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1983 J. Phys. A: Math. Gen. 16 513

(http://iopscience.iop.org/0305-4470/16/3/011)

J. Phys. A: Math. Gen. 16 (1983) 513–519. Printed in Great Britain

Exact propagator for motion confined to a sector

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Received 5 August 1982

Abstract. In certain situations the Feynman path integral 'collapses' into a countable sum over classical paths. This effect is sought in motion confined to a sector (in polar coordinates: $r \geqslant 0$, $0 \leqslant \varphi \leqslant \alpha$). The exact space–time propagator is derived as a sum over a generally non-classical image set, with resulting structure radically dependent on number-theoretic properties of π/α. It is shown that collapse occurs if and only if this number is an integer.

1. Introduction

Let R be a simply-connected region of n-dimensional space, with boundary ∂R, in which a non-relativistic particle moves freely except for perfect boundary reflection. The space–time propagator for the Schrödinger problem is taken to be that solution $K(\boldsymbol{x}, t|\boldsymbol{x}_0, 0)$ to:

$$\mathrm{i}\hbar \frac{\partial K}{\partial t} + \frac{\hbar^2}{2m} \nabla_x^2 K = 0; \qquad \boldsymbol{x}, \boldsymbol{x}_0 \in R \tag{1.1}$$

with short-time behaviour:

$$\lim_{t \to 0^+} K = \delta^n(\boldsymbol{x} - \boldsymbol{x}_0); \qquad \boldsymbol{x}, \boldsymbol{x}_0 \in R \tag{1.2}$$

and boundary conditions:

$$K = 0 \quad \text{if} \quad \boldsymbol{x} \in \partial R \quad \text{or} \quad \boldsymbol{x}_0 \in \partial R. \tag{1.3}$$

This propagator is expressible in terms of the normalised eigenstates $\psi_q(\boldsymbol{x})$ for a particle confined to R, as:

$$K(\boldsymbol{x}, t|\boldsymbol{x}_0, 0) = \sum_q \psi_q(\boldsymbol{x}) \psi_q^*(\boldsymbol{x}_0) \exp(-\mathrm{i}E_q t), \tag{1.4}$$

where q denotes generally a quantum tuple, E_q is the associated energy for state q, and care must be taken to normalise bound states separately from continuum states in the event that R has infinite extent.

In attempting to calculate the exact propagator for a given region, one is tempted to appeal to the Feynman path-integral formalism (Feynman 1948) in which the n-space-dimensional propagator for (smooth) potential function $V(\boldsymbol{x})$ is formally written as a 'sum-over-paths':

$$K(\boldsymbol{x}, t|\boldsymbol{x}_0, 0) = \int A(P) \exp[\mathrm{i}S(P)/\hbar] \partial[P], \tag{1.5}$$

where P generally denotes a single path connecting the space–time endpoints $(\boldsymbol{x}_0, 0)$ and $(\boldsymbol{x}, t)$; $S(P)$ is the classical action for P, and $A(P)$ is a normalisation factor depending only on temporal coordinates (Feynman and Hibbs 1965). One beautiful feature of this formalism is that classical correspondence, at least in an heuristic sense, is immediate. Indeed, we expect that the integral (1.5) will be dominated by paths 'lying near to' classical paths, since $S(P)$ should not vary radically as P ranges over such a sub-collection. The resulting 'reinforcement' that occurs for the classical paths would become more pronounced as $\hbar$ is taken smaller, and this is the essence of the classical correspondence. There are potentials $V(\boldsymbol{x})$ for which the Feynman integral 'collapses' into a single term, and the exact propagator is given for these V by:

$$K(\boldsymbol{x}, t|\boldsymbol{x}_0, 0) = B(t) \exp(\mathrm{i}S/\hbar) \tag{1.6}$$

where here $S = S(\boldsymbol{x}, t|\boldsymbol{x}_0, 0)$ is the classical action. It can be shown that in any number n of dimensions, K has the form (1.6) if and only if the potential is quadratic, that is $V(\boldsymbol{x}) = a(\boldsymbol{x} - \boldsymbol{y})^2 + b$; with $a, b, \boldsymbol{y}$ constant. A vast literature concerned with the validity of the heuristic 'stationary phase' approximation has appeared (DeWitt 1972).

