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Exact propagator for reflectionless potentials

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Abstract. The exact space-time propagator for a general reflectionless potential is obtained in closed form involving error functions. It is indicated how bound states and transmission coefficients may be recovered from asymptotic behaviour of the propagator. A sum rule is derived that shows how the leading terms of the short-time form of the propagator can be used rigorously in a Feynman path integral formalism.

1. Introduction

Reflectionless potentials have been used successfully in various branches of physics, especially in connection with problems of inverse scattering and the theory of solitons (Lamb 1980, Bargmann 1949, Scott *et al* 1973, Gardner *et al* 1974, Moses and Tuan 1959). Recent work has revealed these potentials to be useful in what might be called phenomenological settings, due to certain uniqueness properties forced by an assumption of no reflection. For example, there exists exactly one symmetric, reflectionless potential having a given finite set of bound state energies (Schonfeld *et al* 1980). What is more, algorithms have been written down for computation of such unique potentials in terms of the energy set. These results have been used to construct reflectionless approximations to confining potentials (Quigg and Rosner 1981).

In the present treatment, known properties of reflectionless $V(x)$ and their associated eigenfunctions are used to derive the exact space-time propagator $K(x, t|x_0, 0)$ for the problem. This will be the solution to the time-dependent Schrödinger equation ($\hbar = 2m = 1$):

$$\mathrm{i}\partial K/\partial t = -\partial^2 K/\partial x^2 + V(x)K \tag{1.1}$$

having

$$\lim_{t\to 0^+} K = \delta(x - x_0). \tag{1.2}$$

Exact propagators have been worked out for the (non-reflectionless) potentials $V(x) = ax^2 + bx + c$ (Feynman and Hibbs 1965), $V(x) = ax^2 + b/x^2$ (Khandekhar and Lawande 1975) and for certain time-dependent $V(x, t)$ (Camiz *et al* 1971). In these known cases connection has been achieved with the Feynman path integral formalism, which describes a procedure for propagator construction.

The exact propagator for arbitrary reflectionless $V(x)$ will be computed by the method of summation over eigenstates. This method can be used for the known cases above, as well as for the three-dimensional Coulomb problem (in the latter case the result is a momentum-space Green function) (Blinder 1981, Hostler 1964). It is shown that the Feynman path integral, involving classical action phase terms, gives the exact reflectionless propagator on the basis of a theorem of Truman (1977).

It will be possible to extract information from the propagator via asymptotic evaluation in various regions of the complex time plane. The bound states and the transmission coefficient for scattering can be easily recovered in this fashion. Of special interest is the short-time (classical) limit central to the Feynman formalism. Classical correspondence is achieved through use of a powerful sum rule. Assume that $V(x)$ is reflectionless, with $V(\pm\infty)=0$. Let the N bound states ψ_j have respective energies $-k_j^2$. Then the identity

$$\int_{x_0}^{x} V(u)\,\mathrm{d}u = -4\sum_{n=1}^{N} \psi_n(x)\psi_n(x_0)\sinh(k_n(x-x_0)) \tag{1.3}$$

holds for all real x_0, x. This relation, which we prove in § 2, is typical of the strong restrictions to which reflectionless potentials are subject.

2. Eigenstate structure

A potential $V(x)$ with $V(\pm\infty)=0$ is reflectionless if every solution $\psi_p(x)$ to the one-dimensional Schrödinger equation (real p):

$$-\psi''+V\psi=p^2\psi \tag{2.1}$$

having ingoing structure

$$\psi_p(x) \underset{x\to-\infty}{\sim} \exp(\mathrm{i}px) \tag{2.2}$$

has also the outgoing structure

$$\psi_p(x) \underset{x\to\infty}{\sim} T(p)\exp(\mathrm{i}px). \tag{2.3}$$

The transmission coefficient $T(p)$ will satisfy $TT^*=1$, indicating no reflection. For potentials V having other limits than zero at $x=\pm\infty$, all results are easily modified. It is known (Schonfeld *et al* 1980) that V is uniquely specified by the bound energies E_j together with constants c_j written in terms of the bound states ψ_j as

$$E_j=-k_j^2, \qquad j=1,2,\ldots,N, \qquad c_j=\lim_{x\to\infty}\psi_j(x)\exp(k_jx). \tag{2.4}$$

As noted in § 1, the additional requirement that V be an even function allows the energy spectrum alone to specify V exhaustively, in which case the c_j are themselves determined by the k_j.

