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Combinatorial approach to Feynman path integration

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Abstract. Combinatorial relations can be used to convert the non-relativistic time-sliced Feynman path integral into perturbation expansions. These methods reveal that when the time interval is sliced into N increments, each order of perturbation theory sustains an error $O(1/\sqrt{N})$. In this way we provide exact path integral results for the following potentials: delta-function comb, finite well, tunnelling barrier, and a generalized exponential cusp. For the tunnelling barrier it is seen how the celebrated (-1) reflection factor arises in the limit of infinite barrier height. The one-dimensional Coulomb problem is solved as a limiting case of the exponential cusp. In addition, for power potentials we indicate how this path integral approach yields sometimes divergent, nevertheless asymptotic perturbation expansions.

1. Introduction and nomenclature

Feynman path integration was first proposed (Feynman 1948) as a constructive scheme for evaluation of the non-relativistic spacetime propagator. For one space dimension and time-independent potential $V(x)$ the propagator is the solution $K^{(V)}(x, t|x_0, 0)$ to the Schroedinger equation $(h/2\pi = m = 1)$:

$$\mathrm{i}\frac{\partial K}{\partial t} + \frac{1}{2}\frac{\partial^2 K}{\partial x^2} - V(x)K = 0 \tag{1.1}$$

subject to the impulse condition $K^{(V)}(x, 0|x_0, 0) = \delta(x - x_0)$. The propagator for a free particle $(V = 0)$ is

$$K^{(0)}(x, t|x_0, 0) = \sqrt{\frac{1}{2\pi \mathrm{i}t}} \exp\left(\frac{\mathrm{i}}{2t}(x - x_0)^2\right) \tag{1.2}$$

whose derivation is the elementary starting point of path integral analysis. A vast literature has addressed the issue of non-trivial potentials. To mention a few successful examples, exact path integrals have been carried out for linear and quadratic potentials (Feynman and Hibbs 1965), quadratic plus inverse-square potentials (Khandekar and Lawande 1975), and the delta-function potential (Gaveau and Schulman 1986, Goovaerts *et al* 1973, Bauch 1985). The Coulomb problem in three and higher dimensions has been resolved (Duru and Kleinert 1979, Goovaerts and Devreese 1972, Ho and Inomata 1982) by path integral evaluation of the space-energy Green's function which, as we momentarily discuss, is directly related to $K^{(V)}$. Space-time propagators have also been obtained via path integration for various curved spaces (Schulman 1968, Dowker 1970, 1971). The exact spacetime propagators are known for reflectionless potentials, such as $V(x) = -2\,\mathrm{sech}^2 x$ (Gaveau and

Schulman 1986, Crandall 1983) but as yet there is no satisfactory path integral derivation of such propagators.

In the present treatment we develop, through combinatorial analysis, perturbation expansions that result in path integral solutions for various new settings. We are able to address successfully the following cases: delta-function combs, the finite potential well, the problem of barrier reflection, a generalized exponential cusp, and power potential asymptotics. In particular, the barrier reflection and exponential cusp analyses give rise to new results. For barrier reflection, we show how the much-discussed factor of (-1) corresponding to an infinite wall reflection component arises naturally from the spacetime propagator for a potential step of asymptotically large height. The exponential cusp form we analyse leads to a path integral solution for the one-dimensional Coulomb problem.

We next establish further nomenclature along standard lines (Kleinert 1990). The space-energy Green's function $G^{(V)}(x, x_0, E)$ is a particular solution of

$$\frac{1}{2}\frac{\partial^2 G}{\partial x^2} + (E - V(x))G = \delta(x - x_0). \tag{1.3}$$

The Green's function and spacetime propagator are related as follows:

$$G^{(V)}(x, x_0, E) = -\mathrm{i}\int_0^\infty K^{(V)}(x, t|x_0, 0)\mathrm{e}^{\mathrm{i}Et}\,\mathrm{d}t \tag{1.4}$$

$$\Theta(t)K^{(V)}(x, t|x_0, 0) = \frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty} G^{(V)}(x, x_0, E)\mathrm{e}^{-\mathrm{i}Et}\,\mathrm{d}E. \tag{1.5}$$

The left-hand side in this last relation is the so-called retarded propagator, which vanishes for $t < 0$. To ensure this, the E line integral in (1.5) is to be taken just above the real E-axis. Both G and K contain information about all Schroedinger eigenstates. The usual formal expansions involving the normalized wave functions $\{\Psi_m\}$ and corresponding eigenvalues $\{E_m\}$ are:

$$K^{(V)}(x, t|x_0, 0) = \sum_m \Psi_m(x)\Psi_m^*(x_0)\mathrm{e}^{-\mathrm{i}E_m t} \tag{1.6}$$

$$G^{(V)}(x, x_0, E) = \sum_m \frac{\Psi_m(x)\Psi_m^*(x_0)}{E - E_m + \mathrm{i}\epsilon} \tag{1.7}$$

where it is understood that these sums over quantum numbers m will generally include discrete sums over bound states plus integrals over continuum states. In the common setting for which there exist bound states ($E_m < 0$) and also continuum states ($E \geqslant 0$) one may split the contour in (1.5) to encircle the poles of (1.7) and, separately, to encircle the cut discontinuity on the positive real E axis:

$$K^{(V)}(x, t|x_0, 0) = \sum_m \mathrm{Res}_E(G)|_{E=E_m}\mathrm{e}^{-\mathrm{i}E_m t} + \frac{\mathrm{i}}{2\pi}\int_0^\infty \mathrm{Disc}_E G\,\mathrm{e}^{-\mathrm{i}Et}\,\mathrm{d}E. \tag{1.8}$$

The E-plane poles of G correspond to the bound eigenvalues, with the residues $\mathrm{Res}_E(G)$ involving the spatial wave functions. For the free particle case, the standard solution to (1.3) is:

$$G^{(0)}(x, x_0, E) = \frac{-\mathrm{i}}{\sqrt{2E}}\mathrm{e}^{\mathrm{i}\sqrt{2E}|x-x_0|}. \tag{1.9}$$

The delta-function in (1.3) arises from the fact that $\mathrm{Disc}_x G'|_{x=x_0} = 2$, which is a good checking relation for a proposed Green's function for any continuously differentiable potential. For the free particle there are no bound states, and the branch cut relation

$$\mathrm{Disc}_E G^{(0)}\,\mathrm{d}E = k\,\mathrm{d}k\left(-\frac{\mathrm{i}}{k}\mathrm{e}^{\mathrm{i}k|x-x_0|} - \left(-\frac{\mathrm{i}}{-k}\right)\mathrm{e}^{-\mathrm{i}k|x-x_0|}\right) \tag{1.10}$$

with $k^2 = 2E$ yields, via (1.8), the correct free particle propagator (1.2). We shall have occasion also to describe a transmission coefficient, defined by

$$T(k) = \lim \frac{G^{(V)}(x, x_0, \frac{1}{2}k^2)}{G^{(0)}(x, x_0, \frac{1}{2}k^2)}\bigg|_{x\to\infty, x_0\to-\infty} \tag{1.11}$$

so that this T, and hence a transmission probability $|T|^2$, can also be derived via path integration for certain potentials.