By analogy with the Feynman formalism for smooth potentials, we define the propagator K to be 'collapsed' if it can be written as a *countable sum* of terms (1.6):

$$K(\boldsymbol{x}, t|\boldsymbol{x}_0, 0) = \sum_j B_j(t) \exp[\mathrm{i}S(P_j)/\hbar], \tag{1.7}$$

where $P_1, P_2, \ldots$ are classical paths connecting the space–time endpoints. Relation (1.6) is a special case of collapse, but we shall need the possibility of more than one classical path for the propagators involving bounded regions R, since these latter problems have effective potentials that are singular on the boundary ∂R. The rigid walls allow classical 'bounce' paths in addition to direct paths, with the possibility of infinitely-many bounces.

2. Known collapsed propagators

For free propagation within bounded regions R, all classical paths are straight lines except for reflections. For a path P_j of length L_j the classical action is ($m = \frac{1}{2}$):

$$S(P_j) = L_j^2/4t. \tag{2.1}$$

For one space dimension, K is always collapsed. Let $R = (0, \infty)$, corresponding to one rigid wall at the origin. The exact propagator is ($\hbar = 1$):

$$T = (4\pi \mathrm{i}t)^{-1/2}\{\exp[\mathrm{i}S(P_0)] - \exp[\mathrm{i}S(P_1)]\}, \tag{2.2}$$

where P_0 is the direct path, with $L_0 = |x - x_0|$, and P_1 is the single-bounce path with length $L_1 = x + x_0$. For $R = (-a, a)$ for positive constant a, the quantum-mechanical setting is that of the familiar square-well. It can be shown (Wheeler 1976) that the propagator is:

$$K = (4\pi \mathrm{i}t)^{-1/2} \sum_j (-1)^j \exp[\mathrm{i}S(P_j)], \tag{2.3}$$

where P_j is any path that connects the space–time endpoints via exactly j bounces. There are no other really distinct one-dimensional cases.

In two space dimensions, the expression (2.3) generalises naturally for these known cases:

(i) R is any rectangle,

(ii) R is a 45°–45° right triangle,

(iii) R is a 30°–60° right triangle.

In each case, the exact propagator can be written, as can (2.3), in terms of theta functions, with equivalent representation (1.4) in terms of the bound states of R (Wheeler 1976).

All of these known propagators for one and two space dimensions can be obtained by solving (1.1) and using the method of images. In fact, the solubility of the two-dimensional cases given is intimately connected with the fact that each of the figures can, upon duplication, tessellate the 2-plane.

Generally, a failure of the method of images corresponds to a failure of K to be collapsed. K is most certainly not collapsed for an arbitrary right triangle, for example, although no rigorous results are known. The development of the propagator for a particle in a sector, on which we presently focus our attention, shows that collapse in the sense of (1.7) is a rare occurrence, depending radically on the geometry of the region.

3. Exact sector propagator

A sector will be defined as the two-dimensional region R whose points have polar coordinates (r, φ) satisfying:

$$0 \leqslant r, \qquad 0 \leqslant \varphi \leqslant \alpha, \tag{3.1}$$

so that the region has the appearance of a 'wedge' of interior angle α. The problem of wave diffraction in such a region has been analysed by several investigators (Sommerfeld 1896, Sastry and Chakrabarti 1979). In some limits, our eventual exact result is in agreement with established formulae (Jones 1964).