A complete set of scattering states can be given in terms of the bound states by (Moses and Tuan 1959)

$$\psi_p(x)=T(p)\exp(\mathrm{i}px)\left(1-\mathrm{i}\sum_{n=1}^{N}\frac{c_n\psi_n(x)\exp(-k_nx)}{p+\mathrm{i}k_n}\right). \tag{2.5}$$

Furthermore, a linear relation holds between the bound states, in the form (Gardner *et al* 1974)

$$c_m^{-1}\psi_m(x)=\exp(-k_mx)-\sum_{n=1}^{N}\frac{c_n\psi_n(x)\exp(-k_nx-k_mx)}{k_m+k_n}. \tag{2.6}$$

There are many restricting relations for the potential $V(x)$, among which is the identity (Gardner *et al* 1974)

$$V(x)=2\frac{\mathrm{d}}{\mathrm{d}x}\bigg(\sum_{m=1}^{N} c_m\psi_m(x)\exp(-k_m x)\bigg). \tag{2.7}$$

This can be used together with (2.6) to prove the sum rule (1.3). Note that

$$\tfrac{1}{2}\int_{x_0}^{x} V(u)\,\mathrm{d}u=\sum_{m=1}^{N} c_m(\psi_m(x)\exp(-k_m x)-\psi_m(x_0)\exp(-k_m x_0)). \tag{2.8}$$

By expressing $\psi_m(x_0)$ as a sum (2.6) and symmetrising summands m, n the sum rule is immediately obtained.

A simple example of the above relations is provided by the reflectionless potential

$$V(x)=-2\,\mathrm{sech}^2\,x \tag{2.9}$$

for which the single bound state of energy -1 is

$$\psi_1(x)=2^{-1/2}\,\mathrm{sech}\,x, \tag{2.10}$$

while the continuum states satisfying (2.1), (2.2) are

$$\psi_p(x)=[(\mathrm{i}p-\tanh x)/(\mathrm{i}p+1)]\exp(\mathrm{i}px). \tag{2.11}$$

All of the relations described hold trivially, with the sum rule amounting to the identity $(\tanh x-\tanh x_0)=\mathrm{sech}\,x\;\mathrm{sech}\,x_0\sinh(x-x_0)$. Many other interrelations for V, ψ_j, ψ_p are derived in the references, but the above will suffice for computation and evaluation of the space–time propagator.

3. Propagator construction

The propagator satisfying (1.1), (1.2) is expressible as a sum over eigenstates:

$$K(x,t\,|\,x_0,0)=\sum_{n=1}^{N}\psi_n(x)\psi_n(x_0)\exp(\mathrm{i}k_n^2 t)$$
$$+\frac{1}{2\pi}\int_{-\infty}^{\infty}\psi_p(x)\psi_p^*(x_0)\exp(-\mathrm{i}p^2 t)\,\mathrm{d}p. \tag{3.1}$$

The continuum momentum normalisation factor $(1/2\pi)$ is determined from the observation that the free (V identically zero) propagator is

$$K_0(x,t\,|\,x_0,0)=(4\pi\mathrm{i}t)^{-1/2}\exp\bigg(\frac{\mathrm{i}(x-x_0)^2}{4t}\bigg)$$
$$=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp[\mathrm{i}(p(x-x_0)-p^2t)]\,\mathrm{d}p, \tag{3.2}$$

so that (2.5) and (1.2) demand the equivalent normalisation guaranteeing delta-function behaviour for large positive x_0, x. Insertion of the continuum states (2.5) into the integral results in a complicated expression which can be greatly simplified by the observation that integrals of the form

$$J(x, t) = \int f(p) \exp[\mathrm{i}(px - p^2 t)]\, \mathrm{d}p \tag{3.3}$$

can be thought of as freely propagated waves with initial data $J(x, 0)$. Define the functional F_t to act on initial data $J(x, 0)$ according to

$$J(x, t) = F_t\{J(x, 0)\} = \int_{-\infty}^{\infty} K_0(x, t \mid y, 0) J(y, 0)\, \mathrm{d}y. \tag{3.4}$$

