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LETTER TO THE EDITOR

δ'-function perturbations and Neumann boundary conditions by path integration

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Abstract. δ'-function perturbations and Neumann boundary conditions are incorporated into the path integral formalism. The starting point is consideration of the path integral representation for the one-dimensional Dirac particle together with a relativistic point interaction. The non-relativistic limit yields either the usual δ-function or a δ'-function perturbation; making their strengths infinitely repulsive one respectively obtains either Dirichlet or Neumann boundary conditions in the path integral.

Attempts to incorporate Dirichlet and Neumann boundary conditions into the path integral formalism have been described, for example, in Barut and Duru [1], Clark *et al* [2] and Carreau *et al* [3]. Barut and Duru used a canonical transformation to Hamilton–Jacobi coordinates in a phase-space path integral to perform the path integration as explicitly as possible yielding an integral representation of the Feynman kernel; they could also discuss step potentials within their formalism. In [2, 3] general boundary conditions were addressed, but only for the free particle case.

In a previous paper I have discussed how to implement Dirichlet boundary conditions into the path integral [4]. This was achieved by considering a one-dimensional δ-function perturbation in the path integral. This problem can be solved in a straightforward manner by means of a perturbation expansion [5–9] which can be explicitly summed yielding the corresponding (energy-dependent) Green function $G^{(\delta)}(E)$ in terms of the non-perturbed one $G^{(V)}(E)$, where V refers to an arbitrary potential which can be included [9]. Making the strength of the δ-function infinitely repulsive yields Dirichlet boundary conditions at the location of the δ-function perturbation [10, 11]. It is also desirable to have an analogous representation for a δ'-function perturbation. Making in this case the strength of the coupling infinitely repulsive produces Neumann boundary conditions at the location of the δ'-function. However, the problem becomes awkward if one tries to use reasoning similar to that for the usual δ, for a δ'-function perturbation in the path integral. An expansion into a perturbation expansion yields interrelated complicated terms with no obvious resolution of the summation problem. Alternatively, an approximation of the δ'-function in terms of two normal δ-functions with distance $\epsilon \ll 1$ and performing the limit $\epsilon \to 0$ does not make sense in an obvious way. Bearing this in mind and the fact that the existing literature concerning δ'-function perturbations and Neumann boundary conditions in the path integral does not look satisfactory, something new is needed and one has to look for an appropriate regularization procedure to fill the gap.

In this letter this problem is addressed by means of the path integral representation of the one-dimensional Dirac particle [5]. The incorporation of a point interaction yields a two-parameter family for the corresponding self-adjoint extension [10, 12]: as particular cases, one can choose, say, either the up (electron) or the down (positron) component for the point interaction to act upon. Considering a perturbation expansion for both problems, it is found that they can be explicitly summed in terms of the corresponding Green functions (which are 2×2 matrices). In the non-relativistic limit the former case yields the usual δ-function perturbation, whereas in the latter we obtain the equivalent of a δ'-function perturbation in the path integral. I will concentrate on the latter case.

In the following I will outline how to implement point interactions in the one-dimensional Dirac particle path integral. We automatically obtain in the case of the δ'-function perturbation a correct regularization prescription in terms of the unperturbed Green function $G^{(V)}(E)$. The general method for the time-ordered perturbation expansion is quite simple. We assume that we have a potential $W(x) = V(x) + \widetilde{V}(x)$ in the path integral and we suppose that W is so complicated that a direct path integration is not possible. However, the path integral $K^{(V)}$ corresponding to $V(x)$ is assumed to be known. We expand the path integral containing $\widetilde{V}(x)$ in a perturbation expansion about $V(x)$ in the following way. The initial kernel corresponding to V propagates in time Δt unperturbed, then it interacts with $\widetilde{V}$, propagates again for another time Δt unperturbed, and so on, up to the final state. This gives the series expansion [5–9] ($x \in \mathbb{R}$)

$$
\begin{aligned}
K(x'', x'; T) = K^{(V)}(x'', x'; T) &+ \sum_{n=1}^{\infty} \left(-\frac{\mathrm{i}}{\hbar}\right)^n \left(\prod_{j=1}^{n} \int_{t'}^{t_{j+1}} \mathrm{d}t_j \int_{-\infty}^{\infty} \mathrm{d}x_j\right) \\
&\times K^{(V)}(x_1, x'; t_1 - t')\widetilde{V}(x_1)K^{(V)}(x_2, x_1; t_2 - t_1) \times \cdots \\
&\times \widetilde{V}(x_{n-1})K^{(V)}(x_n, x_{n-1}; t_n - t_{n-1})\widetilde{V}(x_n)K^{(V)}(x'', x_n; t'' - t_n). \qquad (1)
\end{aligned}
$$

