, \tag{11}$$

where $-\mu^2$ is some convenient renormalization scale.
Take the limit as $\epsilon \to 0$, we obtain Krein's formula:

$$\boxed{G(x,y|E) = G_0(x,y|E) + \frac{G_0(x,a|E) G_0(a,y|E)}{\Phi(E)}} \tag{12}$$

where

$$\boxed{\Phi(E) = \frac{1}{\alpha_R} + \int_0^{\infty} K_t(a,a) \left(e^{-t\mu^2} - e^{tE} \right) dt}\,. \tag{13}$$

Eigenfunction Expansion of Green's Functions

Notation:

E_n : Eigenvalues of H_0, $\phi_n(x)$: Eigenfunctions of H_0.
E_n^*: Eigenvalues of H, $\psi_n(x)$: Eigenfunctions of H.

$$G(E) = (H-E)^{-1} 1 = (H-E)^{-1} \sum_n |\psi_n\rangle\langle\psi_n| = \sum_n \frac{|\psi_n\rangle\langle\psi_n|}{E_n^* - E} \; .$$

In coordinate representation:

$$\boxed{G(x,y|E) = \sum_n \frac{\psi_n(x)\overline{\psi_n(y)}}{E_n^* - E}} \; . \tag{14}$$

Poles of Green's function gives the bound state energies E_n^* of the system.

$$\boxed{\mathrm{Res}_{E=E_n^*} G(x,y|E) = \psi_n(x)\overline{\psi_n(y)} = \frac{1}{2\pi i} \oint_{\Gamma_n} G(x,y|E)\, dE} \; . \tag{15}$$

Spectrum of the modified Hamiltonian by delta interaction

Proposition (K. G. Akbas, F. E., O. T. Turgut, 23)

Let $\phi_k(x)$ be the eigenfunction of H_0 associated with the kth eigenvalue E_k, i.e.,

$$H_0\phi_k(x) = E_k\phi_k(x) \ .$$

If $\phi_k(a) \neq 0$ for this particular k, the eigenvalues of the renormalized system are the solutions of

$$\Phi(E) = 0 \ ,$$

and denoted by E_k^*, which lies between E_{k-1} and E_k:

$$E_{k-1} < E_k^* < E_k \ .$$

If $\phi_k(a) = 0$, then

$$E_k^* = E_k \ .$$

For the ground state ($k = 0$), $E_0^* < E_0$.

Spectrum of the modified Hamiltonian by delta interaction

Sketch of the Proof:
Assume for simplicity the spectrum is nondegenarate.
Notice that

$$
\begin{aligned}
\Phi(E) &= \frac{1}{\alpha_R} + \int_0^\infty K_t(a,a) \left(e^{-t\mu^2} - e^{tE} \right) dt \\
&= \frac{1}{\alpha_R} + G_0(a,a|-\mu^2) - G_0(a,a|E) \\
&= \boxed{\frac{1}{\alpha_R} - \sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2 (E+\mu^2)}{(E_n - E)(E_n + \mu^2)}} . \qquad (16)
\end{aligned}
$$

Spectrum of the modified Hamiltonian by delta interaction

Remark

One can show that the above sum is uniformly convergent thanks to the eigenfunction expansion of heat kernel.

Remark

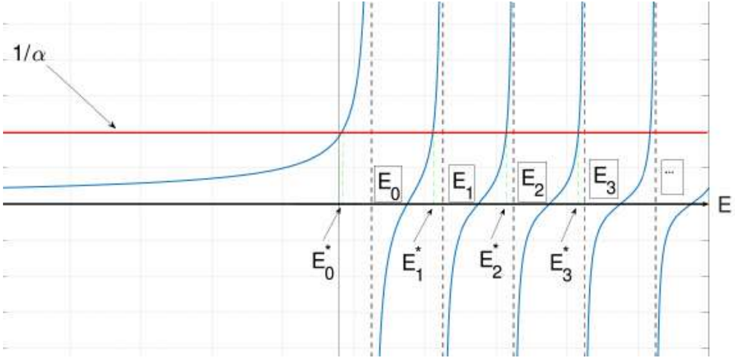
One can show that the truncated version of the above series has no zeros in the upper and lower complex E plane. Thanks to Hurwitz theorem in complex analysis, all zeros of Φ must lie on the real E axis.

$$G(x,y|E) = \underset{\substack{\uparrow \\ \text{poles}}}{G_0(x,y|E)} + \frac{\underset{\substack{\uparrow \\ \text{poles}}}{G_0(x,a|E)}\ \underset{\substack{\uparrow \\ \text{poles}}}{G_0(a,y|E)}}{\Phi(E)}$$

If $\phi_k(a) = 0$, isolate kth term in the sums and expand expressions around $E = E_k$, then poles in the first and second term cancel out. If not, then all poles comes from $\Phi(E) = 0$.