2. Development of the path integral

One way to define the path integral appropriate to $K^{(V)}$ is to slice the time interval $(0, t)$ into N equal increments. For sufficiently regular potentials, one asserts that, in some appropriate sense of limit (Schulman 1981):

$$K^{(V)} = \lim_N K_N(V) \tag{2.1}$$

where the time-sliced propagator is:

$$K_N^{(V)} = \int D[\mathrm{paths}]\mathrm{e}^{\mathrm{i}S[\mathrm{path}]}. \tag{2.2}$$

The path Jacobian $D[\ ]$ and action S are assumed to depend on a coordinate path $(x_0, x_1, \ldots, x_N = x)$ as follows:

$$D[\mathrm{paths}] = \left(\frac{N}{2\pi\mathrm{i}t}\right)^{N/2}\prod_{m=1}^{N-1}\mathrm{d}x_m \tag{2.3}$$

$$\begin{aligned} S[\mathrm{path}] &= \frac{N}{2t}\sum_{m=0}^{N-1}(x_{m+1} - x_m)^2 - \frac{t}{N}\sum_{m=1}^{N-1}V(x_m) \\ &= T[\mathrm{path}] - V[\mathrm{path}]. \end{aligned} \tag{2.4}$$

Note that some authors prefer to take the second summation in (2.4) from $m = 0$, which involves an extra term involving $V(x_0)$ that is unimportant to our ultimate analysis. On the idea that $V(x)$ vanishes sufficiently rapidly for large $|x|$, which is the essential idea underlying perturbation expansions, we invoke the obvious formal relation

$$\int_{-\infty}^{\infty} f(x)\exp\left(-\mathrm{i}\frac{t}{N}V(x)\right)\mathrm{d}x = \int_{-\infty}^{\infty} f(x)\,\mathrm{d}x + \int_{-\infty}^{\infty} f(x)\left(\exp\left(-\mathrm{i}\frac{t}{N}V(x)\right) - 1\right)\mathrm{d}x \tag{2.5}$$

and conclude that the N-time-slice propagator is:

$$K_N^{(V)} = \sum_{m\in M_{N-1}} \int D[\text{paths}]e^{iT[\text{path}]} \prod_{j\in m} \left(\exp\left(-i\frac{t}{N}V(x_j)\right) - 1\right) \tag{2.6}$$

where M_{N-1} consists of all ordered subsets of the symbols $\{1, 2, 3, \ldots, N-1\}$, incuding the empty set (in which case the product is defined to be 1). Now any non-empty subset m, with card $(m) = j$, having elements $\{m_0, \ldots, m_{j-1}\}$ can be uniquely characterized by a $(j+1)$-tuple:

$$\begin{aligned} L(m) &= \{m_0, m_1 - m_0, \ldots, m_{j-1} - m_{j-2}, N - m_{j-1}\} \\ &= \{L_0, \ldots, L_j\}. \end{aligned} \tag{2.7}$$

We extend this assignment by defining, for the empty set m, $L = \{L_0\} = \{N\}$. Note that the elements of L always sum to N. Now the integral (2.2) can be reduced via the identity:

$$\int_{-\infty}^{\infty} \exp\left(ia\left(\frac{(y-z)^2}{A} + \frac{(z-w)^2}{B}\right)\right) dz = \sqrt{\frac{\pi i}{a}}\sqrt{\frac{AB}{A+B}} \exp\left(ia\frac{(y-w)^2}{A+B}\right) \tag{2.8}$$

which in (2.6) applies to any integration over dx_j when j is not an element of the subset m, for such integrations do not involve the potential. It follows that

$$\begin{aligned} K_N^{(V)} = \sum_{j=0}^{N-1} \left(\frac{N}{2\pi i t}\right)^{(j+1)/2} \sum_{L_0+\ldots+L_j=N} \prod_{h=0}^{j} L_h^{-1/2} \\ \times \int e^{iT(y,L)} \prod_{k=1}^{j} \left(\exp\left(-i\frac{t}{N}V(y_k)\right) - 1\right) dy_k \end{aligned} \tag{2.9}$$

where

$$T(y, L) = \frac{N}{2t} \sum_{m=0}^{j} \frac{(y_{m+1} - y_m)^2}{L_m} \tag{2.10}$$

with $y_0 = x_0$, $y_{j+1} = x$; and each L_i is a positive integer. The $j = 0$ case of the combined integral and k-product in (2.9) is just 1, which observation amounts to an immediate derivation of the free particle propagator (1.2). In the free case (2.8) effectively reduces the path integral (2.6) completely.

The representation (2.9) is central to the combinatorial derivations that follow. But alternative representations are also useful. We observe that (2.9) involves convolutions, and we are moved to define:

$$W(k, t) = \frac{iN}{2\pi t} \int_{-\infty}^{\infty} \left(\exp\left(-i\frac{t}{N}V(x)\right) - 1\right) e^{-ikx}\, dx \tag{2.11}$$

whence an alternative form of the time-sliced propagator is

$$\begin{aligned} K_N^{(V)} = \frac{1}{2\pi} \sum_{j=0}^{N-1} \left(\frac{-it}{N}\right)^j \sum_{L_0+\ldots+L_j=N} \int \prod_{h=0}^{j} dk_h \exp\left(-\frac{it}{2N}L_h k_h^2\right) \\ \times e^{i(k_j x - k_0 x_0)} \prod_{q=0}^{j-1} W(k_{q+1} - k_q, t) \end{aligned} \tag{2.12}$$

where, again, any empty products are 1 and the L_l are positive integers.

The basic formulae (2.9) and (2.12) are exact expressions—subject to appropriate convergence criteria—for the N-fold time-sliced spacetime propagator. One could conceivably argue that N should immediately be taken to infinity, in which case various established perturbation expansions would result. But there is some value in keeping N finite for the moment. For one thing, any numerical evaluations of path integrals that assume finite N can be assessed for their accuracy, if we are careful to establish how a finite N affects a perturbation expansion. It is the problem of the large-N limit to which we now turn.

3. Combinatorial relations

Our representations of the time-sliced propagator $K_N^{(V)}$ involve combinatorial sums over order-$(j+1)$ partitions of N. With a view to representation (2.9) we consider, for vectors $\boldsymbol{d} = \{d_0, \ldots, d_j\}$ the sum

$$S_{Nj}(\boldsymbol{d}) = \sum_{L_0+\ldots+L_j=N} \prod_{m=0}^{j} L_m^{-1/2} \exp\left(\mathrm{i}\frac{N\mathrm{d}_m^2}{L_m}\right). \tag{3.1}$$

This sum is difficult to analyse in any exact sense, but rigorous asymptotic analysis can be performed. We shall be able to give the leading large-N term of (3.1). Take first the special case:

$$S_{Nj}(\mathbf{0}) = \sum_{L_0+\ldots+L_j=N} \frac{1}{\sqrt{L_0\ldots L_j}}. \tag{3.2}$$

If we approximate this sum by a surface integral over an appropriate section of the $(j+1)$-dimensional sphere of radius $\sqrt{N}$, we arrive at an estimate

$$S_{Nj}(\mathbf{0}) = \frac{\pi^{(j+1)/2}}{\Gamma((j+1)/2)} N^{(j-1)/2} + E(N, j) \tag{3.3}$$

where nothing is known *a priori* about the error term $E(N, j)$. But we can observe that

$$S_{Nj}(\mathbf{0}) = \sum_{L=1}^{N-j} \frac{1}{\sqrt{L}} S_{N-L,j-1}(\mathbf{0}). \tag{3.4}$$

We then apply this identity recursively to the estimate (3.3). It turns out to be enough to provide a sufficiently sharp estimate of the sum:

$$\sigma_{Nj} = \sum_{L=1}^{N-j} \frac{1}{\sqrt{L}} (N-L)^{(j-2)/2}. \tag{3.5}$$

Such an estimate can be obtained by writing this last sum as an integral of the function $[L]^{-1/2}(N-[L])^{j/2-1}$ where [ ] denotes greatest integer. One may show in this way that, for example

$$\left| \sigma_{Nj} - B\left(\frac{1}{2}, \frac{j}{2}\right) N^{(j-1)/2} \right| < 6N^{(j-2)/2} \tag{3.6}$$

where B denotes the beta function. One may in turn provide an estimate on the error term

$$|E(N,j)| < C^j N^{(j-2)/2} \tag{3.7}$$

where C is an absolute constant. The precise nature of the E term is still mysterious, but what we can say is that

$$S_{Nj}(0) = \frac{\pi^{(j+1)/2}}{\Gamma((j+1)/2)} N^{(j-1)/2} \left(1 + O\left(\frac{1}{\sqrt{N}}\right)\right) \tag{3.8}$$

where the implicit big-O constant is absolute, meaning both j- and N-independent.