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 the path integral representation for the one-dimensional Dirac particle [5, 13–17] ($p_x = -\mathrm{i}\hbar\partial_x$):

$$
\begin{aligned}
K^{(V)}(x'', x'; T) &= \left\langle x'' \left| \exp\left[-\frac{\mathrm{i}}{\hbar}T(c\sigma_x p_x + mc^2\sigma_z + V(x))\right]\right| x'\right\rangle \\
&= \int_{x(t')=x'}^{x(t'')=x''} \mathcal{D}v(t) \exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t'}^{t''} V(x)\,\mathrm{d}t\right). \qquad (2)
\end{aligned}
$$

V may be a matrix-valued potential. The support property of the measure $\mathcal{D}v$ is defined in such a way that the motion it describes selects paths of N steps each of length $c\epsilon$ ($\epsilon = T/N$ in the lattice representation) that start at x' in the direction α, and end at x'' in the direction β, where α and β take the values 'right' and 'left'. The path integration then is a summation over all reversings of directions [5]. $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices. We introduce the Green function $G^{(V)}(E)$ with its matrix representation

$$
G^{(V)}(x'', x'; E) = \begin{pmatrix} G_{11}^{(V)}(x'', x'; E) & G_{12}^{(V)}(x'', x'; E) \\ G_{21}^{(V)}(x'', x'; E) & G_{22}^{(V)}(x'', x'; E) \end{pmatrix}. \qquad (3)
$$

We first consider a δ-function perturbation in the electron ('+') component, i.e. $V_+ = -\alpha \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \delta(x - a)$. By inserting it into the path integral and summing the perturbation expansion we obtain

$$G^{(\delta_+)}(x'',x';E) = G^{(V)}(x'',x';E) + \frac{1}{1/\alpha - G_{11}^{(V)}(a,a;E)} \times \begin{pmatrix} G_{11}^{(V)}(a,x';E)G_{11}^{(V)}(x'',a;E) & G_{11}^{(V)}(a,x';E)G_{12}^{(V)}(x'',a;E) \\ G_{21}^{(V)}(a,x';E)G_{11}^{(V)}(x'',a;E) & G_{21}^{(V)}(a,x';E)G_{12}^{(V)}(x'',a;E) \end{pmatrix}. \tag{4}$$

Similarly for the positron ('−') component, i.e. $V_- = (4m^2c^2\beta/\hbar^2)\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\delta(x-a)$ (the constants have been chosen for convenience),

$$G^{(\delta_-)}(x'',x';E) = G^{(V)}(x'',x';E) - \frac{1}{\hbar^2/4m^2c^2\beta + G_{22}^{(V)}(a,a;E)} \times \begin{pmatrix} G_{12}^{(V)}(a,x';E)G_{21}^{(V)}(x'',a;E) & G_{12}^{(V)}(a,x';E)G_{22}^{(V)}(x'',a;E) \\ G_{22}^{(V)}(a,x';E)G_{21}^{(V)}(x'',a;E) & G_{22}^{(V)}(a,x';E)G_{22}^{(V)}(x'',a;E) \end{pmatrix}. \tag{5}$$

Let us assume for simplicity that the component $G_{11}^{(V)}(E)$ in (3) is known and V is a scalar, we can then derive

$$G_{12}^{(V)}(x,y;E) = \frac{c}{mc^2+V+E} p_x G_{11}^{(V)}(x,y;E) \tag{6}$$

$$G_{22}^{(V)}(x,y;E) = \frac{-1}{mc^2+V+E}\left(\frac{c^2}{mc^2+V+E} p_x p_y G_{11}^{(V)}(x,y;E) + \delta(x-y)\right). \tag{7}$$

From these representations it is easily seen that if $G_{11}^{(V)}(E)$ is of O(1) for $c \to \infty$, $G_{12}^{(V)}(E)$ and $G_{22}^{(V)}(E)$ vanish for $c \to \infty$ as they are $\propto 1/c$ and $\propto 1/c^2$, respectively.