Spectrum of the modified Hamiltonian by delta interaction

Plot the graphs of $1/\alpha_R$ and $\sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2 (E+\mu^2)}{(E_n - E)(E_n+\mu^2)}$ versus E:



Spectrum of the modified Hamiltonian by delta interaction

If Γ_k is the closed contour anticlockwise oriented around each simple pole E_k^*, then

$$\psi_k(x)\overline{\psi_k(y)} = \frac{1}{2\pi i} \oint_{\Gamma_k} G(x,y|E) \, dE \; . \tag{17}$$

• From the explicit expression of the Green's function and the residue theorem, we obtain

$$\boxed{\psi_k(x) = \frac{G_0(x,a|E_k^*)}{\left(-\frac{d\Phi(E)}{dE}\Big|_{E=E_k^*} \right)^{1/2}}} . \tag{18}$$

• Remark: These functions are not in the domain of H_0, if you compute the kinetic energy it is divergent, yet they are square integrable. They become singular when $x \to a$.
• If $\phi_k(a) = 0$, the corresponding eigenfunction $\psi_k(x) = \phi_k(x)$.

Orthonormality of Eigenfunctions

Proposition

Let ϕ_n be orthonormal set of eigenfunctions of H_0, i.e.,

$$\begin{aligned} H_0\phi_n &= E_n\phi_n \\ \int_{\mathcal{M}} \overline{\phi_n(x)}\phi_m(x)\, d\mu(x) &= \delta_{nm}. \end{aligned} \tag{19}$$

Then, the eigenfunctions ψ_n for H_0 modified by a delta interaction supported at $x = a$ are orthonormal, that is,

$$\int_{\mathcal{M}} \overline{\psi_n(x)}\psi_m(x)\, d\mu(x) = \delta_{nm} \;, \tag{20}$$

where $D = 2, 3$.

Orthonormality of Eigenfunctions

Sketch of the Proof:

$$\int_{\mathcal{M}} \overline{\psi_n(x)}\, \psi_m(x)\, d\mu(x)$$
$$= \frac{1}{\left(-\left.\frac{d\Phi(E)}{dE}\right|_{E=E_n^*}\right)^{1/2}\left(-\left.\frac{d\Phi(E)}{dE}\right|_{E=E_m^*}\right)^{1/2}} \sum_k \frac{|\phi_k(a)|^2}{(E_k - E_n^*)(E_k - E_m^*)}$$

Here

$$\left.\frac{d\Phi(E)}{dE}\right|_{E=E_k^*} = -\sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2}{(E_n - E_k^*)^2} \,. \tag{21}$$

Hence, $\psi_n(x)$ are normalized.

Orthonormality of Eigenfunctions

• For $n \neq m$, we first formally decompose the expression in the summation with a cut-off N as a sum of two partial fractions

$$\sum_{k=0}^{N} \frac{|\phi_k(a)|^2}{(E_k - E_n^*)(E_k - E_m^*)} = \frac{1}{(E_n^* - E_m^*)} \sum_{k=0}^{N} |\phi_k(a)|^2 \left(\frac{1}{E_k - E_n^*} - \frac{1}{E_k - E_m^*} \right)$$
$$= \frac{1}{(E_n^* - E_m^*)} \left[G_0^N(a, a|E_n^*) - G_0^N(a, a|E_m^*) \right] \qquad (22)$$

Each term is divergent as $N \to \infty$. Motivated by this, we add and subtract

$$\frac{1}{\alpha_R} + G_0^N(a, a| - \mu^2)$$

to the above expression and obtain in the limit $N \to \infty$

$$\int_{\mathcal{M}} \overline{\psi_n(x)} \psi_m(x) \, d\mu(x) = \frac{(\Phi(E_n^*) - \Phi(E_m^*))}{(E_n^* - E_m^*)} \left(-\frac{d\Phi(E)}{dE}\bigg|_{E_n^*} \right)^{-1/2} \left(-\frac{d\Phi(E)}{dE}\bigg|_{E_m^*} \right)^{-1/2}$$

Since the zeroes of the function Φ are the bound state of the modified system, that is, $\Phi(E_n^*) = 0$ and $\Phi(E_m^*) = 0$ for all n, m (when $n \neq m$).

