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Path Integration via Summation of Perturbation Expansions and Applications to Totally Reflecting Boundaries, and Potential Steps

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The path integral for the propagator is expanded into a perturbation series, which can be exactly summed in the case of δ-function perturbations giving a closed expression for the (energy-dependent) Green function. Making the strength of the δ-function perturbation infinite repulsive produces a totally reflecting boundary, hence giving a path integral solution in half spaces in terms of the corresponding Green function. The example of the Woods-Saxon potential serves by an appropriate limiting procedure to obtain the Green function for the step potential and the finite potential well in the half space, respectively.

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Although the technique of exactly computing Feynman path integrals seems to reach a saturation point as far as generic Lagrangians with smooth long-range potentials are concerned, there are still a whole range of problems which lack a systematic approach. Boundary problems and piece-wise constant potentials belong to these classes of problems. Steps forward to a solution of the latter have been taken by, e.g., Barut and Duru [1], for the former, e.g., by Clark, Menikoff, and Sharp [2] and Carreau, Farhi, and Guttmann [3]. Barut and Duru obtained a formula for the propagator for some piece-wise constant potentials via a canonical transformation to Hamilton-Jacobi coordinates, however, left with one (or more) additional integration(s) over momenta. In Refs. [2,3] boundary conditions could be implemented into the path integral by means of cleverly chosen δ-function perturbations in the Lagrangian generating the corresponding boundary conditions. However, it is often more appropriate to consider the (energy-dependent) Green function $G(E)$ instead of the propagator $K(T)$. For instance, the whole range of problems where a space-time transformation [4–6] must be performed demonstrate the convenient use of the Green function $G(E)$.

In this paper I discuss boundary problems with Dirichlet boundary conditions in path integral problems by explicitly stating closed formulas for the Green functions. As we will see the corresponding formulas can be derived by implementing a δ-function perturbation into the path integral, which leads to an exactly summable perturbation expansion. Making the strength of the δ-function perturbation be infinite repulsive produces an impenetrable boundary; i.e., Dirichlet boundary conditions are generated. It is possible to consider arbitrary one-dimensional potential problems as long as the Green function for the problem without boundaries is known. The specific example of the smooth step and the Woods-Saxon potential then gives by an appropriate limiting procedure the path integral solution for the step potential and finite potential well in the half space, respectively.

The general method for the time-ordered perturbation expansion is quite simple. We assume that we have a potential $W(x)=V(x)+\tilde{V}(x)$ in the path integral and we suppose that W is so complicated that a direct path integration is not possible. However, the path integral corresponding to $V(x)$ is assumed to be known. We expand the path integral containing $\tilde{V}(x)$ in a perturbation expansion about $V(x)$ in the following way. The initial kernel corresponding to V propagates in Δt time unperturbed, then interacts with $\tilde{V}$, propagates again in another Δt time unperturbed, and so on, up to the final state.

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This gives the series expansion [7,8] ($x \in \mathbb{R}$)

$$K(x'',x';T)=\int_{x(t')=x'}^{x(t'')=x''}\mathcal{D}x(t)\exp\left\{\frac{i}{\hbar}\int_{t'}^{t''}\left[\frac{m}{2}\dot{x}^2-V(x)-\tilde{V}(x)\right]dt\right\},$$
$$=K^{(V)}(x'',x';T)+\sum_{n=1}^{\infty}\left[-\frac{i}{\hbar}\right]^n\left[\prod_{j=1}^{n}\int_{t'}^{t_{j+1}}dt_j\int_{-\infty}^{\infty}dx_j\right]$$
$$\times K^{(V)}(x_1,x';t_1-t')\tilde{V}(x_1)K^{(V)}(x_2,x_1;t_2-t_1)\times\tilde{V}(x_{n-1})\times\cdots$$
$$\times K^{(V)}(x_n,x_{n-1};t_n-t_{n-1})\times\tilde{V}(x_n)K^{(V)}(x'',x_n;t''-t_n)\,. \tag{1}$$

I have ordered time as $t'=t_0<t_1<t_2<\cdots<t_{n+1}=t''$ and paid attention to the fact that $K(t_j-t_{j-1})$ is different from zero only if $t_j>t_{j-1}$. We consider now an arbitrary one-dimensional potential $V(x)$ with an additional δ-function perturbation [9] $W(x)=V(x)-\gamma\delta(x-a)$. The path integral for this potential problem reads

$$K^{(\delta)}(x'',x';T)=\int_{x(t')=x'}^{x(t'')=x''}\mathcal{D}x(t)\exp\left\{\frac{i}{\hbar}\int_{t'}^{t''}\left[\frac{m}{2}\dot{x}^2-V(x)+\gamma\delta(x-a)\right]dt\right\}. \tag{2}$$

We have assumed that the path integral (Feynman kernel, respectively) $K^{(V)}$ for the potential V is known, including its Green function,

$$G^{(V)}(x'',x';E)=\frac{i}{\hbar}\int_0^{\infty}dT\,e^{iET/\hbar}K^{(V)}(x'',x';T)\,. \tag{3}$$