We consider the limit $c \to \infty$ in $G^{(\delta_\pm)}(E)$. On the one hand we know that the path integral representation (2) gives the usual one-dimensional path integral in non-relativistic quantum mechanics [5, 13–17]:

$$\int_{x(t')=x'}^{x(t'')=x''} \mathcal{D}v(t) \exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t'}^{t''} V(x)\,\mathrm{d}t\right) \to \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \int_{x(t')=x'}^{x(t'')=x''} \mathcal{D}x(t) \exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t'}^{t''}\left[\frac{m}{2}\dot{x}^2 - V(x)\right]\mathrm{d}t\right\} \qquad (c \to \infty) \tag{8}$$

where $V(x)$ is the non-relativistic limit of $V(x)$. In the language of stochastic processes, the measure $\mathcal{D}v$ yields in the limit $c \to \infty$ the measure $\mathcal{D}W[x]$ (W being a Wiener process, taken in real time, respectively, Wick rotated) which following [5] is interpreted in the usual way as $\mathcal{D}x \exp((\mathrm{i}/\hbar)\int_{t'}^{t''} \dot{x}^2\,\mathrm{d}t)$, see, e.g., [18]. In the present case we find [10, 12] $V_+(x) \to V_\alpha(x) = -\alpha\delta(x-a)$, and $V_-(x) \to V_\beta(x) = -\beta\delta'(x-a)$, respectively. However, we find that only the (1, 1) component in the Green functions remains finite, all others vanish. Furthermore, we find $G_{11}^{(\delta_+)}(E) \to G^{(\delta)}(E)$ and $G_{11}^{(\delta_-)}(E) \to G^{(\delta')}(E)$, where $G^{(\delta)}(E)$ is the Green function for a potential problem V with the usual δ-function perturbation in non-relativistic quantum mechanics, and $G^{(\delta')}(E)$ is the Green function for a potential problem V together with a δ'-function perturbation, respectively. Putting everything together we obtain for the latter an explicit path integral representation yielding

$$G_V^{(\delta')}(x'',x';E)=\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}T\,\mathrm{e}^{\mathrm{i}ET/\hbar}\int_{x(t')=x'}^{x(t'')=x''}\mathcal{D}x(t)$$
$$\times\exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t'}^{t''}\left[\frac{m}{2}\dot{x}^2-V(x)+\beta\delta'(x-a)\right]\mathrm{d}t\right\} \tag{9}$$
$$=G^{(V)}(x'',x';E)-\frac{G^{(V)}_{,x'}(x'',a;E)G^{(V)}_{,x''}(a,x';E)}{\hat{G}^{(v)}_{,x'x''}(a,a;E)+1/\beta} \tag{10}$$

$$\hat{G}^{(v)}_{,xy}(a,a;E)=[\partial_x\partial_y G^{(V)}(x,y;E)-2m\delta(x-y)/\hbar^2]|_{x=y=a}. \tag{11}$$

The path integral (9) has thus been *derived* in a unique way through the regularization (5) in the limit $c\to\infty$. Note that (11) automatically yields the correct (ultra-violet) regularization of the formal expression '$G^{(V)}_{,xy}(a,a;E)$'. For $V\equiv 0$, i.e. the free particle, we obtain the explicit representation

$$G_0^{(\delta')}(x'',x';E)=\frac{1}{\hbar}\sqrt{-\frac{m}{2E}}\exp\left(-\sqrt{\frac{-2mE}{\hbar}}|x''-x'|\right)$$
$$-\frac{m^2}{\hbar^4}\frac{\exp[-(\sqrt{-2mE}/\hbar)(|x''-a|+|a-x'|)]}{1/\beta-m\sqrt{-2mE}/\hbar^3}\,\mathrm{sign}(x''-a)\,\mathrm{sign}(x'-a). \tag{12}$$

For the propagator we obtain (using [19] p 246)

$$\int_{x(t')=x'}^{x(t'')=x''}\mathcal{D}x(t)\exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t'}^{t''}\left[\frac{m}{2}\dot{x}^2+\beta\delta'(x-a)\right]\mathrm{d}t\right\}$$
$$=\sqrt{\frac{m}{2\pi\mathrm{i}\hbar T}}\exp\left(\frac{\mathrm{i}m}{2\hbar T}|x''-x'|^2\right)$$
$$+\sqrt{\frac{m}{2\pi\mathrm{i}\hbar T}}\exp\left[\frac{\mathrm{i}m}{2\hbar T}(|x''-a|+|x'-a|)^2\right]\times\mathrm{sign}(x''-a)\,\mathrm{sign}(x'-a)$$
$$+\frac{\hbar^2}{2m\beta}\exp\left[-\frac{\hbar^2}{m\beta}(|x''-a|+|x'-a|)+\frac{\mathrm{i}}{\hbar}\frac{\hbar^6}{2m^3\beta^2}T\right]$$
$$\times\,\mathrm{erfc}\left\{\sqrt{\frac{m}{2\mathrm{i}\hbar T}}\left[(|x''-a|+|x'-a|)-\frac{\mathrm{i}\hbar^3 T}{m^2\beta}\right]\right\}\mathrm{sign}(x''-a)\,\mathrm{sign}(x'-a) \tag{13}$$