The result (3.8) is enough to solve specialized path integral problems, such as the problem of the delta-function potentials' ground state energy in section 4, but we still need to address the general sum (3.1). There is an attractive method for obtaining heuristic initial estimates of general sums involving functions f_m:

$$Q_{Nj} = \sum_{L_0+\ldots+L_j=N} \prod_{m=0}^{j} f_m(L_m). \tag{3.9}$$

One integrates over $\delta(L_0 + \ldots + L_j - N)$ to infer a large-N behaviour:

$$Q_{Nj} \sim \frac{1}{2\pi} \int \mathrm{d}k\, \mathrm{e}^{-\mathrm{i}kN} \prod_{m=0}^{j} \int_0^\infty f_m(L)\, \mathrm{e}^{\mathrm{i}kL}\, \mathrm{d}L. \tag{3.10}$$

For the combinatorial sum (3.1) this delta-function method may be applied, together with the integral identity:

$$\int_0^\infty \exp\left(\mathrm{i}kL + \mathrm{i}\frac{Nd^2}{L}\right) \frac{\mathrm{d}L}{\sqrt{L}} = \sqrt{\frac{\pi}{\mathrm{i}k}}\, \mathrm{e}^{-2|d|\sqrt{Nk}} \qquad \mathrm{Im}(k) > 0 \tag{3.11}$$

to give a convenient contour representation of the leading term:

$$S_{Nj}(\boldsymbol{d}) \sim N^{(j-1)/2} \pi^{(j+1)/2} \frac{\mathrm{i}}{2\pi} \oint_C (-z)^{-(j+1)/2} \mathrm{e}^{-z} \mathrm{e}^{-2\sqrt{\mathrm{i}z}(|d_0|+\cdots+|d_j|)}\, \mathrm{d}z \tag{3.12}$$

where the contour C circles the origin counter-clockwise, sufficiently tightly enclosing the positive real z-axis. Note that for $\boldsymbol{d} = 0$ we recover, via the standard contour representation of $1/\Gamma$, the original leading term estimate in (3.3). By series expansion of the $\boldsymbol{d}$-dependent exponential, one may use error function representations (Abramowitz and Stegun 1965) to perform the contour integral. Further error analysis of the style embodied in (3.4)–(3.7) gives the general estimate:

$$S_{Nj}(\boldsymbol{d}) = N^{(j-1)/2} \pi^{(j+1)/2} 2^{j-1} i^{j-1}\mathrm{erfc}(D\sqrt{-\mathrm{i}}) \left(1 + O\left(\frac{1}{\sqrt{N}}\right)\right) \tag{3.13}$$

where $D = |d_0| + \ldots + |d_j|$, and $i^n\mathrm{erfc}$ is the iterated error function of order n. For fixed $\boldsymbol{d}$ the implicit O constant is independent of both j and N. For $\boldsymbol{d} = 0$, hence $D = 0$, the result (3.13) is consistent with (3.8).

The integral (3.12) can be used to establish large-N limits for the sliced-time propagator. Starting with (2.9), and observing that $\mathrm{e}^{-\mathrm{i}tV/N} - 1 = -\mathrm{i}tV/N + O(1/N^2)$, we arrive after some straightforward manipulations to a formal perturbation series for the space-energy Green's function:

$$G^{(V)}(x, x_0, E) = \sum_{j=0}^{\infty} \left(\frac{-\mathrm{i}}{\sqrt{2E}}\right)^{j+1}$$
$$\times \int \exp(\mathrm{i}\sqrt{2E}(|x_1 - x_0| + |x_2 - x_1| \ldots + |x - x_j|)) \prod_{m=1}^{j} V(x_m)\,\mathrm{d}x_m \quad (3.14)$$

with the empty integral defined to be $\mathrm{e}^{\mathrm{i}|x-x_0|\sqrt{(2E)}}$, which rule gives the $j = 0$ term as the correct free Green's function (1.9). The perturbation expansion will be recognized as nothing new, amounting essentially to iteration of a standard Lippman–Schwinger scattering expansion (Schiff 1968) for non-relativistic settings. The point, however, is that we have shown that for every j, the jth term in (3.14) is approximated to $O(1/\sqrt{N})$ by the time-sliced propagator. This means that whenever one can sum the perturbation series, one can in principle trace back to the original path integral definition, and so claim that the path integral has been resolved.

An alternative analysis, again using partitions $\mathbf{L}$ of N, starts with (2.12), uses the delta-function method embodied in (3.10), and results in a second representation for the space-energy Green's function:

$$G^{(V)}(x, x_0, E) = \frac{1}{2\pi} \sum_{j=0}^{\infty} \int \mathrm{e}^{\mathrm{i}(k_j x - k_0 x_0)} \prod_{m=0}^{j-1} V^{\sim}(k_{m+1} - k_m) \prod_{h=0}^{j} \frac{\mathrm{d}k_h}{E - \frac{1}{2}k_h^2 + \mathrm{i}\epsilon} \quad (3.15)$$

where the empty m-product is defined as 1 and $V^{\sim}$ is the transformed potential:

$$V^{\sim}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} V(x)\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x. \quad (3.16)$$

This second expansion (3.15) is also standard, in fact it gives rise to instructional Feynman diagrams for non-relativistic scattering. But again, if a problem can be solved with this expansion, the solution can in principle be recast in terms of the original time-sliced propagator.

Before we proceed to solutions for specific potentials, we establish another kind of combinatorial relation. For given complex T, integer M, integers $b_0, b \epsilon [0, M-1]$, and a collection of complex numbers $U_0, \ldots, U_{M-1}$; consider a function of complex z:

$$g(b, b_0, z) = \sum_{j=0}^{\infty} z^j \sum_{b_i \epsilon [0, M-1]} U_{b_1} \ldots U_{b_j} T^{|b_1 - b_0| + \ldots + |b - b_j|} \quad (3.17)$$

where the second sum is over tuples $\{b_1, \ldots, b_j\}$, and the empty second sum for $j = 0$ is defined to be $T^{|b-b_0|}$. In the theory of connected graph combinatorics and adjacency matrices (Stanley 1986, Buhler 1992) one considers all graphs connecting $b_0 \to b_1 \to \ldots \to b_j \to b$ to arrive at a matrix representation

$$g(b, b_0, z) = \left(\frac{\boldsymbol{T}}{1 - z\boldsymbol{U}\boldsymbol{T}}\right)_{bb_0} \quad (3.18)$$

where the $\boldsymbol{T}$ matrix has elements $\boldsymbol{T}_{ij} = T^{|i-j|}$ and the $\boldsymbol{U}$ matrix is diagonal, with $\boldsymbol{U}_{ii} = U_i$; both matrices being M-by-M. The resemblance of the combinatorial sum (3.17) to the perturbation expansion (3.14) is evident. We shall be able to apply the result (3.18) to various problems in which the potential may be thought of as a dense comb of delta functions. For such problems path integration comes down to an exercise in matrix algebra.