Now, introducing the Green function $G^{(\delta)}(E)$ of the perturbed system similarly to (3), it is easy to sum up the emerging geometric power series due to the convolution theorem of the Fourier transformation, and we obtain [10]

$$G^{(\delta)}(x'',x';E)=G^{(V)}(x'',x';E)-\frac{G^{(V)}(x'',a;E)G^{(V)}(a,x';E)}{G^{(V)}(a,a;E)-1/\gamma}, \tag{4}$$

where it is assumed that $G^{(V)}(a,a;E)$ actually exists. The energy levels E_n of the perturbed problem $W(x)$ are therefore determined in a unique way by the denominator of $G^{(\delta)}(E)$. Radial problems, of course, can be discussed in a completely analogous way. It is straightforward to incorporate more than one δ-function perturbation and obtain the Green function for N δ-function perturbations, which can be proven by induction.

In (4) we now consider the limit $\gamma\to-\infty$, which has the effect that an impenetrable wall appears [2] at $x=a$. We set $\lim_{\gamma\to-\infty}G^{(\delta)}(E)\equiv G^{(\mathrm{Wall})}(E)$; i.e., we obtain

$$G^{(\mathrm{Wall})}(x'',x';E)=G^{(V)}(x'',x';E)-\frac{G^{(V)}(x'',a;E)G^{(V)}(a,x';E)}{G^{(V)}(a,a;E)}. \tag{5}$$

Repeating the procedure for the twofold δ-function perturbation Green function, we consider for two δ-function perturbations with strengths $\gamma_{1,2}$ located at $x=a,b$, respectively, the limit $\lim_{\gamma_1,\gamma_2\to-\infty}G^{(\delta_2)}(E)\equiv G^{(\mathrm{Box})}(E)$ and we obtain the Green function for the motion in the box $a<x<b$. By the same method it is possible to consider motion constraint by radial boxes and rings, respectively, with the corresponding radial Green function $G_l^{(V)}(E)$ taken into account.

We consider the "smooth-step" potential. Its path integral solution is given by [11,12] ($b,R,V_0>0$ constants)

$$\frac{i}{\hbar}\int_0^{\infty}dT\,e^{iET/\hbar}\int_{x(t')=x'}^{x(t'')=x''}\mathcal{D}x(t)\exp\left\{\frac{i}{\hbar}\int_{t'}^{t''}\left[\frac{m}{2}\dot{x}^2+\frac{V_0}{1+e^{(x-b)/R}}\right]dt\right\}$$
$$=\frac{2mR}{\hbar^2}\frac{\Gamma(m_1)\Gamma(m_1+1)}{\Gamma(m_1+m_2+1)\Gamma(m_1-m_2+1)}$$
$$\times\left[\frac{1}{2}\left(1-\tanh\frac{x'-b}{2R}\right)\right]^{(m_1-m_2)/2}\left[\frac{1}{2}\left(1+\tanh\frac{x'-b}{2R}\right)\right]^{(m_1+m_2)/2}$$
$$\times\left[\frac{1}{2}\left(1-\tanh\frac{x''-b}{2R}\right)\right]^{(m_1-m_2)/2}\left[\frac{1}{2}\left(1+\tanh\frac{x''-b}{2R}\right)\right]^{(m_1+m_2)/2}$$
$$\times{}_2F_1\left(m_1,m_1+1;m_1-m_2+1;\frac{1}{2}\left(1-\tanh\frac{x_>-b}{2R}\right)\right)$$
$$\times{}_2F_1\left(m_1,m_1+1;m_1+m_2+1;\frac{1}{2}\left(1+\tanh\frac{x_<-b}{2R}\right)\right), \tag{6}$$

with $x_{>,<}$ the larger or smaller of x',x''. Here we denote $m_{1,2}=\sqrt{2m}R(\sqrt{-E-V_0}\pm\sqrt{-E})/\hbar$. With a barrier at

$x=a$, such that we consider motion in the half space $x>a$, we obtain that the Green function of the Woods-Saxon potential is given by (5), and the bound state energy levels are determined by (with $0<|E_n|<V_0$)

$$ {}_2F_1\left(\beta_n-i\lambda_n,\beta_n-i\lambda_n+1;1+2\beta_n;\frac{1}{2}\left(1-\tanh\frac{a-b}{2R}\right)\right)=0. \tag{7}$$

Here we denote $\beta^2=\beta^2(E)=-2mER^2/\hbar^2$, $\lambda^2=\lambda^2(E)=2m(E+V_0)R^2/\hbar^2$, $\beta_n=\beta(E_n)$, and $\lambda_n=\lambda(E_n)$.

