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LETTER TO THE EDITOR

Derivation of the time-dependent propagator for the three-dimensional Schrödinger equation with one point interaction

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Abstract. An explicit formula for the time-dependent propagator of the Schrödinger equation with one point interaction in three dimensions is given. The derivation is based on the inverse Laplace transformation applied to the corresponding resolvent.

Recently Gaveau and Schulman [3, 6] have derived the time-dependent propagator for the one-dimensional Schrödinger equation with one point interaction (see also [4]). Here we extend their result to the corresponding three-dimensional problem.

It is well known that the Schrödinger Hamiltonian H_α with a point interaction of strength $\alpha \in \mathbb{R}$, placed at the origin of $\mathbb{R}^3$, can be rigorously constructed as a lower-bounded and self-adjoint operator in $L^2(\mathbb{R}^3)$ using various techniques (see, e.g., [1] and references therein).

For the convenience of the reader we report the explicit formula for the integral kernel of the resolvent of H_α

$$(H_\alpha+\lambda)^{-1}(x,x') = G_\lambda(x-x') + \left(\alpha+\frac{\sqrt{\lambda}}{4\pi}\right)^{-1} G_\lambda(x')G_\lambda(x) \tag{1}$$

where $x, x' \in \mathbb{R}^3\backslash\{0\}$, $x \neq x'$, and G_λ is the integral kernel of the free resolvent defined as

$$G_\lambda(x-x') \equiv \frac{\mathrm{e}^{-\sqrt{\lambda}|x-x'|}}{4\pi|x-x'|} \qquad x \neq x'. \tag{2}$$

Formula (1) holds in particular for $\lambda > 0$, except for $\lambda = (4\pi\alpha)^2$ if $\alpha < 0$.

From (1) the spectral properties of H_α are easily derived. The continuous spectrum of H_α is purely absolutely continuous and coincides with the interval $[0, +\infty)$ while the point spectrum is empty if $\alpha \geqslant 0$ and $\{-(4\pi\alpha)^2\}$ if $\alpha < 0$. The normalized eigenfunction associated with the negative eigenvalue is given by

$$\Psi_\alpha(x) = \sqrt{-2\alpha}\,\frac{\mathrm{e}^{4\pi\alpha|x|}}{|x|}. \tag{3}$$

For $\alpha = 0$ the Hamiltonian exhibits a zero-energy resonance.

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The result of this letter is the following: Let

$$K(x,x';t)\equiv\frac{\mathrm{e}^{-|x-x'|^2/4\mathrm{i}t}}{(4\pi\mathrm{i}t)^{3/2}}\qquad t>0\qquad x,x'\in\mathbb{R}^3 \tag{4}$$

and

$$K_\alpha(x,x';t)\equiv\begin{cases} K(x,x';t)+\dfrac{1}{|x||x'|}\displaystyle\int_0^\infty \mathrm{e}^{-4\pi\alpha u}(u+|x|+|x'|) \\ \quad\times K(u+|x|+|x'|,0;t)\,\mathrm{d}u & \text{for } \alpha>0 \\ K(x,x';t)+\dfrac{2\mathrm{i}t}{|x||x'|}K(|x|+|x'|,0;t) & \text{for } \alpha=0 \\ K(x,x';t)+\Psi_\alpha(x)\Psi_\alpha(x')\,\mathrm{e}^{\mathrm{i}t(4\pi\alpha)^2} \\ \quad+\dfrac{1}{|x||x'|}\displaystyle\int_0^\infty \mathrm{e}^{4\pi\alpha u}(u-|x|-|x'|)K(u-|x|-|x'|,0;t)\,\mathrm{d}u \\ & \text{for } \alpha<0 \end{cases} \tag{5}$$

then for every $f\in L^2(\mathbb{R}^3)$

$$(\mathrm{e}^{-\mathrm{i}tH_\alpha}f)(x)=\lim_{R\to\infty}\int_{|x'|<R}\mathrm{d}x'\,f(x')K_\alpha(x,x';t) \tag{6}$$

where the limit in (6) is taken in the L^2 sense.

Proof. Taking the inverse Laplace transform of the resolvent (1) we can compute the semigroup generated by H_α

$$\begin{aligned}(\mathrm{e}^{-zH_\alpha}f)(x)&=L^{-1}[((H_\alpha+\cdot)^{-1}f)(x)](z)\\ &=\int_{\mathbb{R}^3}\mathrm{d}x'\,f(x')L^{-1}[(H_\alpha+\cdot)^{-1}(x,x')](z)\\ &=\int_{\mathbb{R}^3}\mathrm{d}x'\,f(x)\bigg[\frac{\exp(-|x-x'|^2/4z)}{(4\pi z)^{3/2}}+\frac{1}{|x||x'|4\pi(\pi z)^{1/2}}\\ &\quad\times\bigg(\exp[-(|x|+|x'|)^2/4z]-4\pi\alpha\int_0^\infty\mathrm{d}u\,\exp(-4\pi\alpha u)\\ &\quad\times\exp[-(u+|x|+|x'|)^2/4z]\bigg)\bigg]\end{aligned} \tag{7}$$

where $\Re z>0$ and L^{-1} denotes the inverse Laplace transformation. The last equality in (7) has been obtained using equations (29.3.82), (29.3.88) and (7.4.2) of [2]. We now distinguish three cases.

Case $\alpha=0$. Using the standard 'iε' trick (see, e.g., [5] p 59) from (7) we immediately get formula (6).

Case $\alpha>0$. Integrating by parts in (7) we obtain

$$\begin{aligned}(\mathrm{e}^{-zH_\alpha}f)(x)&=\int_{\mathbb{R}^3}\mathrm{d}x'\,f(x')\bigg[\frac{\exp(-|x-x'|^2/4z)}{(4\pi z)^{3/2}}+\frac{1}{|x||x'|}\int_0^\infty\mathrm{d}u\\ &\quad\times\exp(-4\pi\alpha u)(u+|x|+|x'|)\,\frac{\exp[-(u+|x|+|x'|)^2/4z]}{(4\pi z)^{3/2}}\bigg]\end{aligned} \tag{8}$$

and then we proceed as in the previous case.

Case $\alpha < 0$. The convergence of the last integral in (7) could now seem problematic. However, extracting the specific contribution of the bound state (3), we get

$$\frac{\alpha}{|x||x'|(\pi z)^{1/2}} \int_0^\infty \mathrm{d}u \exp(-4\pi\alpha u) \exp[-(u+|x|+|x'|)^2/4z]$$

$$= -\Psi_\alpha(x)\Psi_\alpha(x') \exp(z(4\pi\alpha)^2) - \frac{\alpha}{|x||x'|(\pi z)^{1/2}} \int_0^\infty \mathrm{d}u$$

$$\times \exp(4\pi\alpha u) \exp[-(u-|x|-x'|)^2/4z]. \qquad (9)$$

Substituting (9) in (7) and using again the 'iε' trick we get (6), concluding the proof. □

To conclude we remark that, following the line of [6], formula (6) can be used to describe the explicit time evolution of a wavepacket, e.g., a Gaussian wavepacket, comparing it with the usual time-independent scattering theory and, moreover, to investigate the meaning of the semiclassical approximation for H_α.

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