4. Delta-function potentials

Perhaps the most direct derivation of a ground state energy from a time-sliced propagator is to apply the special combinatorial case (3.8) to the $K_N^{(V)}$ representation (2.9) for the potential $V(x) = -A\delta(x)$. Here, A is a positive real constant, and one might wish to preserve rigour by approximating V by a very narrow, appropriately deep potential well; though the asymptotics are not particularly illuminating and are best handled via the finite well solution that we discuss later. The correct observation is that, on the basis of (2.9), and for spatial endpoints $x = x_0 = 0$

$$K_N^{(v)}(0, t|0, 0) \sim \sum_{j=0}^{\infty} \left(\frac{N}{2\pi \mathrm{i}t}\right)^{(j+1)/2} \left(\mathrm{i}A\frac{t}{N}\right)^j S_{Nj}(\mathbf{0}) \tag{4.1}$$

which, from (3.8) results in

$$K^{(V)}(0, t|0, 0) = \frac{1}{\sqrt{2\pi \mathrm{i}t}} + A\sqrt{\frac{\mathrm{i}t}{2}} \exp\left(\mathrm{i}\frac{A^2 t}{2}\right) \operatorname{erfc}\left(-A\sqrt{\frac{\mathrm{i}t}{2}}\right) \tag{4.2}$$

where we have made use of standard series expansions for erfc() (Ambramowitz and Stegun 1965). From the eigenfunction expansion (1.6) we can employ the Feynman–Kac limit (Schulman 1981), that is $t = -\mathrm{i}s \to -\mathrm{i}\infty$, to infer a leading term $\Psi\Psi^* \mathrm{e}^{-sE_0}$, so that the ground state has energy

$$E_0 = -A^2/2. \tag{4.3}$$

For more general spacetime endpoints, one may use the general combinatorial form (3.13) to express the complete spacetime propagator in terms of error functions. The expansion (4.1) is preserved but with $\mathbf{0}$ replaced by $\boldsymbol{d} = \{x_0, 0, \ldots, 0, x\}$ when $j > 0$, and by $\boldsymbol{d} = \{x - x_0\}$ for $j = 0$. The propagator has been obtained separately via Laplace transforms and iterated error function identities by Bauch (1985). But within the present context there is a convenient way to derive this propagator. We appeal to the space-energy form (3.14). Trivial integrations for the delta-function potential at hand result in

$$G^{(V)}(x, x_0, E) = \frac{-\mathrm{i}}{\sqrt{2E}} \mathrm{e}^{\mathrm{i}\sqrt{2E}|x-x_0|} + \frac{A}{\sqrt{2E}} \frac{1}{\sqrt{2E} - \mathrm{i}A} \mathrm{e}^{\mathrm{i}\sqrt{2E}(|x|+|x_0|)}. \tag{4.4}$$

As expected, there is a pole for the energy (4.3), and the ground state wave function can be seen to be the well-known exponential cusp. One may apply with care the cut relation (1.8) to obtain the exact spacetime propagator as:

$$K^{(V)}(x, t|x_0, 0) = K^{(0)}(x, t|x_0, 0) + \frac{A}{\sqrt{2\pi \mathrm{i}t}} \int_0^{\infty} \mathrm{e}^{Au} \exp\left(\frac{\mathrm{i}}{2t}(u + |x| + |x_0|)^2\right) \mathrm{d}u \tag{4.5}$$

in agreement with known results (Gaveau and Schulman 1986).

We next turn to the problem of the delta-function comb. Define the potential

$$V(x) = -\frac{A}{M} \sum_{m=0}^{M-1} \delta\left(x - \frac{m}{M}\right) \tag{4.6}$$

where M simply counts the number of delta-functions in the problem. Using (3.14) and the combinatorial analysis starting with (3.17), we can obtain the space-energy Green's function for spacetime endpoints lying precisely on delta locations. Assume that $b_0 = Mx_0$ and $b = Mx$ are integers lying in $[0, \ldots, M-1]$. Then the exact Green's function for such spatial endpoints is

$$G^{(V)}(x, x_0, E) = -\frac{\mathrm{i}}{k}\left(\frac{\boldsymbol{T}_M}{\mathbf{1} - z\boldsymbol{T}_M}\right)_{bb_0} \tag{4.7}$$

where $k = \sqrt{(2E)}$, $z = \mathrm{i}A/Mk$, and $\boldsymbol{T}_m$ for $m\epsilon[0, M-1]$ is generally the $m \times m$ matrix having $\boldsymbol{T}_{cd} = T^{|c-d|}$, where $T = \mathrm{e}^{\mathrm{i}k/M}$. On the other hand, for any spatial endpoints that straddle the entire comb, that is $x > (M-1)/M$, $x_0 < 0$, we have

$$G^{(V)}(x, x_0, E) = -\frac{\mathrm{i}}{k}\left(\frac{\boldsymbol{T}_M}{\mathbf{1} - z\boldsymbol{T}_M}\right)_{0,M-1} \exp\left(\mathrm{i}k\left(x - x_0 - \frac{(M-1)}{M}\right)\right). \tag{4.8}$$

Note that for coupling constant $A \to 0$, both (4.7) and (4.8) approach the correct free Green's function (1.9). For this problem, and to a greater extent the ensuing problem of the finite well, we require some matrix algebra. Detailed analysis of the matrix $\mathbf{1} - z\boldsymbol{T}_m$ results in the following relations, which serve to determine completely the inverse of the full matrix $\mathbf{1} - z\boldsymbol{T}_M$. Define

$$D_m = \det(\mathbf{1} - z\boldsymbol{T}_m) \tag{4.9}$$

Then one may establish, via row- and column-reduction, the following recursion (Mayer 1992):

$$D_m = (1 - z + (1+z)T^2)D_{m-1} - T^2 D_{m-2} \tag{4.10}$$

where $D_0 = 1$, $D_1 = 1 - z$. Furthermore, by analysing minors one finds that the diagonal elements of $(\mathbf{1} - z\boldsymbol{T}_M)^{-1}$ satisfy:

$$(\mathbf{1} - z\boldsymbol{T}_M)^{-1}_{aa} = \frac{T^2 D_{M-1} + (1 - T^2)D_a D_{M-1-a}}{D_M} \tag{4.11}$$

while the off-diagonal elements, for say $M > a > b \geqslant 0$, satisfy:

$$(\mathbf{1} - z\boldsymbol{T}_M)^{-1}_{ab} = \frac{T^{a-b}}{z}\frac{(D_{b+1} - D_b)(D_{M-a} - D_{M-a-1})}{D_M}. \tag{4.12}$$

The Green's function may now be deduced in terms of these relations for the full matrix inverse using:

$$\frac{-\boldsymbol{T}}{\mathbf{1} - z\boldsymbol{T}} = \frac{\mathbf{1}}{z} - \frac{1}{z}\frac{1}{\mathbf{1} - z\boldsymbol{T}}. \tag{4.13}$$

From (4.12) and (4.8) one may conclude that for straddling endpoints $x > (M-1)/M$, $x_0 < 0$:

$$G^{(V)}(x, x_0, E) = \frac{G^{(0)}(x, x_0, E)}{D_M}. \tag{4.14}$$

This result can now be shown to imply known delta-comb results. From the recurrence (4.10) and the definition

$$w = \frac{1 - z + (1 + z)T^2}{2T} \tag{4.15}$$

we can use standard relations for the Chebyshev polynomial of the second kind (Abramowitz and Stegun 1965) to deduce an alternative recurrence:

$$D_m = T^m(U_m(w) - (1 + z)TU_{m-1}(w)). \tag{4.16}$$

This, together with the identity

$$U_m^2 - 2wU_mU_{m-1} + U_{m-1}^2 = 1 \tag{4.17}$$

is enough to establish, via (4.14) and (1.11), the transmission probability for an M delta-function comb (Griffiths and Taussig 1992):

$$|T(k)|^{-2} = 1 + \left(\frac{A}{Mk}\right)^2 U_{M-1}^2\left(\cos\frac{k}{M} - \frac{A}{kM}\sin\frac{k}{M}\right). \tag{4.18}$$

One might wonder whether the exact Green's function (4.14) can be used, in the spirit of (4.4)–(4.5), to obtain the spacetime propagator for the comb. The answer is yes: in principle, one may always obtain an expression for $K^{(V)}$ in terms of a finite number of error function integrals. This analysis shows that the spacetime propagator for the delta-function comb can be completely resolved via path integration: for given M, one computes D_M, then performs the discontinuity calculus. One may expand this approach to allow more general matrices U in the general formula (3.18). There is the option of expressing any potential as a sufficiently dense comb, with the elements of U varying according to the specific potential. To exemplify the dense comb limit we next turn to the problem of the finite well.

5. Finite well potential

The previous results enable a complete path integral solution for the finite well:

$$V(x) = \begin{cases} 0 & x < 0 \\ -A & 0 \leqslant x < 1 \\ 0 & x \geqslant 1 \end{cases} \tag{5.1}$$

where A is a positive constant, although results for the finite potential step ($A < 0$) can be inferred via analytic continuation. We represent V by an extremely dense delta-function comb of the type (4.6). We assume that the large-M limits of (4.7), (4.8) for the comb will give the correct space-energy Green's function for the well. Whether a dense comb approximation to a potential is valid is problematic; but at least our eventual solution will satisfy the fundamental Schroedinger definition (1.3).