$$=\frac{\hbar^2}{m\beta}\exp\left[-\frac{\hbar^2}{m\beta}(|x''-a|+|x'-a|)+\frac{\mathrm{i}}{\hbar}\frac{\hbar^6}{2m^3\beta^2}T\right]\mathrm{sign}(x''-a)\,\mathrm{sign}(x'-a)$$
$$+\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}p\exp\left(-\mathrm{i}\frac{p^2\hbar}{2m}T\right)\left(\sin px'\sin px''+\cos px'\cos px''\right.$$
$$\left.+\frac{\mathrm{i}mp\beta/\hbar^2}{1+\mathrm{i}pm\beta/\hbar^2}\mathrm{e}^{\mathrm{i}p(|x'-a|+|x''-a|)}\,\mathrm{sign}(x''-a)\,\mathrm{sign}(x'-a)\right). \tag{14}$$

For $\beta > 0$, there is one bound state which has energy $E = -\hbar^6/2m^3\beta^2$. The case $\beta = 0$, i.e. the free particle on the real line is easily recovered in equations (12) and (14). This case is also reproduced in (13) by a proper $\beta \to 0$ limiting procedure, which (14) provides.

Repeating the procedure for N-fold δ'-function perturbations similarly gives (compare also [10], $a_i \neq a_j$ $(i \neq j)$)

$$\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}T\,\mathrm{e}^{\mathrm{i}TE/\hbar}\int_{x(t')=x'}^{x(t'')=x''}\mathcal{D}x(t)\exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t'}^{t''}\left[\frac{m}{2}\dot{x}^2 - V(x) + \sum_{j=1}^{N}\beta_j\delta'(x-a_j)\right]\mathrm{d}t\right\}$$
$$= \frac{\begin{vmatrix} G^{(V)}(x'',x';E) & G^{(V)}_{,x'}(x'',a_1;E) & \dots & G^{(V)}_{,x'}(x'',a_N;E) \\ G^{(V)}_{,x''}(a_1,x';E) & \hat{G}^{(v)}_{,x'x''}(a_1,a_1;E)+1/\beta_1 & \dots & G^{(V)}_{,x'x''}(a_1,a_N;E) \\ \vdots & \vdots & \ddots & \vdots \\ G^{(V)}_{,x''}(a_N,x';E) & G^{(V)}_{,x'x''}(a_N,a_1) & \dots & \hat{G}^{(v)}(a_N,a_N;E)+1/\beta_N \end{vmatrix}}{\begin{vmatrix} \hat{G}^{(v)}_{,x'x''}(a_1;a_1;E)+1/\beta_1 & \dots & G^{(V)}_{,x'x''}(a_1,a_N;E) \\ \vdots & \ddots & \vdots \\ G^{(V)}_{,x'x''}(a_N,a_1;E) & \dots & \hat{G}^{(v)}_{,x'x''}(a_N,a_N;E)+1/\beta_N \end{vmatrix}} \qquad (15)$$

Of course, any combination of N-fold δ-function and M-fold δ'-function perturbations is possible yielding a closed expression in terms of the corresponding Green functions.

Now making the coupling of the δ'-function perturbation infinitely repulsive produces Neumann boundary conditions at $x = a$, thus decoupling the regions $(-\infty, a)$ and (a, ∞), i.e.

$$\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}T\,\mathrm{e}^{\mathrm{i}ET/\hbar}\int_{x(t')=x'}^{x(t'')=x''}\mathcal{D}^{(N)}_{x=a}x(t)\exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t'}^{t''}\left[\frac{m}{2}\dot{x}^2 - V(x)\right]\mathrm{d}t\right\}$$
$$= G^{(V)}(x'',x';E) - G^{(V)}_{,x'}(x'',a;E)G^{(V)}_{,x''}(a,x';E)/\hat{G}^{(v)}_{,x'x''}(a,a;E). \qquad (16)$$

The notation $\mathcal{D}^{(N)}_{x=a}$ stands for Neumann boundary conditions at $x = a$, and for the corresponding Green function in shorthand we write $G^{(V,N)}_{x=a}(E)$. Note that $\lim_{\gamma\to-\infty} G^{(\delta)}(E) = G^{(V,D)}_{x=a}(E)$, where D stands for Dirichlet boundary conditions [4, 11]. Of course, any combination of boundary conditions of a particle moving in the box $a < x < b$ is allowed yielding closed expression in terms of the corresponding Green functions.

