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Exact Time-Dependent Green's Function for the Half-Plane Barrier

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Let G be the *time-dependent* quantum mechanical propagator for a particle that is free except for a half-plane barrier with a straight edge. A closed-form exact expression for G is presented in terms of the Fresnel integral for the case where the initial and final positions lie in a plane perpendicular to the edge. G is not expressible as a sum over classical paths.

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The time-dependent Green's function is the quantity $G(x,t;y)=\langle x|\exp(-itH/\hbar)|y\rangle$ and is the object calculated in the Feynman sum over histories. With $it/\hbar$ replaced by appropriate real parameters it provides a solution for the heat or the diffusion equation as well as the Schrödinger equation. It is known in exact form in few cases and in every one of those (that I know of) reduces to the form

$$\sum_\alpha \left(\frac{\partial^2 S_\alpha(x,t;y)}{\partial x\,\partial y}\right)^{1/2} \exp\left(\frac{iS_\alpha(x,t;y)}{\hbar}\right),$$

where $S_\alpha(x,t;y)$ is the action along a *classical* path, satisfying the Euler-Lagrange equations, starting from y at time 0 and arriving at x at time t; the (denumerable) sum is over all such classical paths.[1] Moreover, the known examples are either the free particle or the harmonic oscillator in one form or another.[2] It may be worth emphasizing here that I am discussing the *time-dependent* propagator and not the apparently more tractable object, the energy-dependent Green's function, related by a Fourier transform; closed-form solutions for the latter have been known for the Coulomb potential for some time[3] and although there are signs that the time-dependent propagator is coming under control[4] it is as yet unknown.

In this article I present an exact, closed-form (in terms of a Fresnel integral) solution for the time-dependent propagator for a particle subject to an infinite half-plane barrier. This problem is of considerable importance in optics where Sommerfeld's exact solution[5] of the time-independent problem is the starting point for Keller's geometric diffraction theory.[6] My solution bears a great resemblance to Sommerfeld's, as presented by Lewis and Boersma,[7] suggesting that other exact solutions known in optics[8,9] may also provide closed formulas for the time-dependent Green's function for the Schrödinger equation. However, my derivation of it[10] did not rely on knowledge of Sommerfeld's form and by rights should only be an asymptotic solution (for $\hbar\to 0$) rather than an exact result. The Fourier transform ($t\to E$) connecting the various expressions is done by stationary phase and I know of no *a priori* reason for exactness to obtain on both ends of the approximation. In fact, the main purpose of Ref. 10 is to justify Keller's method in geometries that are not exactly solved.

The geometry is illustrated in Fig. 1. The third dimension has been dropped and the barrier is the negative y axis. The initial and final points are $\vec{a}=(\rho_a,\theta_a)$ and $\vec{b}=(\rho_b,\theta_b)$, respectively. Define the following quantities:

$$\omega_1 = \tfrac{1}{2}(\theta_a + \theta_b), \quad \omega_2 = \tfrac{1}{2}(\theta_a - \theta_b) - \tfrac{1}{2}\pi, \quad m = \left(\frac{\rho_a \rho_b}{t\hbar}\right)^{1/2} \sin\omega_2, \quad n = \left(\frac{\rho_a \rho_b}{t\hbar}\right)^{1/2} \sin\omega_1, \tag{1}$$

and the function

$$h(u) = (i\pi)^{-1/2} \int_{-\infty}^{u} \exp(iv^2) dv. \tag{2}$$

Let the mass of the particle be $\frac{1}{2}$. Then the exact Green's function is

$$G(\vec{b}, t; \vec{a}) = (4\pi i \hbar t)^{-1} \exp[i(\rho_a + \rho_b)^2/4\hbar t]\{\exp(-im^2)h(-m) \mp \exp(-in^2)h(-n)\}, \tag{3}$$

where the upper (lower) sign corresponds to Dirichlet (Neumann) boundary conditions on the barrier. The derivation of (3) given in Ref. 10 is entirely irrelevant since it is only asymptotic ($\hbar \to 0$) to the first two leading orders $[O(1)$ and $O(\sqrt{\hbar})]$. Instead, having by whatever means gotten (3), we apply $H - i\hbar\,\partial/\partial t = -\nabla^2 - i\hbar\,\partial/\partial t$ to it, check if that is zero, and also check that the boundary conditions are satisfied. In fact, the two terms in G individually satisfy Schrödinger's equation as can be verified by straightforward application of $-\nabla^2 - i\hbar\,\partial/\partial t$. The only feature of that tedious exercise that might not be done by a computer programmed to take derivatives is to notice that the final result of taking those derivatives, namely,

$$(\text{const})\exp[i(\rho_a + \rho_b)^2/4t]\,t^{-2}(\rho_a/\rho_b)\int_0^\infty ds\,(\tfrac{1}{2}i - s^2 - su)\exp(is^2 + 2isu),$$

with $\hbar = 1$ and $u = (\rho_a \rho_b / t)^{1/2} \sin\omega_2$ (for the first term in G), is in fact zero. This is because

$$\int_0^\infty ds(\tfrac{1}{2}i - s^2 - su)\exp(is^2 + 2isu) = \int_0^\infty ds \frac{d}{ds}\left(\frac{is}{2}\exp(is^2 + 2isu)\right) \tag{4}$$

and the contribution at $s = \infty$ drops out by the usual regularization procedures, e.g., giving $\hbar$ or m small imaginary parts.[11] The satisfying of the boundary conditions is verified by noting that one can obtain the second term in G from the first by the transformation $\theta_a \to 3\pi - \theta_a$ (the barrier is at angle $3\pi/2$).