The idea is to compute (4.7), (4.8) in the dense comb limit, $M \to \infty$. We first observe that any sequence satisfying a recurrence such as (4.10) can be represented by:

$$D_m = \alpha_+ r_+^m + \alpha_- r_-^m \tag{5.2}$$

where $r_\pm$ are roots of a certain quadratic equation, which equation can be obtained by inserting the ansatz (5.2) into the recurrence. In fact, for the previous delta comb definitions $z = \mathrm{i}A/kM$, $T = \mathrm{e}^{\mathrm{i}k/M}$ we have

$$\begin{aligned} r_\pm &= \frac{v \pm c}{2} \\ v &= 1 - z + (1+z)T^2 \\ c &= \sqrt{v^2 - 4T^2} \\ \alpha_\pm &= \frac{1 \pm u}{2c} \\ u &= 1 - z - (1+z)T^2. \end{aligned} \tag{5.3}$$

These relations can now be used to express (4.7), (4.8) in terms of $r_\pm$, by proper use of the matrix relations (4.11), (4.12). Taking the large-M dense comb limit is an intricate and tedious task, so we simply state the final result as follows. For spatial endpoints $0 \leqslant x_0 \leqslant x \leqslant 1$, the finite well Green's function arises from (4.7) as:

$$G^{(V)}(x, x_0, E) = \frac{-\mathrm{i}}{kR} \frac{h(x_0)h(1-x)}{R\cos R - \mathrm{i}a \sin R} \tag{5.4}$$

and $k = \sqrt{(2E)}$ and

$$\begin{aligned} a &= k + \frac{A}{k} \\ R &= \sqrt{2A + k^2} \end{aligned} \tag{5.5}$$

with the function h defined by:

$$h(z) = R\cos Rz - \mathrm{i}k \sin Rz. \tag{5.6}$$

For $0 \leqslant x \leqslant x_0 \leqslant 1$, one reverses the roles of the spacetime endpoints on the right-hand side of (5.4). The space-energy Green's function (5.4) is exact for the given constraints on the spatial endpoints. Further analysis in the style that led to (4.8) gives the finite well Green's function for arbitrary spacetime endpoints as:

$$\begin{aligned} G^{(V)}(x, x_0, E) &= \Delta(x, x_0) G^{(0)}(x, x_0, E) \\ &\quad + \mathrm{e}^{\mathrm{i}k(|x|+|x_0|-c(x)-c(x_0))} \left(G^{(V)}(c(x), c(x_0), E) + \frac{\mathrm{i}}{k}\Delta(x, x_0) \right) \end{aligned} \tag{5.7}$$

where

$$c(z) = \begin{cases} 1 & z \geqslant 1 \\ z & 0 \leqslant z \leqslant 1 \\ 0 & z \leqslant 0 \end{cases}$$

$$\Delta(x, y) = \begin{cases} 1 & ((x > 1) \text{ and } (y > 1)) \text{ or } ((x < 0) \text{ and } (y < 0)) \\ 0 & \text{otherwise.} \end{cases} \tag{5.8}$$

Note that $0 \leqslant c(\ ) \leqslant 1$ so that (5.7) can always be computed from (5.4). Regardless of all the convergence problems encountered in our path integral derivation of the exact Green's function (5.7), one can check that this $G^{(V)}$ solves (1.3), in particular the boundary-discontinuity relation $\mathrm{Disc}_x G'|_{x=x_0} = 2$ is satisfied always. When x_0, x both lie within the well, this discontinuity arises from the re-ordering rule (remark after (5.6)). The transmission coefficient is obtained immediately from the limit relation (1.11) as:

$$T(k) = \mathrm{e}^{-\mathrm{i}k} \frac{R}{R \cos R - \mathrm{i}a \sin R} \tag{5.9}$$

giving the inverse transmission probability

$$|T(k)|^{-2} = 1 + \left(\frac{A}{Rk} \right)^2 \sin^2 R. \tag{5.10}$$

This standard result for the finite well can be derived independently from the comb formula (4.18) by considering the large-M asymptotics of Chebyshev polynomials (Griffiths 1992).

The bound states of the finite well are signified by the E-poles of (5.7). Evidently the bound states correspond to occurrences in (5.4) of

$$\begin{aligned} \mathrm{i}a &= R \cot R \\ &= R(\cot R/2 - \tan R/2)/2 \end{aligned} \tag{5.11}$$

which amounts to

$$(R \tan R/2 + \mathrm{i}k)(R \cot R/2 - \mathrm{i}k) = 0. \tag{5.12}$$

It is interesting that the path integral analysis gives just one transcendental pole relation (5.11) which turns into a pair of transcendental root relations (5.12). Indeed the standard textbook solution for even and odd states involves, respectively, the tan, cot root relations of (5.12) (Schiff 1968). At the poles, the internal sinusoidal bound state wave functions are the residues; namely the h functions in (5.4). The Green's function (5.7) is also correct for $A \to -A$, but the usual rule, that $\mathrm{Im}(k) > 0$, rules out any bound states.

The dense comb analysis has given us a valuable by-product, a means by which certain iterated integrals of the type (3.14) can be obtained in closed form. For the finite well, one could avoid *a priori* the dense comb picture, and start from (3.14) where each spatial integral is performed over [0,1]. It is enough to evaluate the generating function:

$$f(x, x_0, z, k) = \sum_{j=0}^{\infty} z^j \int_0^1 \ldots \int_0^1 \mathrm{e}^{\mathrm{i}k(|x_1 - x_0| + \ldots + |x - x_j|)} \, \mathrm{d}x_1 \ldots \mathrm{d}x_j \tag{5.13}$$

where the empty integral is defined to be $\mathrm{e}^{\mathrm{i}k|x-x_0|}$, and $\mathrm{Im}(k) > 0$. Instead of appealing to the dense comb limit, we merely use the combinatorial generating function (3.17) to solve the somewhat forbidding calculus problem of evaluating f. One has:

$$f(x, x_0, z, k) = \lim_{M \to \infty} g\left(Mx, Mx_0, \frac{z}{M} \right) \tag{5.14}$$

with $\boldsymbol{T} = \mathrm{e}^{\mathrm{i}k/M}$, $\boldsymbol{U} = \mathbf{1}$, and for each M the $\boldsymbol{T}$ and $\boldsymbol{U}$ matrices are each $M \times M$. As before, the relations (5.2)–(5.3) and (4.10)–(4.13) result in a closed form for the generating function f. For spatial endpoints $x_0 \leqslant x$ in [0,1] we obtain:

$$f(x, x_0, z, k) = \frac{1}{\rho} \frac{h(x_0) h(1-x)}{\rho \cos \rho - \mathrm{i}\alpha \sin \rho} \tag{5.15}$$

where $\rho = \sqrt{(k^2 - 2ikz)}$, $\alpha = k - iz$. An attractive special case is the exact evaluation of (5.13) for both spatial endpoints vanishing:

$$f(0,0,z,k) = \frac{\rho - ik\tan\rho}{\rho - i\alpha\tan\rho}. \tag{5.16}$$

One need only to establish this case of the generating function (5.13) to infer a path integral solution for all of the bound state energies. Each energy pole appears because our well is centred at 1/2, so that both even and odd wave bound state functions are non-zero at the origin.