Completeness of Eigenfunctions of the modified Hamiltonian by delta interaction

Proposition

Let ϕ_n be a complete set of eigenfunctions of H_0, i.e.,

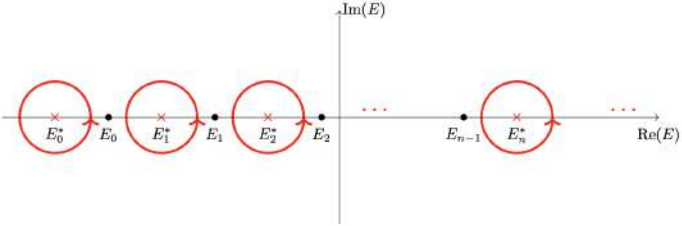
$$\begin{aligned} H_0 \phi_n &= E_n \phi_n \\ \sum_{n=0}^{\infty} \overline{\phi_n(x)} \phi_n(y) &= \delta(x-y) \; . \end{aligned} \tag{23}$$

Then, the eigenfunctions ψ_n of H_0 modified by a delta-interaction supported at $x = a$, form a complete set, that is,

$$\sum_{n=0}^{\infty} \overline{\psi_n(x)} \psi_n(y) = \delta(x-y) \; . \tag{24}$$

Original Contours around E_k^*

Sketch of the Proof: Let Γ_n be the counter-clockwise oriented closed contours around each simple pole E_n^* and $\Gamma_n \cap \Gamma_m = \emptyset$ for $n \neq m$, as shown in the figure below.



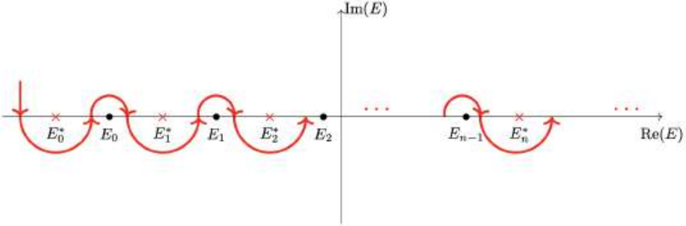
Then, the projection onto the associated eigenspace is given by the formula (17), and thanks to Krein's formula, we have

$$\sum_{n=0}^{\infty} \overline{\psi_n(x)}\psi_n(y) = \frac{1}{2\pi i} \sum_{n=0}^{\infty} \oint_{\Gamma_n \supset E_n^*} \left(G_0(x,y|E) + \frac{G_0(x,a|E)G_0(a,y|E)}{\Phi(E)} \right) dE.$$

Completeness of Eigenfunctions of H

• Note that the total expression in the Krein's formula has only poles at E_n^*'s; however, when we think of it as the sum of two separate expressions, we have the original eigenvalues, E_n, reappearing as poles.

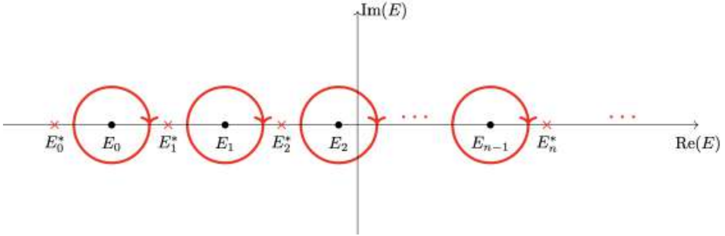
• The first in the above contour integral *vanishes since the poles* E_n *of* G_0 *are all located outside* of each Γ_n. For simplicity, we assume that all $E_k^* \neq E_k$ from now on. Note that thanks to the denominators we can elongate the contours to ellipses that extend to infinity along the imaginary direction (on the complex E-plane):



Completeness of Eigenfunctions of H

• Note that we have *no poles of the Green's function on the left part of the line* $E_0^* + i\mathbb{R}$ *nor any zeros of* $\Phi(E)$, the product of two Green's functions decay rapidly as $|E| \to \infty$ along the negative real direction as well as along the imaginary directions, hence we have no contributions from the contours at infinity for these deformations. This observation allows us to change the contour as described below.