Now denote the first bound-state sum in (3.1) by K_b, and insert the full wavefunctions (2.5) into the integral of (3.1) to get

$$\begin{aligned} K(x, t \mid x_0, 0) = {} & K_\mathrm{b} + K_0 + \sum_m c_m \psi_m(x) \exp(-k_m x) F_t\{-\theta(x_0 - x) \exp(-k_m |x - x_0|)\} \\ & + \sum_n c_n \psi_n(x_0) \exp(-k_n x_0) F_t\{-\theta(x - x_0) \exp(-k_n |x - x_0|)\} \\ & + \sum_{m,n} c_m c_n \psi_n(x_0) \psi_m(x) \exp(-k_n x_0 - k_m x) F_t\{I_{mn}(x - x_0)\} \end{aligned} \tag{3.5}$$

where the function I_{mn} is defined by

$$I_{mn}(s) = (k_m + k_n)^{-1} (\theta(s) \exp(-k_n s) + \theta(-s) \exp(-k_m |s|)). \tag{3.6}$$

The functional F_t is patently linear, so we can write

$$K(x, t \mid x_0, 0) = K_\mathrm{b} + K_0 + G(x, x_0, t) + G(x_0, x, t) \tag{3.7}$$

where we put $s = x - x_0$ and define G by

$$\begin{aligned} G(x, x_0, t) = {} & \sum_m c_m \psi_m(x) \exp(-k_m x) \\ & * \left(F_t\{\theta(-s) \exp(+k_m s)\} - 1 + \sum_n \frac{c_n \psi_n(x_0) \exp(-k_n x_0)}{k_m + k_n} \right). \end{aligned} \tag{3.8}$$

The final two terms conveniently simplify due to the identity (2.6). Furthermore, the functional can now be evaluated from (3.4) and (3.2) as

$$F_t\{\theta(-s) \exp(k_m s)\} = \tfrac{1}{2} \exp(k_m s + \mathrm{i} k_m^2 t)(1 - \mathrm{erf}(R_m^-(s))) \tag{3.9}$$

where

$$R_m^{\pm}(s) = (\mathrm{i}t)^{1/2} (k_m \pm \mathrm{i}s/2t) \tag{3.10}$$

and erf is the standard error function:

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-u^2)\, \mathrm{d}u. \tag{3.11}$$

It is interesting that the simplification arising from (2.6) actually cancels the leading bound state terms of (3.1). Performing this cancellation we get the exact reflectionless propagator, from (3.7), as:

$$\begin{aligned} K(x, t \mid x_0, 0) = {} & K_0(x, t \mid x_0, 0) + \tfrac{1}{2} \sum_{n=1}^{N} \psi_n(x) \psi_n(x_0) \exp(\mathrm{i} k_n^2 t) \\ & * \{\mathrm{erf}[(\mathrm{i}t)^{1/2}(k_n + \mathrm{i}(x - x_0)/2t)] + \mathrm{erf}[(\mathrm{i}t)^{1/2}(k_n - \mathrm{i}(x - x_0)/2t)]\}. \end{aligned} \tag{3.12}$$

The expression has finitely many terms, and the bound state component of the propagator is now 'hidden' in the error-function part. Note that if there are no bound states the sum is interpreted as empty, in which case the free propagator results (the unique reflectionless potential with no bound states and $V(\pm\infty)=0$ is the zero potential). A special case is discussed in detail in Crandall and Litt (1983).

Some asymptotic regions of interest for evaluation of K are the short-time limit:

$$t \to 0^+, \qquad x_0, x \text{ fixed} \tag{3.13}$$

and the scattering limit:

$$-x_0, x, t \to \infty, \qquad q = (x - x_0)/2t \text{ fixed.} \tag{3.14}$$

The denominator '2' in this last expression allows q to be a measure of momentum, since $m = \frac{1}{2}$ in present units. In these, or in any other asymptotic regions, it is important that the location of the argument to erf be properly interpreted. Consider the expression

$$\mathrm{erf}[(\mathrm{i}t)^{1/2}(k + \mathrm{i}s/2t)] \tag{3.15}$$

in the short-time limit. It would appear that for positive s, k the argument lies in the octant $\pi/2 < \theta < 3\pi/4$, but this gives incorrect results. For consistent evaluation, one may attribute to the time variable a negative imaginary part, that is t replaced by $t(1 - \mathrm{i}\varepsilon)$, in which case the short-time limit of (3.15) has argument lying in the octant $3\pi/4 < \theta < \pi$. The argument for s negative will lie in the octant $-\pi/4 < \theta < 0$. This method of evaluation is equivalent to modifying $\hbar$, as some investigators have indicated for even the free particle propagator (Feynman and Hibbs 1965).