6. Tunnelling barrier

Consider the finite barrier potential

$$V(x) = \begin{cases} B & x \geqslant 0 \\ 0 & x < 0 \end{cases} \tag{6.1}$$

where B is a positive constant. We can evaluate the Green's function representation (3.14) on the basis of the generating function:

$$F(x, x_0, z, k) = \sum_{j=0}^{\infty} z^j \int_0^{\infty} \ldots \int_0^{\infty} e^{ik(|x_1 - x_0| + \ldots + |x - x_j|)}\, dx_1 \ldots dx_j \tag{6.2}$$

with the empty integral defined as per the remarks following (5.13). In terms of the corresponding finite well generating function (5.13) we scale the integrals in (6.2) to obtain:

$$F(x, x_0, z, k) = \lim_{Y\to\infty} f\left(\frac{x}{Y}, \frac{x_0}{Y}, Yz, Yk\right) \tag{6.3}$$

for both x, $x_0 \geqslant 0$, one concludes from (5.15) that:

$$F(x, x_0, z, k) = \frac{e^{ik|x-x_0|Q}(1 + 1/Q) + e^{ik|x+x_0|Q}(1 - 1/Q)}{1+Q} \tag{6.4}$$

where

$$Q = \sqrt{1 - \frac{2iz}{k}}. \tag{6.5}$$

For $x_0 \leqslant 0$ and $x \geqslant 0$ the defining relation is:

$$F(x, x_0, z, k) = e^{-ikx_0} F(x, 0, z, k) \tag{6.6}$$

and when both x, $x_0 \leqslant 0$ we have

$$F(x, x_0, z, k) = e^{-ik(x+x_0)} F(0, 0, z, k). \tag{6.7}$$

The generating function (6.2) thus yields the complete space-energy Green's function as:

$x \geqslant x_0 \geqslant 0$:

$$G^{(V)}(x, x_0, E) = -\frac{\mathrm{i}}{k}\frac{k}{k+R}\left(\mathrm{e}^{\mathrm{i}R(x+x_0)}\left(1-\frac{k}{R}\right)+\mathrm{e}^{\mathrm{i}R(x-x_0)}\left(1+\frac{k}{R}\right)\right)$$

$x \geqslant 0 \geqslant x_0$:

$$G^{(V)}(x, x_0, E) = -\frac{2\mathrm{i}}{k+R}\mathrm{e}^{\mathrm{i}(Rx-kx_0)}$$

$x, x_0 \leqslant 0$:

$$G^{(V)}(x, x_0, E) = G^{(0)}(x, x_0, E) - \mathrm{i}\frac{k}{R}\frac{k-R}{k+R}\mathrm{e}^{-\mathrm{i}k(x+x_0)} \tag{6.8}$$

where

$$R = \sqrt{k^2 - 2B}. \tag{6.9}$$

The space-energy Green's function (6.8) allows us to resolve the long-standing problem of just how the spacetime propagator acquires a reflection term for an infinitely high barrier. Assume that both x, $x_0 < 0$, so we are considering propagation for spacetime endpoints both to the left of the barrier. One may perform the discontinuity integral (1.8) for the third Green's function representation of (6.8). This procedure is intricate, involving discontinuous Weber–Schafheitlin integrals relevant to the study of Bessel functions. The formal result is, for time $t = 0$,

$$K^{(V)}(x, 0|x_0, 0) = \delta(x - x_0) + 2\theta(x + x_0)\frac{J_2((-x - x_0)\sqrt{2B})}{x + x_0} \tag{6.10}$$

where J_2 is the Bessel function of order 2. For the given spatial endpoints this initial condition propagates according to the free time-dependent Schroedinger equation, so that

$$K^{(V)}(x, t|x_0, 0) = K^{(0)}(x, t|x_0, 0) - \frac{2}{\sqrt{2\pi \mathrm{i}t}} \times \int_0^\infty \mathrm{d}u\, \frac{J_2(u\sqrt{2B})}{u}\exp\left(\frac{\mathrm{i}}{2t}(u + |x| + |x_0|)^2\right). \tag{6.11}$$

This is the exact spacetime propagator for spatial endpoints x, $x_0 \leqslant 0$. Finally we can see how the spacetime propagator acquires a reflection factor of (-1) due to an infinite barrier. Indeed, as $B \to \infty$, we can use the interesting representation:

$$\lim_{C\to\infty} 2J_2(Cz)/z = \delta(z). \tag{6.12}$$

This follows from the relation (Abramowitz and Stegun 1965):

$$\frac{J_2(Cz)}{z} = \frac{C}{4}(J_1(Cz) + J_3(Cz)). \tag{6.13}$$

Indeed, the right-hand side has integral 1/2 over $z\in[0,\infty]$, the area being progressively more localized near the origin as $C\to\infty$. We infer that for infinite barrier height the propagator (6.11) becomes:

$$K^{(0)}(x,t|x_0,0)=\sqrt{\frac{1}{2\pi it}}\exp\left(\frac{i}{2t}(x-x_0)^2\right)-\sqrt{\frac{1}{2\pi it}}\exp\left(\frac{i}{2t}(x+x_0)^2\right). \tag{6.14}$$

The exact solution (6.11) shows that contributions to the celebrated (−) sign in (6.14) for the reflection term come from various depths into the potential step, in a complicated way. In fact, there is a kind of Gibb's phenomenon: the (−1) reflection coefficient is in actuality, for large finite B, an oscillatory term made up from stationary points of the (6.11) integrand. Such stationary points arise from the local minima and maxima of the appropriate Bessel functions. Asymptotic analysis of the reflection coefficient is difficult, but analysis of the integral (6.11) for large B gives at least the leading reflection term:

$$-\left(1+\frac{i(x+x_0)\sqrt{2}}{t\sqrt{B}}+O\left(\frac{1}{B}\right)\right) \tag{6.15}$$

showing again the limit (−1) as $B\to\infty$.

7. Generalized exponential cusp and the Coulomb problem

We now consider the generalized exponential cusp potential

$$V(x)=\sum_{n=1}^{\infty}a_n e^{-\lambda n|x|} \tag{7.1}$$

where $\lambda>0$ and $\{a_i\}$ are constants. We shall be able to solve special cases of this potential including the single exponential cusp, $V(x)=-Be^{-\lambda|x|}$ and a more complicated cusp:

$$V(x)=-\frac{Z\lambda Ae^{-\lambda|x|}}{1-Ae^{-\lambda|x|}} \tag{7.2}$$

whose limit $A\to 1^-$, $\lambda\to 0^+$ provides a solution for the Coulomb potential $V(x)=-Z/|x|$.

We define an iterated integral:

$$I_j(x,x_0,k)=\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}e^{ik(|x_1-x_0|+\ldots+|x-x_j|)}\prod_{m=1}^{j}V(x_m)\,dx_m \tag{7.3}$$

where the empty case $j=0$ is defined as usual by $I_0(x,x_0,k)=e^{ik|x-x_0|}$. We next establish a closure relation for the particular integrals $I_j(x,0,k)$, in the sense that each such integral turns out to be a polynomial in $e^{-\lambda|x|}$. To this end we observe:

$$\int_{-\infty}^{\infty}e^{-n\lambda|b|}e^{ik|x-b|}e^{(ik-m\lambda)|b|}\,db=f_{m+n}e^{ik|x|}-g_{m+n}e^{(ik-(m+n)\lambda)|x|} \tag{7.4}$$

where

$$f_\mu = \frac{1}{\mu\lambda - 2ik} + \frac{1}{\mu\lambda} \qquad g_\mu = \frac{-1}{\mu\lambda - 2ik} + \frac{1}{\mu\lambda} \tag{7.5}$$

from which it follows that

$$I_j(x, 0, k) = X^T M^j Y e^{ik|x|} \tag{7.6}$$

where X is the vector $\{1, e^{-\lambda|x|}, e^{-2\lambda|x|}, \ldots\}$, Y is the vector $\{1, 0, 0, \ldots\}$, and M is the matrix:

$$M = \begin{bmatrix} F_0 & F_1 & F_2 \ldots \\ -a_1 g_1 & 0 & 0 \ldots \\ -a_2 g_2 & -a_1 g_z & 0 \ldots \\ \ldots & & \end{bmatrix} \tag{7.7}$$

with

$$F_\nu = \sum_{j=1}^{\infty} a_j f_{\nu+j}. \tag{7.8}$$

In view of these relations the generating function:

$$H(x, 0, z, k) = \sum_{j=0}^{\infty} z^j I_j(x, 0, k) \tag{7.9}$$

takes the form:

$$H(x, 0, z, k) = X^T (\mathbf{1} - zM)^{-1} Y e^{ik|x|}. \tag{7.10}$$

In the case $a_n = a^n$, where a is constant, analysis of the matrix M results in:

$$H(x, 0, z, k) = X^T C \frac{e^{ik|x|}}{\det(\mathbf{1} - zM)} \tag{7.11}$$

where the vector C is:

$$C = \{1, -ag_1 z, a^2 g_2 z(zg_1 - 1), -a^3 z g_3 (zg_1 - 1)(zg_2 - 1), \ldots\} \tag{7.12}$$

while the determinant is:

$$\det(\mathbf{1} - zM) = 1 - af_1 z + a^2 f_2 z(zg_1 - 1) - a^3 f_3 z(zg_1 - 1)(zg_2 - 1) + \ldots. \tag{7.13}$$