A complete set of eigenstates for the sector of angle α can be obtained via the method of separation of the Schrödinger equation (1.1), as ($\hbar = 2m = 1$):

$$\psi_{\nu,E}(r, \varphi) = C_\nu(E) \sin \nu\varphi J_\nu(r\sqrt{E}), \tag{3.2}$$

where E is the (non-negative) energy, J_ν is the Bessel function of order ν, and $C_\nu(E)$ is a normalisation number, to be determined. The index ν takes on particular values:

$$(\alpha\nu/\pi) \in Z^+, \tag{3.3}$$

which ensures that each eigenfunction vanishes on the boundary of the sector, that is along each ray $\varphi = 0$ and $\varphi = \alpha$. Consider the space-time function K_α defined by:

$$K_\alpha(r, \varphi, t | r_0, \varphi_0, 0) = \frac{1}{\alpha} \int_0^\infty \mathrm{d}E \exp(-\mathrm{i}Et) \times \sum_\nu J_\nu(r\sqrt{E}) J_\nu(r_0\sqrt{E}) \sin \nu\varphi \sin \nu\varphi_0 \tag{3.4}$$

where the summation is over the values of ν allowed by (3.3). On the basis of (3.2) it is evident that K_α solves the Schrödinger equation (1.1) in r, φ, t. What we shall presently show is that for two interior points $\boldsymbol{r}$, $\boldsymbol{r}_0$ of the sector

$$\lim_{t\to 0^+} K_\alpha = \delta^2(\boldsymbol{r}-\boldsymbol{r}_0), \tag{3.5}$$

so that in fact K_α is the exact space–time propagator for the sector. It is interesting that this implies each eigenstate has equal energy-normalisation $C_\nu(E)=\sqrt{1/\alpha}$

The demonstration of (3.5) is somewhat intricate. We start with the integral identity (Gradshteyn and Ryzhik 1965):

$$\begin{aligned} G_\nu &= \int_0^\infty \exp(-\mathrm{i}Et) J_\nu(r\sqrt{E}) J_\nu(r_0\sqrt{E})\,\mathrm{d}E \\ &= (\mathrm{i}t)^{-1} I_\nu\,(rr_0/2\mathrm{i}t)\exp[\mathrm{i}(r^2+r_0^2)/4t], \end{aligned} \tag{3.6}$$

where I_ν is the modified Bessel function of order ν. Keeping in mind the correct values of ν (3.3) in all summations, we have:

$$\begin{aligned} \sum_\nu G_\nu \exp(\mathrm{i}\nu\omega) &= (\mathrm{i}t)^{-1}\exp[\mathrm{i}(r^2+r_0^2)/4t]\sum_\nu I_\nu\left(\frac{rr_0}{2\mathrm{i}t}\right)\exp(\mathrm{i}\nu\omega) \\ &\underset{t\to 0^+}{\sim} (\pi \mathrm{i} t r r_0)^{-1/2}\exp[\mathrm{i}(r-r_0)^2/4t]\sum_\nu \exp[\mathrm{i}\omega\nu], \end{aligned} \tag{3.7}$$

where we have used standard asymptotic expansion of $I_\nu(z)$ as $z\to -\mathrm{i}\infty$. The final sum can be evaluated with the Poisson identity:

$$\sum_{k\in Z}\exp(\mathrm{i}kz) = 2\pi\sum_{j\in Z}\delta(2\pi j - z). \tag{3.8}$$

Then the assignment $\omega=\varphi\pm\varphi_0$ establishes (3.5).

4. Sum over images

In order to determine possible collapse of the exact propagator into a countable summation (1.7) we must attempt to cast the Bessel integral as a sum of free propagators, each summand corresponding to a classical path within the sector.

Let $q=\alpha/\pi$. If q happens to be rational, say a/b, define a space–time function:

$$\begin{aligned} S_\alpha(r,\varphi,t|r_0,\varphi_0,0) &= \frac{1}{2\pi a}\int_0^\infty \mathrm{d}E\exp(-\mathrm{i}Et) \\ &\quad\times\sum_{\nu\in Z^+/a} J_\nu(r\sqrt{E})J_\nu(r_0\sqrt{E})\cos[\nu(\varphi-\varphi_0)] \\ &\quad+\frac{1}{4\pi a}\int_0^\infty \mathrm{d}E\exp(-\mathrm{i}Et)J_0(r\sqrt{E})J_0(r_0\sqrt{E}). \end{aligned} \tag{4.1}$$