• Using the interlacing theorem we mentioned, we can, so to speak, flip the contour while preserving the result of integration and then deform the contour to the one $\Gamma^\sharp$ that consists of isolated closed contours $\Gamma_n^\sharp$ around each isolated eigenvalue E_n of the initial Hamiltonian H_0 with opposite orientation, as shown.



Completeness of Eigenfunctions of H

$$\frac{1}{2\pi i}\sum_{n=0}^{\infty}\oint_{\Gamma_n^{\sharp}\supset E_n} dE \; \left(g_n(x,a \mid E) + \frac{\overline{\phi_n(a)}\,\phi_n(x)}{E_n - E} \right)$$
$$\times \left(\frac{E_n - E}{(g(\mu) + D_n(\alpha_R, E))(E_n - E) - |\phi_n(a)|^2} \right) \left(g_n(a,y \mid E) + \frac{\overline{\phi_n(y)}\,\phi_n(a)}{E_n - E} \right) \; .$$

$$\begin{aligned} g_n(x,y \mid E) &:= \sum_{k\neq n} \frac{\phi_k(x)\,\overline{\phi_k(y)}}{E_k - E} \\ g(\mu) &:= \sum_{k} \frac{|\phi_k(a)|^2}{E_k + \mu^2} \\ D_n(\alpha_R, E) &:= \frac{1}{\alpha_R} - \sum_{k\neq n} \frac{|\phi_k(a)|^2}{E_k - E} . \end{aligned}$$

Completeness of Eigenfunctions of H

$$\frac{1}{2\pi i} \sum_{n=0}^{\infty} \oint_{\Gamma^n_{\text{dual}} \supset E_n} \left(\text{holomorphic part} + \frac{|\phi_n(a)|^2 \, \overline{\phi_n(y)} \, \phi_n(x)}{E_n - E} \right)$$
$$\times \left(\frac{1}{(g(\mu) + D(\alpha_R, E))(E_n - E) - |\phi_n(a)|^2} \right) dE.$$

Applying the residue theorem, we obtain

$$\sum_{n=0}^{\infty} \overline{\psi_n(x)} \psi_n(y) = \frac{1}{2\pi i} \sum_{n=0}^{\infty} \frac{\phi_n(x)\overline{\phi_n(y)}}{-|\phi_n(a)|^2} \left(-2\pi i |\phi_n(a)|^2 \right) = \sum_{n=0}^{\infty} \overline{\phi_n(x)} \phi_n(y) = \delta(x-y).$$

where the minus sign is due to the opposite orientation of the deformed contour.

Some Further Ideas

• We can write the resulting renormalized Hamiltonian in this basis:

$$H = \sum_{k \notin \mathcal{N}}^{\infty} E_k^* \, (H_0 - E_k^*)^{-1} |a\rangle \left(\frac{d\Phi(E)}{dE} \Big|_{E_k^*} \right)^{-1} \langle a| (H_0 - E_k^*)^{-1} + \sum_{k \in \mathcal{N}} E_k |\phi_k\rangle\langle\phi_k| .$$

• Theorem: let H be a closed hermitian operator acting on $\mathcal{H}$ with domain $D(A)$. Assume that $D(A)$ contains an orthonormal (Schauder) basis of $\mathcal{H}$ (complete orthonormal set) whose elements are eigenvectors of H. Then H is self-adjoint.

• Let us suppose that initially the system is prepared in the eigenstate $G_0(x, a|E_k^*(a))$, $E_k^*(a)$ referring to the energy for this case. A sudden perturbation means that the system has no time to readjust itself, so the wave function remains as it is, but should be decomposed in terms of the new eigenbasis $G_0(x, b|E_m^*(b))$'s to calculate the probability of finding the system in the new energy eigenstate $E_m^*(b)$.

Summary

• The standard route is to construct the Green's function and establish that the Hamiltonian defined by this expression is self-adjoint. By the spectral theorem, there is a complete set of eigenfunctions!

• We prove directly by means of the explicit expression of the constructed Green's function that the corresponding Hamiltonian still has a complete set of eigenfunctions. Completeness remain valid after renormalization. For this we use the completeness property of the eigenfunctions of the initial Hamiltonian H_0, having only a discrete spectrum, and an interlacing theorem for the poles of the new Green's function.

• As a result, we thus establish the self-adjointness of the resulting Hamiltonian in a novel way.

• It would be possible to consider the sudden perturbation approximation for systems where the support of the delta interaction is suddenly changed.

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