Behaviour in regions (3.13) and (3.14) can now be analysed using known asymptotics for the error function (Abramowitz and Stegun 1970). Keeping in mind the definition (3.10) we obtain, in the short-time limit,

$$\mathrm{erf}(R_n^+(x - x_0)) + \mathrm{erf}(R_n^-(x - x_0)) \underset{t \to 0^+}{\sim} 8\mathrm{i}tK_0(x, t \,|\, x_0, 0)\frac{\sinh(k_n(x - x_0))}{(x - x_0)}(1 + \mathrm{O}(t)) \tag{3.16}$$

where $\mathrm{O}(t)$ indicates an error term that is absolutely bounded by At for a constant A, any x_0, x. For the scattering limit the result is

$$\mathrm{erf}(R_n^+(x - x_0)) + \mathrm{erf}(R_n^-(x - x_0)) \underset{(3.14)}{\sim} -2K_0(x, t \,|\, x_0, 0)\exp(-\mathrm{i}tk_n^2) * \left(\frac{\exp[k_n(x - x_0)]}{k_n - \mathrm{i}q} + \frac{\exp[k_n(x_0 - x)]}{k_n + \mathrm{i}q}\right). \tag{3.17}$$

A third asymptotic region is especially easy to analyse. Take

$$t \to -\mathrm{i}\infty \tag{3.18}$$

which can be used to recover bound state information. The sum of the two error functions in (3.12) is asymptotic to +2. For this region, the propagator behaves according to

$$K(x, -\mathrm{i}z \,|\, x_0, 0) \underset{z \to \infty}{\sim} \sum_n \psi_n(x)\psi_n(x_0)\exp(k_n^2 z), \tag{3.19}$$

having ground state leading term.

4. Recovery of transmission coefficient

In the scattering region of space–time indicated by (3.14) the sum-over-eigenstates (3.1) will go into

$$K \sim \int T(p) \exp[\mathrm{i}p(x-x_0)] \exp(\mathrm{i}p^2 t)\, \mathrm{d}p. \tag{4.1}$$

Stationary-phase evaluation of this integral gives the formal relation between transmission coefficient $T(p)$ and the propagator:

$$T(q) \underset{\substack{t\to\infty \\ -x_0\to\infty}}{\sim} \frac{K(x_0+2qt\,|\,x_0, 0)}{K_0(x_0+2qt\,|\,x_0, 0)}. \tag{4.2}$$

We presently show this to be correct for the calculated reflectionless propagator on the basis of (3.17). We have

$$K \sim K_0\left[1-\sum_n \psi_n(x)\psi_n(x_0)\left(\frac{\exp[k_n(x-x_0)]}{k_n-\mathrm{i}q}+\frac{\exp[-k_n(x-x_0)]}{k_n+\mathrm{i}q}\right)\right]. \tag{4.3}$$

From the eigenstate behaviour implied by (2.4) we have

$$K \sim K_0\left(1-\sum_n \frac{c_n^2}{k_n-\mathrm{i}q}\right). \tag{4.4}$$

The factor in parentheses has the required pole structure of the transmission coefficient $T(q)$, and is in fact precisely this coefficient on the basis of relations for the c_n given in Lamb (1980) and Schonfeld *et al* (1980).