If q is irrational, we use instead:

$$S_\alpha(r,\varphi,t|r_0,\varphi_0,0) = \frac{1}{2\pi}\int_0^\infty \mathrm{d}E\exp(-\mathrm{i}Et)\int_0^\infty \mathrm{d}s\,J_s(r\sqrt{E})J_s(r_0\sqrt{E})\cos[s(\varphi-\varphi_0)]. \tag{4.2}$$

The importance of these functions will be apparent shortly. Using asymptotic methods of the last section, it is straightforward to show that for interior points $\boldsymbol{r}_0$, $\boldsymbol{r}$ of the sector:

$$\lim_{t\to 0^+} S_\alpha = \delta^2(\boldsymbol{r}-\boldsymbol{r}_0). \tag{4.3}$$

The functions S_α are not, however, solutions to the propagator problem because they do not satisfy the sector boundary conditions (1.3). When q is rational the first summation in (4.1) can be split into two parts, one for integral ν. The result is:

$$S_\alpha = \frac{1}{a}\tilde{K} + \frac{1}{2\pi a}\int_0^\infty \mathrm{d}E\,\exp(-\mathrm{i}Et) \sum_{\substack{\nu\notin Z^+\\ \nu\in Z^+/a}} J_\nu(r\sqrt{E})J_\nu(r_0\sqrt{E})\cos[\nu(\varphi-\varphi_0)], \tag{4.4}$$

where $\tilde{K}$ is the (single direct path) free propagator:

$$\tilde{K}(r,\varphi,t|r_0,\varphi_0,0) = (4\pi\mathrm{i}t)^{-1}\exp[\mathrm{i}(\boldsymbol{r}-\boldsymbol{r}_0)^2/4t]. \tag{4.5}$$

The separation of the function S_α into such parts is not possible when q is irrational.

Next we define a set of image points in the plane (not necessarily lying in the sector itself) by:

$$I_\alpha(\boldsymbol{r}) = \{(r, k\varphi+2\mu\alpha): \mu\in Z; k=\pm 1\}. \tag{4.6}$$

This set, which depends on a fixed point $\boldsymbol{r}$ in the sector, is distributed over a circle of radius r, and is finite if q is rational, otherwise infinite. The importance of the functions S_α can now be revealed as follows. Trigonometric identities applied to the integrands of the definitions of the S_α yield the exact propagator K_α from (3.4) as a sum over the image set (4.6):

$$K_\alpha = \sum_{\boldsymbol{p}\in I_\alpha(\boldsymbol{r})} (-1)^k S_\alpha(\boldsymbol{p}, t|\boldsymbol{r}_0, 0). \tag{4.7}$$

We are now in a position to address the issue of collapse. As might be anticipated, the results will depend strongly on the number-theoretic properties of $q=\alpha/\pi$.

5. The collapsing cases

It is evident from the first term in (4.4) that collapse will occur only if $a=1$, because collapse entails that the sum (4.7) consists only of free propagators expressible in terms of classical actions. For $a=1$, that is sector angle $\alpha=\pi/b$ for a positive integer b, the exact sector propagator is, from (4.7):

$$K_\alpha(\boldsymbol{r},t|\boldsymbol{r}_0,0) = \sum_{\mu=0}^{b-1}\tilde{K}\left(r, \frac{2\pi\mu}{b}+\varphi, t\middle| r_0,\varphi_0,0\right) - \sum_{\mu=0}^{b-1}\tilde{K}\left(r,\frac{2\pi\mu}{b}-\varphi, t\middle| r_0,\varphi_0,0\right). \tag{5.1}$$

There are exactly $2b$ classical paths, exactly half of which are paths with an odd number of bounces. It is easy to see on geometrical grounds that for any initial point $\boldsymbol{r}_0$ in the sector interior, classical rays with b bounces have this amusing property: they strike the final point $\boldsymbol{r}$ with the same angle (with respect to the horizontal x axis, say) at which they leave the initial point. Studies in the references (McGuire 1964) make the connection between this classical property and the absence of diffractive effects in wave equations for the sector. The equal-angle property of the rays is not true when the sector angle is not of the form π/b. Indeed, the space–time function S_α in (4.4) is, in the obvious sense, made up of a proportion $(1-1/a)$ diffractive waves and a proportion $(1/a)$ of what we might call non-diffractive component (the 'free' part of this function).