The generating function for the case $a_n = a^n$ is thus

$$H(x, 0, z, k) = e^{ik|x|} P(a\, e^{-\lambda|x|}, z)/[P(a, z) + (i\lambda a/k) P_{,1}(a, z)] \tag{7.14}$$

where

$$P(y, z) = 1 - yg_1 z + y^2 g_2 z(zg_1 - 1) - y^3 g_3 z(zg_1 - 1)(zg_2 - 1) + \cdots \tag{7.15}$$

and $P_{,1}$ denotes the derivative with respect to the second argument of P.

Now we can apply the generating function result (7.14) to specific potentials. We conclude that the Green's function (3.14) for the potential:

$$V(x) = -\frac{Z\lambda A\, \mathrm{e}^{-\lambda|x|}}{1 - A\, \mathrm{e}^{-\lambda|x|}} \tag{7.16}$$

is:

$$G^{(V)}(x, 0, E) = \frac{Q(|x|)}{Q'(0)} \tag{7.17}$$

where Q can be expressed in terms of the Gauss hypergeometric function as:

$$Q(y) = \mathrm{e}^{iky}\, {}_2F_1(-s_-, -s_+, 1 - s_- - s_+, A\, \mathrm{e}^{-\lambda y}) \tag{7.18}$$

where

$$s_\pm = \frac{ik}{\lambda}\left(1 \pm \sqrt{1 - \frac{2\lambda Z}{k^2}}\right). \tag{7.19}$$

Further analysis along these lines results in a more general Green's function for the potential (7.16). For $x > 0 > x_0$:

$$G^{(V)}(x, x_0, E) = \frac{Q(x)Q(-x_0)}{Q'(0)Q(0)}. \tag{7.20}$$

Consider the potential obtained as $A \to 1^-$:

$$V(x) = -\frac{Z\lambda\, \mathrm{e}^{-\lambda|x|}}{1 - \mathrm{e}^{-\lambda|x|}} \tag{7.21}$$

where Z denotes, in view of future results, a constant nuclear charge. The bound state energies for odd eigenstates will correspond to the zeros of $Q(0)$ in (7.20) while the even states correspond to the zeros of $Q'(0)$. Using standard relations for the Gauss hypergeometric function, for example:

$${}_2F_1(a, b, c, 1) = \frac{\Gamma(c)\Gamma(c - b - a)}{\Gamma(c - a)\Gamma(c - b)} \tag{7.22}$$

valid for $\mathrm{Re}(c - a - b) > 0$ (Henrici 1977), we find that the odd parity energy values correspond to poles of $\Gamma(1 - s_-)$; namely as values:

$$E = -\frac{1}{2}\left(\frac{Z}{n} - n\frac{\lambda}{2}\right)^2 \tag{7.23}$$

for $n = 1, 2, \ldots$. These odd-parity bound energies E only exist when the expression being squared in (7.23) is positive. What about the even states for the potential (7.21)? These correspond to zeros of Q' and are extremely difficult to analyse. The best estimate we have been able to obtain on the basis of hypergeometric function theory is that the ground state energy for the potential (7.16) behaves in the $A \to 1^-$ limit as:

$$E \sim -2Z^2 \log^2(1 - A) \tag{7.24}$$

which means that for the potential (7.21) the ground state 'falls to the centre' as A approaches 1. *In the Coulomb limit of (7.21), namely* $\lambda \to 0^+$, *we see that the even states above the* missing ground state coalesce with odd states, and the Bohr energies:

$$E = -\frac{1}{2}\frac{Z^2}{n^2} \tag{7.25}$$

remain. This coalescing of states can be understood in terms of degeneracy. Every bound state for the one-dimensional Coulomb problem is two-fold degenerate. This is because the wave function to the left of the origin—at which origin all wave functions must vanish—can have a sign factor ± 1 with respect to the wave function on the right hand side.

The bound state Coulomb wave functions can be derived as follows. The residues of (7.20) for the potential (7.21) at the Bohr poles (7.23) give the bound state wave function $\Psi_n(x)$ proportional to

$${}_2F_1\left(-n, \frac{2Z}{\lambda n}, 1-n+\frac{2Z}{\lambda n}, \mathrm{e}^{-\lambda|x|}\right)\exp\left(-\left(\frac{Z}{n}-\frac{n\lambda}{2}\right)|x|\right). \tag{7.26}$$

Up to a normalization constant this is the exact wave function for (7.21). The expression (7.26) can in turn be expressed in terms of Jacobi polynomials $P^{(-1,2Z/\lambda n)}(2e^{-\lambda|x|}-1)$ to yield, in the limit $\lambda \to 0^+$, Coulomb bound state wave functions for $x > 0$ as:

$$\Psi(x) = \mathrm{e}^{-Zx/n} x L^1_{n-1}\left(2Z\frac{x}{n}\right) \tag{7.27}$$

where L is the associated Legendre polynomial. These observations amount to a solution of the one-dimensional Coulomb problem. It should be pointed out that Coulomb perturbation expansions have been previously analysed by (Goovaerts and Devreese 1972) who developed such expansions in terms of certain density integrals of the propagator.

One more special limit of (7.16) deserves attention. The single exponential cusp potential

$$V(x) = -B\mathrm{e}^{-\lambda|x|} \tag{7.28}$$

can be solved using these methods. One way is to assume the potential (7.16) and take the limit $A \to 0$, with the nuclear charge $Z \sim B/(\lambda A)$. The result from (7.20) is, for $x > 0 > x_0$:

$$G^{(V)}(x, x_0, E) = -\frac{1}{\sqrt{2B}}\frac{J_\nu(\alpha\,\mathrm{e}^{-\beta x})J_\nu(\alpha\,\mathrm{e}^{+\beta x_0})}{J'_\nu(\alpha)J_\nu(\alpha)} \tag{7.29}$$

where $\beta = \lambda/2$, $\alpha = (1/\lambda)\sqrt{(8B)}$, $\nu = -2ik/\lambda$, $k = \sqrt{(2E)}$. The even bound energies correspond to zeros of $J'_\nu(\alpha)$, while odd bound energies correspond to zeros of $J_\nu(\alpha)$. In particular it is straightforward to show that there exists exactly one bound state if and only if B is positive but satisfies

$$\sqrt{8B} \leqslant \lambda z_{01} \tag{7.30}$$

where z_{01} denotes the first positive zero of J_0.

The transmission coefficient from (1.11) can be obtained via standard Bessel function asymptotics as (Abramowitz and Stegun 1965):

$$T(k) = \frac{-ik}{\sqrt{2B}}\left(\frac{2B}{\lambda^2}\right)^{-2ik/\lambda}\frac{1}{\Gamma^2(1+\nu)}\frac{1}{J_\nu((1/\lambda)\sqrt{8B})J'_\nu((1/\lambda)\sqrt{8B})}. \tag{7.31}$$

In summary, these methods show that the generalized exponential cusp (7.1) can be resolved for the particular form (7.21), which leads to the Coulomb case and to the single exponential cusp case.