5. Validity of the Feynman path integral

In this section it will be shown that the leading terms of the short-time form of K can be used rigorously in a path integral formulation. Consider the straight-line path connecting space–time endpoints $(x_0, 0)$ and (x, t):

$$y(\tau) = x_0 + (x-x_0)\tau/t, \qquad 0 \leqslant \tau \leqslant t, \tag{5.1}$$

and define the classical action for this path by

$$\bar{S}(x, t\,|\,x_0, 0) = \int_0^t [T(y(\tau)) - V(y(\tau))]\, \mathrm{d}\tau, \tag{5.2}$$

where T, V are kinetic and potential energies respectively. It is known that a particular definition of the Feynman path integral is valid for this straight-line action, provided the potential $V(x)$ is sufficiently well behaved. Specifically, define for integers M the parameters $x_M = x$ and $\tau = t/M$, and define the Mth-order path integral to be the $(M-1)$-fold integral

$$K_M(x, t\,|\,x_0, 0) = (4\pi \mathrm{i}\tau)^{-M/2} \int \prod_{j=0}^{M-1} \mathrm{d}x_j \exp[\mathrm{i}\bar{S}(x_{j+1}, \tau\,|\,x_j, 0)]. \tag{5.3}$$

Then if V is the Fourier transform of a measure of bounded absolute variation,

$$K = \lim_M K_M \tag{5.4}$$

exists and is the exact propagator satisfying (1.1), (1.2) (Truman 1977). From the sum rule (1.3) we can write, by inspecting the limit $x_0 \to x$,

$$V(x) = -4 \sum_{n=1}^{N} k_n \psi_n^2(x). \tag{5.5}$$

This means that the Fourier transform of V is a finite sum of Fourier transforms of exponentially decaying functions (by (2.4)). Therefore the transform of V is itself of bounded variation, and this establishes the validity of the limit (5.4) for any reflectionless potential. Now we shall turn to the problem of evaluating the propagator (3.12) in the short-time limit.

Insertion of the asymptotic form (3.16) into the exact propagator expression (3.16) gives

$$K(x, t\,|\,x_0, 0) \underset{t\to 0^+}{\sim} K_0 * \left(1 + 4\mathrm{i}t \sum_{n=1}^{N} \psi_n(x)\psi_n(x_0) \frac{\sinh(k_n(x - x_0))}{x - x_0} + \mathrm{O}(t^2)\right). \tag{5.6}$$

The importance of the sum rule (1.3) in the classical limit is now evident. The short-time limit can be immediately written as

$$K(x, t\,|\,x_0, 0) \underset{t\to 0^+}{\sim} K_0 * \left(1 - \mathrm{i}t(x - x_0)^{-1} \int_{x_0}^{x} V(u)\,\mathrm{d}u + \mathrm{O}(t^2)\right). \tag{5.7}$$

It is interesting that the sum rule has suggested in a natural way that we use the straight-line classical action. Indeed, the potential term in (5.7) is just the straight-line form, and we write:

$$K(x, t\,|\,x_0, 0) \underset{t\to 0^+}{\sim} (4\pi \mathrm{i}t)^{-1/2} \exp[\mathrm{i}\tilde{S} + \mathrm{O}(t^2)]. \tag{5.8}$$

This is the intended result, that the short-time form (5.8) is, in leading terms, sufficiently accurate to allow a rigorously defined path integral (5.3).

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References

Abramowitz M and Stegun I 1970 *Handbook of Mathematical Functions, NBS Series Appl. Math. #55* USDC
Bargmann V 1949 *Rev. Mod. Phys.* **21** 488
Blinder S M 1981 *J. Math. Phys.* **22** 306
Camiz P, Geradi A, Marchioro C, Presutti E and Scacciatelli E 1971 *J. Math. Phys.* **12** 2040
Crandall R E and Litt B 1983 *Ann. Phys.* **146** 458
Feynman R P and Hibbs A R 1965 *Quantum mechanics and path integrals* (New York: McGraw-Hill)
Gardner C S, Greene J M, Kruskal M D and Miura R M 1974 *Comm. Pure Appl. Math.* **27** 97
Hostler L 1964 *J. Math. Phys.* **5** 1235
Khandekhar D C and Lawande S V 1975 *J. Math. Phys.* **16** 384
Lamb G L 1980 *Elements of Soliton Theory* (New York: Wiley)
Moses H E and Tuan S F 1959 *Nuovo Cimento* **13** 197
Quigg C and Rosner J L 1981 *Phys. Rev.* D **23** 2625
Schonfeld J F, Kwong W and Rosner J L 1980 *Ann. Phys.* **128** 1
Scott A C, Chu F Y F and McLaughlin D W 1973 *Proc. IEEE* **61** 1443
Truman A 1977 *J. Math. Phys.* **18** 1499