A point of interest in the form (3) is that it is not a sum over classical paths. True, the small-$\hbar$ asymptotic expansion shows it to consist of direct, reflected, and diffracted rays, a feature exploited by Keller,[6] but this neat division is only possible asymptotically. To see this recall[7] the large-u asymptotic expansion of h,

$$h(u) \sim \Theta(u) - \tfrac{1}{2}\pi^{-1/2} e^{i\pi/4} \exp(iu^2) u^{-1} \sum_{n=0}^{\infty} a_n (iu^2)^{-n},$$

where Θ is the step function, $a_0 = 1$, and $a_n = (n - \frac{1}{2})a_{n-1}$ for $n > 0$. When applied to (3) this gives firstly two Θ functions whose arguments are positive in the case where there is an unobstructed direct path from $\vec{a}$ to $\vec{b}$ or a reflected path off the barrier, respectively. The first term from each asymptotic series is $O(\sqrt{\hbar})$ and together they yield what Keller calls the diffracted ray. The remaining terms do not correspond to any classical path even with Keller's generalization of that notion to diffracted rays. Moreover, the above expression for h breaks down on the "shadow boundary" ($\vec{b}$ falls on the line $\vec{a}O$) and G is given by half the direct ray plus the "diffraction" portion of the reflected-ray term. It does not seem useful to me to think of this as a sum over classical paths in view of the complicated auxiliary prescriptions used (half of one term, a different por-

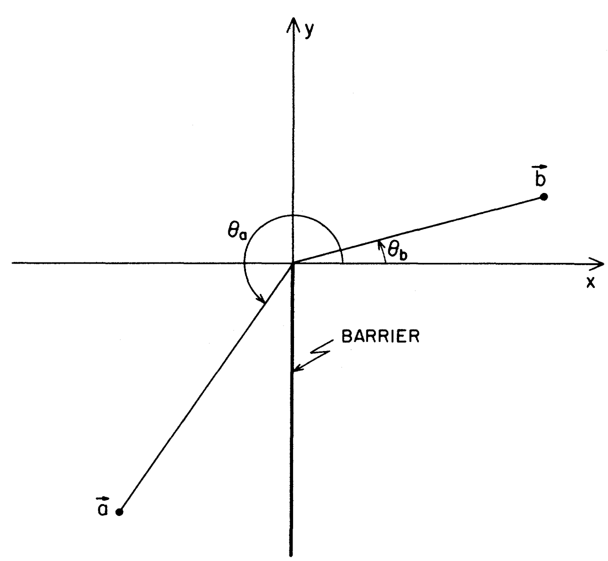

FIG. 1. The barrier (on which the propagator G or its normal derivative vanishes) is the negative y axis and $\vec{a}$ and $\vec{b}$ are the spatial arguments of G.

tion of the other). It is true, however, that (3) is a sum of terms individually satisfying the Schrödinger equation and combined to satisfy the boundary conditions. Sommerfeld[5] provided an elegant rendering of this sum as a generalized method of images with the basic partial differential equation defined on a two-sheeted Riemann surface. (Similar techniques are useful in path integration; see Ref. 1, p. 224).

Sommerfeld's presentation also shows that his exact half-plane solution is not an isolated result and in fact it is only one of a large class of exactly solved problems known today,[8,9] for example the wedge (interior or exterior), the cylinder, the obliquely incident ray on an edge [i.e., not requiring both $\vec{a}$ and $\vec{b}$ of (3) to be in a single plane normal to the knife edge], or even an infinity of parallel edges. It is my expectation that many of these problems will also lead to closed-form solutions for the time-dependent propagator.

As a problem in quantum mechanics I know of no reason why the half-plane barrier should have any great intrinsic interest. It is offered here, firstly, because it adds to the small number of exact solutions and any exact solution is a kind of laboratory on which ideas can be tested (e.g., exactness of the sum over classical paths) as well as a starting point for perturbations. Secondly, I expect this exact solution to lead to others, some of which may have greater intrinsic physical relevance. Finally, it should be observed that $t \to -it$ converts (3) to a solution of the heat equation for which the kind of boundary-value problem formulated may be a realistic model of a physical situation.

[1]For further discussion with references, see L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981), in particular Sec. 6, appendix.

[2]The solved time-dependent forced harmonic oscillator has of course been quite useful in many problems and the solved free particle may be moving on rather complicated manifolds (in particular group manifolds of Lie groups). In addition the method of images may be used to build up further interesting exact solutions. See Ref. 1.

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[5]A. J. W. Sommerfeld, *Optics* (Academic, New York, 1954).

[6]J. B. Keller, in *Calculus of Variations and its Applications*, edited by L. M. Graves (McGraw-Hill, New York, 1958).

[7]R. M. Lewis and J. Boersma, J. Math. Phys. 10, 2291 (1969).

[8]G. L. James, *Geometrical Theory of Diffraction for Electromagnetic Waves*, IEE Electromagnetic Waves Series I (Peregrinus, Stevenage, United Kingdom, 1980).

[9]M. Born and E. Wolf, *Principles of Optics* (Pergamon, New York, 1975), 5th ed., Chap. 11.

[10]L. S. Schulman, in Proceedings of the Symposium on Wave-Particle Dualism, Perugia, 1982 (to be published). In this calculation I discard terms which though smaller than $O(\sqrt{\hbar})$ are definitely not zero. Apparently there is a fortuitous cancellation of errors.

[11]I. M. Gelfand and A. M. Yaglom, J. Math. Phys. 1, 48 (1960), Sec. 2. In the present application the expression $\exp(iv^2)$ in the definition (2) of h becomes $\exp[i(1+i\epsilon)v^2]$, and $\epsilon \downarrow 0$ only after the limits on the v integration [or s in (4)] are taken.