8. Power potentials

The previous derivations have involved potentials for which perturbation expansions generally converge. One might ask about power potentials, e.g.

$$V(x) = fx^n \tag{8.1}$$

where f is a constant coupling strength. As is well known, the linear ($n = 1$) and quadratic ($n = 2$) cases were solved at the inception of path integral analysis (Feynman and Hibbs 1965). It turns out that the perturbation series developments (3.14) and (3.15) can give meaningful results for the power potentials, though in some cases the perturbation expansions are merely asymptotic. Our analysis begins with the formal representation of the transform (3.16) for the potential in terms of the nth derivative of the delta function:

$$V^{\sim}(k) = f i^n \delta^{(n)}(k). \tag{8.2}$$

With a view to the representation (3.15) we consider what one might call a cascaded integral:

$$I_j^{(n)} = \int_{-\infty}^{\infty} \frac{\mathrm{d}z}{1+z^2} \partial^n \frac{1}{1+z^2} \cdots \partial^n \frac{1}{1+z^2} \tag{8.3}$$

where j occurrences of the derivative operator are understood. Alternatively, with a view to (3.14) we define:

$$E_j^{(n)} = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathrm{e}^{-|b_1|-|b_2-b_1|-\ldots-|b_j|} \prod_{m=1}^{j} b_m^n \,\mathrm{d}b_m \tag{8.4}$$

with the $j = 0$ case defined as $E_0^{(n)} = 1$. For both spatial endpoints vanishing, the formal expansions in terms of these iterated intgrals I, E are, for the space-energy propagator:

$$K^{(V)}(0, t|0, 0) = \frac{1}{\sqrt{2\pi \mathrm{i} t}} \sum_{j=0}^{\infty} \left(\frac{-f t^{1+n/2} \mathrm{i}^{1+3n/2}}{2^{n/2}} \right)^j \frac{1}{\Gamma(\frac{1}{2} + (1+n/2)j)} \frac{I_j^{(n)}}{\sqrt{\pi}} \tag{8.5}$$

and, for the space-energy Green's function:

$$G^{(V)}(0, 0, E) = \sum_{j=0}^{\infty} (-1)^j \left(\frac{\mathrm{i}}{\sqrt{2E}} \right)^{nj+j+1} f^j E_j^{(n)}. \tag{8.6}$$

These expansions are related through the identity:

$$I_j^{(n)} = \frac{\pi}{(2i^n)^j} E_j^{(n)}. \tag{8.7}$$

If both n and j are odd, both sides of this relation vanish.

Consider first the linear potential (8.1) with $n = 1$. It can be shown by means of elementary calculus (Mayer 1992) that

$$\begin{aligned} I_j^{(1)} &= 0 && j \text{ odd} \\ &= \left(-\frac{1}{12}\right)^{j/2} \frac{\sqrt{\pi}}{(j/2)!} \Gamma\left(\frac{3j+1}{2}\right) && j \text{ even}. \end{aligned} \tag{8.8}$$

From this it follows from (8.5) that:

$$K^{(V)}(0,t|0,0) = \frac{1}{\sqrt{2\pi i t}} e^{-if^2t^3/24} \tag{8.9}$$

which is the correct propagator for both spatial endpoints vanishing (Schulman 1981). It is of interest that this linear case involves a generally convergent perturbation expansion, a property unfortunately not enjoyed by potentials of any higher integral power.

For the quadratic potential, take $n = 2$, $f = 1/2$ in (8.1). One may derive a generating function:

$$f^{(2)}(z) = \sum_{j=0}^{\infty} z^j I_j^{(2)} \tag{8.10}$$

through complicated analysis, the result being:

$$f^{(2)}(z) = \frac{\pi}{2z^{1/4}} \frac{\Gamma(\frac{1}{4}(1+1/\sqrt{z}))}{\Gamma(\frac{1}{4}(3+1/\sqrt{z}))} \tag{8.11}$$

and conclude that the Green's function for both spatial endpoints vanishing is:

$$G^{(V)}(0,0,E) = -\frac{1}{2} \frac{\Gamma(\frac{1}{4} - E/2)}{\Gamma(\frac{3}{4} - E/2)} \tag{8.12}$$

which shows poles at $E = 1/2, 5/2, 9/2, \ldots$ corresponding to the even-parity bound states. Along these lines it is possible to obtain the odd-parity energies by deducing that:

$$\left.\frac{\partial^2 G^{(V)}(x, x_{,0} E)}{\partial x \partial x_0}\right|_{x=x_0=0} = -2\frac{\Gamma(\frac{3}{4} - E/2)}{\Gamma(\frac{1}{4} - E/2)}. \tag{8.13}$$

These results are in agreement with the known representation of the one-dimensional harmonic oscillator G in terms of Whittaker functions (Kleinert 1990). It has to be admitted that (8.10) is an asymptotic expansion of (8.11); the series is generally divergent. These analyses give the quadratic potential propagator (8.5) as:

$$K^{(V)}(0,t|0,0) = 1 + \frac{t^2}{12} + \frac{t^4}{160} + \frac{61t^6}{120\,960} + \cdots \tag{8.14}$$

which is in fact an asymptotic expansion for small t of the well known result:

$$K^{(V)}(0,t|0,0) = \sqrt{\frac{t}{\sin t}}. \tag{8.15}$$

The expansion (8.14) does not converge for $t \geqslant \pi$, in fact the expansion fails at the first caustic of (8.15).

Finally, the elusive quartic potential fx^4 turns out to have a propagator expansion, from (8.1) and (8.5) of the form:

$$K^{(V)}(0,t|0,0) = \frac{1}{\sqrt{2\pi i t}} \left(1 + \frac{ift^3}{10} - \frac{23f^2t^6}{840} - \frac{3403if^3t^9}{240\,240} + \ldots\right). \tag{8.16}$$

One would hope that Feynman–Kac limits using (1.6) and (8.16) could resolve the as yet unknown quartic ground state. But judging from the limited convergence radius of (8.14) for the solved oscillator, this program is not a promising one. Nevertheless, it is conceivable that some method such as that of Padé approximants could be applied to the expansion (8.16) to give numerical estimates for the quartic ground state. It is possible, for example, to work out sufficient recursion relations for the cascaded integral (8.3) to obtain hundreds of terms in the expansion (8.16). What (8.16)—being a short-time expansion—tells us is information about the semi-classical picture. It should be possible to develop accordingly a higher-order WKB expansion theory using the short-time series.

9. Open problems

We have addressed the problems of the delta comb, finite well, tunnelling barrier, and—via an exponential cusp formalism—the Coulomb problem. Our results for power potentials appear to yield correct asymptotic expansions but such expansions cannot necessarily be given closed form analytic solutions.

Open problems, then, include the problem of deducing bound state energies from asymptotic expansions such as (8.16). Results on anharmonic oscillators might evolve from appropriate redefinition of the differential operators in (8.3). Another open problem involves reflectionless potentials such as $V(x) = -2\,\mathrm{sech}^2 x$. These potentials can be put in the generalized exponential form (7.1) but the ensuing matrix algebra is difficult; there is currently no clear path integral derivation of the propagator, even though the Green's functions for such potentials are easy to derive independently from the known propagator forms (Gaveau and Schulman 1986, Crandall 1983) by application of the cut discontinuity relation (1.8).

Another problem of note is that of the quantum pendulum, with potential $V(x) = -\cos(x)$. This problem should be solvable via iterated integrals such as (8.3), where one must replace the derivative operators with shift operators. Again, this analysis has not been carried out, but the various methods herein look promising for such periodic potentials.

Yet another promising case is the inverted Gaussian potential $V(x) = -Ae^{-x^2}$. It is a tantalizing fact that the representation (2.12) involves integrals each of which can be expressed in closed form, as appropriate Jacobian determinants, in the large-N limit. Yet the perturbation series remains unsummed.

Finally, though we have applied the combinatorial adjacency matrix relations (3.17), (3.18) for very special potentials, it should be possible to derive more general results. It is apparently possible to obtain differential equations for the space-energy propagator's numerator and denominator for some U matrices not the identity (Mayer 1992). The zeros of the analytic denominator would of course provide the energy poles. This work is still in progress, but we remain optimistic that such a combinatorial matrix approach will lead to exact solutions for more general potentials.

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