It is no surprise, therefore, that each of the solved collapsing cases for polygons given in § 2 involves interior angles of the form π/b. The plane-tessellating property of such polygons goes into the property, for the sector, that the latter must tessellate the half-plane.

6. Edge diffraction

Consider the case $\alpha = 2\pi$. This is the problem of a diffracting 'knife-edge' running along the $+x$ axis. As a by-product of the sector analysis, we can write out the exact solution to the diffraction problem.

From (4.4) we see that the exact $\alpha = 2\pi$ propagator will be $\frac{1}{2}$ collapsed and $\frac{1}{2}$ diffractive, since $a = 2$, $b = 1$. The integral in (4.4) can be evaluated to give:

$$S_{2\pi} = \tilde{K}[\tfrac{1}{2} + (2\mathrm{i})^{-1/2} F\{(rr_0/t)\cos[(\varphi - \varphi_0)/2]\}], \tag{6.1}$$

where F is the Fresnel integral (Abramowitz and Stegun 1970):

$$F(z) = C(z) + \mathrm{i}S(z) = \int_0^z \exp(\mathrm{i}\pi y^2/2)\,\mathrm{d}y. \tag{6.2}$$

The exact propagator $K_{2\pi}$ is then obtained from (4.7) where there are two image points. These correspond to the direct path from $\boldsymbol{r}_0$ to $\boldsymbol{r}$, which is sometimes classically possible; and a second path from $\boldsymbol{r}_0$ to the reflection of $\boldsymbol{r}$ through the knife-edge, which is also sometimes possible. That at least one of these paths is always classically possible is suggested by the factor of $\frac{1}{2}$ in (6.1).

Generally we expect the collapse to fail in Schrödinger problems for which the classical rays sometimes disappear as the initial and final points are moved within the region R. One reason for the failure is that paths not continuously defined cannot be the sole contributors to a sum such as (1.7), since the latter must itself be continuous. Still, it appears that such situations can still be salvaged by appeal to a non-classical 'image set' as was done in the derivation of (4.7).

7. Conclusion

We have seen that the space–time propagator for motion in a sector of angle α can be found exactly as a sum over a generally non-classical image set. This propagator collapses into a sum of free terms over $2b$ possible classical paths if and only if the angle is $\alpha = \pi/b$. In general, if the angle has the form $\pi a/b$ then the exact propagator is in a certain sense made up of a $(1/a)$ collapsed part and a $(1-1/a)$ diffractive part. This is in keeping with known results concerning closed two-dimensional polygonal regions: in each solved case every interior angle is of the form π/b.

It would be interesting to find a general sum-over-images formalism for application to all problems of free motion in bounded regions R. It is very likely that diffractive effects would dominate the propagators in the vast majority of cases. Finally, it would be very useful to extend the Feynman path integral formalism in such a way that these results could be obtained via stationary-phase methods, without recourse to the structure of the eigenstates for the region.

References

Abramowitz M and Stegun I 1970 *Handbook of Mathematical Functions*, NBS # 55
DeWitt C 1972 *Commun. Math. Phys.* **28** 47
Feynman R P 1948 *Rev. Mod. Phys.* **20** 367
Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)
Gradshteyn I S and Ryzhik I M 1965 *Table of Integrals, Series, and Products* (New York: Academic Press)
Jones D S 1964 *The Theory of Electromagnetism* (New York: Pergamon)
McGuire J B 1964 *J. Math. Phys.* **5** 622
Sastry V and Chakrabarti A 1979 *J. Math. Phys.* **20** 2123
Sommerfeld A 1896 *Math. Ann.* **47** 317
Wheeler N A 1976 *Summer Research Notes, Reed College*