In the limit $R\to 0$ the smooth-step potential transforms into the step potential $V^{(\mathrm{PS})}(x)=[\Theta(x-b)-1]V_0$ with step height V_0. We obtain for the Green function $G^{(\mathrm{PS})}(E)(k\to\lambda/R,\chi\to\beta/R)$

$$\begin{aligned} G^{(\mathrm{PS})}(x'',x';E)=&\Theta(b-x')\Theta(b-x'')\frac{1}{\hbar}\left(-\frac{m}{2(E+V_0)}\right)^{1/2}e^{-ik(x_<-b)}\left(e^{ik(x_>-b)}-\frac{\chi+ik}{\chi-ik}e^{-ik(x_>-b)}\right)\\ &+\Theta(x'-b)\Theta(x''-b)\frac{1}{\hbar}\left(-\frac{m}{2E}\right)^{1/2}e^{-\chi(x_>-b)}\left(e^{\chi(x_<-b)}+\frac{\chi+ik}{\chi-ik}e^{-\chi(x_<-b)}\right)\\ &+\Theta(x_>-b)\Theta(b-x_<)\frac{1}{\hbar}\frac{\sqrt{2m}}{\sqrt{-E}+\sqrt{-E-V_0}}e^{-ik(x_<-b)}e^{-\chi(x_>-b)} \end{aligned} \tag{8}$$

[alternatively we can write $e^{2i\arctan(k/\chi)}=(\chi+ik)/(\chi-ik)$]. The continuity of the Green function at the location of the step at $x=b$ is easily checked.

Considering now a totally reflecting barrier at $x=a<b$ we obtain for the potential well (PW) in the half space $x>a$ the Green function

$$\begin{aligned} G^{(\mathrm{PW})}(x'',x';E)=&\Theta(b-x')\Theta(b-x'')\frac{1}{\hbar}\left(-\frac{m}{2(E+V_0)}\right)^{1/2}\\ &\times\left\{e^{-ik(x_<-b)}\left(e^{ik(x_>-b)}-\frac{\chi+ik}{\chi-ik}e^{-ik(x_>-b)}\right)-\left(e^{2ik(a-b)}-\frac{\chi+ik}{\chi-ik}\right)^{-1}\right.\\ &\left.\times\left(e^{ik(x''-b)}-\frac{\chi+ik}{\chi-ik}e^{-ik(x''-b)}\right)\left(e^{ik(x'-b)}-\frac{\chi+ik}{\chi-ik}e^{-ik(x'-b)}\right)\right\}\\ &+\Theta(x'-b)\Theta(x''-b)\left\{\frac{1}{\hbar}\left(-\frac{m}{2E}\right)^{1/2}e^{-\chi(x_>-b)}\left(e^{\chi(x_<-b)}+\frac{\chi+ik}{\chi-ik}e^{-\chi(x_<-b)}\right)\right.\\ &\left.-\frac{2}{\hbar}\frac{\sqrt{-2m(E+V_0)}}{(\sqrt{-E}+\sqrt{-E-V_0})^2}\left(e^{2ik(a-b)}-\frac{\chi+ik}{\chi-ik}\right)^{-1}e^{-\chi(x''-b)-\chi(x'-b)}\right\}\\ &+\Theta(x_>-b)\Theta(b-x_<)\frac{1}{\hbar}\frac{\sqrt{2m}}{\sqrt{-E}+\sqrt{-E-V_0}}\\ &\times\left\{e^{-ik(x_<-b)}e^{-\chi(x_>-b)}-\left(e^{2ik(a-b)}-\frac{\chi+ik}{\chi-ik}\right)^{-1}\left(e^{ik(x_<-b)}-\frac{\chi+ik}{\chi-ik}e^{-ik(x_<-b)}\right)e^{-\chi(x_>-b)}\right\}. \end{aligned} \tag{9}$$

Again, the continuity at $x=b$ and the boundary conditions of the Green function are easily checked. The bound state energy levels are determined by the poles of $G^{(\mathrm{PW})}$ yielding to the well-known result [13] $k/\chi=-\tan k(b-a)$.

In this paper I have presented a perturbation expansion approach to path integral problems with Dirichlet boundary conditions. The use of a perturbation expansion was necessary because the construction of the Feynman kernel of a Dirichlet problem by means of the "mirror" principle fails generally because the entire kernel does not have the required reflection symmetry. I obtained closed formulas of the corresponding Green functions for arbitrary systems put into half spaces, boxes, radial boxes, and rings, respectively. Particularly, in the case of radial boxes we can consider the corresponding motion inside a radial box outside a hard sphere. Of course, numerous examples could serve to demonstrate the power of the presented formalism; for example, the linear potential in the half space, the radial harmonic oscillator including a $1/r^2$

term inside a radial box, motion under the influence of an Aharonov-Bohm solenoid outside a hard disk located at the origin, and many more.

As examples of the technique I chose the cases of the smooth-step potential, respectively the Woods-Saxon potential, which gave the path integral solution in terms of the corresponding Green functions for the step potential and the finite potential well in the half space, respectively. These two examples are of considerable importance, because the treatment of piece-wise constant potentials in the path integral have been very rudimentary up to now. Hence, two examples of an entire new class of quantum mechanical problems are added to the list of exactly solvable path integrals [5]. The present treatment also has in contrast to Ref. [1] the advantage of stating explicitly simple quantization conditions for bound state solutions.

What remains is a thorough discussion of, say, Neumann boundary conditions in the path integral along the lines presented here for Dirichlet problems. This topic, however, will be addressed elsewhere.

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