It is now obvious how to describe potential problems with absolute value dependence, i.e. $V = V(|x|)$. Combining the results for Dirichlet and Neumann boundary conditions we obtain the general formula

$$\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}T\,\mathrm{e}^{\mathrm{i}ET/\hbar}\int_{x(t')=x'}^{x(t'')=x''}\mathcal{D}x(t)\exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t'}^{t''}\left[\frac{m}{2}\dot{x}^2 - V(|x|)\right]\mathrm{d}t\right\}$$
$$= G^{(V)}(x'',x';E) - \tfrac{1}{2}[G^{(V,D)}_{x=0}(x'',x';E) + G^{(V,N)}_{x=0}(x'',x';E)]. \qquad (17)$$

If the potential V already contains only even powers in x, such as the harmonic oscillator, the last two terms in (17) cancel. Simple examples for the general case are, for instance, the double oscillator $V(x) = \frac{1}{2}m\omega^2(|x| - a)^2$, the one-dimensional Coulomb problem

$V(x) = k|x|$, or the symmetric potential well. For the one-dimensional Coulomb problem one obtains, e.g., the quantization condition

$$K_\nu\left(\frac{2}{3}\frac{\sqrt{2mk}}{\hbar}\left(-\frac{E_n}{k}\right)^{3/2}\right) = 0 \tag{18}$$

with $\nu = \frac{1}{3}, \frac{2}{3}$ for the odd and even wavefunctions, respectively

In this letter I have presented a perturbation expansion approach to the problem of δ'-function perturbations and Neumann boundary conditions in the context of path integrals. This was achieved by considering the path integral representation of the one-dimensional Dirac particle with a δ-function perturbation in the electron and positron components, respectively V_+ and V_-. I obtained the closed formulae (4), (5) for both problems in terms of the corresponding energy-dependent Green function. For V_- a δ'-function perturbation emerged in the non-relativistic limit in the path integral (9). Of course, both Green functions represent Krein's formula for the problem in question. This shows in a nice way that in comparison to the Schrödinger equation approach a properly defined (and regularized if necessary) path integral provides a global picture of the problem in question, thus giving comprehensive information about the physical system. However, whereas Krein's formulae are usually derived by means of functional-analytical methods [10], we obtain them by summing perturbation expansions. The necessary ingredients are the path integral formulation of the one-dimensional Dirac particle, including its non-relativistic limit, and knowledge of Green's function for the one-dimensional free Dirac particle. No additional assumptions have been made. An analogous discussion for the electron component yields a δ-function perturbation in the path integral and Dirichlet boundary condition, respectively. The formalism can be repeated in an obvious way to incorporate multiple δ- and δ'-function perturbations, and one can consider motion in a box $a < x < b$ with any combination of Dirichlet and Neumann boundary conditions at the walls of the box. Analogously to [11] one can also generalize our method to higher dimensions to derive path integral formulations for δ'-function perturbations, Dirichlet and Neumann boundary conditions along lines and hyperplanes, etc.

I could also derive a general expression for potentials with absolute value dependence by combining the results from Dirichlet and Neumann boundary conditions, cf (17). In general, only the corresponding Green function can be stated.

The definition of the path integral of the δ'-function perturbation and its (energy-dependent) Green function via the path integral representation of the one-dimensional Dirac particle looks at first sight circumstantial. However, specific regularization prescriptions of singular potentials are familiar for path integrals: for instance, the $1/r$ potential requires in a proper path integral representation a regularization through the Kustaanheimo–Stiefel transformation [20], and the $1/r^2$ potential by means of the Besselian functional weight [8, 21]. In the path integral formulation the usual δ-function perturbation is quite a simple object [9] in comparison to the δ'-function perturbation as shown in this letter. It must be regularized by removing an ultraviolet divergence, cf (11). In fact both point interactions describe a particular kind of boundary condition of the wavefunctions in their domains at the location of the interaction. The even more singular two-and three-dimensional point interactions also require a regularization prescription by means of their Green functions [10], i.e. the removal of an ultraviolet divergence.

The outcome of regularization (11) is quite satisfactory, and it shows that the 'sum over paths' in an exact summation of a perturbation expansion offers possibilities for the solution of problems which go beyond the usual 'Gaussian sum over paths'.

The achieved results for a proper approach to δ- and δ'-function perturbations, and Dirichlet and Neumann boundary conditions respectively, in the language of Feynman path integrals properly combined cover a wide range of problems in path integral techniques. What remains is to develop a path integral formalism to incorporate general boundary conditions, where Dirichlet and Neumann boundary conditions are but special cases of multiple boundary conditions on the real line (e.g. combinations of step potentials). These open questions will be the subject of future investigations.

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