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Using symbolic manipulation to evaluate Feynman's path integral for an interaction of the form $\mathbf{F}(t)\cdot\mathbf{r}$

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Obtaining Feynman's path integral, which is a representation for the system's Green's function, is essential for many physical problems. In this paper, a symbolic algebra program is presented to evaluate analytically Feynman's path integral for an interaction of the form $\mathbf{F}(t)\cdot\mathbf{r}$. Such an interaction governs the motion of an electron in the field of one or more lasers as well as in a static electric field. © *1996 American Institute of Physics.* [S0894-1866(96)01801-0]

INTRODUCTION

Feynman's path integral approach to quantum mechanics[1,2] is a beautiful and unique formalism that has been widely applied to many physical and mathematical problems in areas such as quantum field theory,[3] statistics,[4] and stochastic processes.[5] We present here a concise formulation of Feynman's path integral for an interaction of the form $\mathbf{F}(t)\cdot\mathbf{r}$, where $\mathbf{F}(t)$ may be a constant. This formulation comprises two steps. First, we employ the Green's function method of potential scattering theory[6] to obtain the classical path. Second, the path integral is evaluated analytically along the classical path using Mathematica.[7] Using the classical path to evaluate the path integral in this way has been noted as a particularly simple and effective approach.[8] Having an analytical result for the path integral (which is a representation of the system's Green's function) permits one to keep track of the physical significance of each term.

The interaction $\mathbf{F}(t)\cdot\mathbf{r}$ is encountered frequently in physical problems. It arises whenever a particle is driven by a time-dependent force such as, for instance, when a charged particle moves in some combination of time-dependent and time-independent electric fields in the electric dipole approximation. The complexity of this type of path integral depends on the complexity of $\mathbf{F}(t)$. Four special cases are discussed in this paper as examples of the use of this method. For either a constant electric field or a monochromatic laser electric field, the first two special cases, the path integrals are not difficult to obtain. Our results are compared to results obtained by others for these cases. On the other hand, for a charged particle moving in both a static electric field and either a circularly or a linearly polarized laser electric field, the third and fourth special cases, one finds that the Feynman's path integrals comprise tens of terms. These latter cases arise when one investigates the laser photodetachment of negative ions in the presence of a static electric field. Green's functions for these cases have not been presented previously, except in limiting cases, as we discuss below. Even more complicated cases (such as those involving more than one laser field) may be treated with our code.

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I. THEORY

Consider an N-dimensional system with a Lagrangian of the form

$$L(\dot{x}_1,\dot{x}_2,\ldots,\dot{x}_N;x_1,x_2,\ldots,x_N;t)$$
$$=\frac{1}{2}m\dot{\mathbf{x}}^2+\mathbf{F}(t)\cdot\mathbf{x}=\frac{1}{2}m\sum_{i=1}^{N}\dot{x}_i^2+\sum_{i=1}^{N}F_i(t)x_i, \tag{1}$$

where m is the mass of the particle, $\mathbf{x}$ is the N-dimensional generalized coordinate of the particle, and $\mathbf{F}(t)$ is the N-dimensional generalized external force acting on the particle. Feynman's path integral expression for the kernel (Green's function) between point (x_i,τ) and point (x_i',τ') is[2]

$$K(x_i,\tau;x_i',\tau')=\theta(\tau-\tau')\left[\frac{m}{2\pi\hbar i(\tau-\tau')}\right]^{N/2}$$
$$\times\exp\left(\frac{i}{\hbar}I(x_i,\tau;x_i',\tau')\right), \tag{2}$$

where the action is defined by

$$I(x_i,\tau;x_i',\tau')=\int_{\tau'}^{\tau}L(\dot{x}_1,\dot{x}_2,\ldots,\dot{x}_N;x_1,x_2,\ldots,x_N;t)dt, \tag{3}$$

and where the Heaviside function $\theta(\tau-\tau')$ ensures that causality is obeyed.

In order to obtain the kernel in Eq. (2), the action in Eq. (3) needs to be worked out. Our two-step approach for evaluating the action follows.

A. Solving for the classical path

The above physical problem can be described by Newton's equations

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$$m\frac{d^2}{dt^2}x_i(t)=F_i(t),\quad i=1,2,\ldots,N. \tag{4}$$

According to the Green's function method[6] for potential scattering, the solution of Eq. (4) can be written as

$$x_i(t)=x_{i0}(t)+\frac{1}{m}\int_{\tau'}^{\tau}G_0(t,t')F_i(t')dt', \tag{5}$$

where $x_{i0}(t)$ is the solution of the homogeneous equation,

$$\frac{d^2}{dt^2}x_{i0}(t)=0,\quad i=1,2,\ldots,N, \tag{6}$$

where

$$x_i=x_i(\tau),\quad x_i'=x_i(\tau'),\quad i=1,2,\ldots,N, \tag{7}$$

and where $G_0(t,t')$ is the Green's function, which satisfies

$$\frac{\partial^2}{\partial t^2}G_0(t,t')=\delta(t-t'). \tag{8}$$

Solving Eqs. (6), (7), and (8), one gets, respectively,

$$x_{i0}(t)=\frac{x_i'(\tau-t)+x_i(t-\tau')}{\tau-\tau'}, \tag{9}$$

and

$$G_0(t,t')=-\frac{1}{\tau-\tau'}[(\tau-t)(t'-\tau')\theta(t-t') +(\tau-t')(t-\tau')\theta(t'-t)]. \tag{10}$$

Hence, we have the classical path of this particle:

$$x_i(t)=\frac{x_i'(\tau-t)+x_i(t-\tau')}{\tau-\tau'} +\frac{1}{m}\int_{\tau'}^{\tau}G_0(t,t')F_i(t')dt'. \tag{11}$$

B. Obtaining the action

The action for this problem is

$$I(x_i,\tau;x_i',\tau')=\int_{\tau'}^{\tau}L(\dot{x}_1,\dot{x}_2,\ldots,\dot{x}_N;x_1,x_2,\ldots,x_N;t)dt, \tag{12}$$

$$=\sum_{i=0}^{N}\int_{\tau'}^{\tau}\left(\frac{1}{2}m\dot{x}_i(t)+F_i(t)x_i(t)\right)dt. \tag{13}$$

Inserting the classical path defined by Eq. (11) into Eq. (13), integrating by parts, and using Eq. (4), we obtain

$$\begin{aligned}I(x_i,\tau;x_i',\tau')&=\frac{m}{2}\frac{(\mathbf{x}-\mathbf{x}')^2}{\tau-\tau'}+\int_{\tau'}^{\tau}dt\,\mathbf{F}(t)\cdot\left(\mathbf{x}\frac{t-\tau'}{\tau-\tau'}+\mathbf{x}'\frac{\tau-t}{\tau-\tau'}\right)\\&\quad+\frac{1}{2m}\int_{\tau'}^{\tau}dt\int_{\tau'}^{\tau}dt'\,G_0(t,t')\mathbf{F}(t)\cdot\mathbf{F}(t'),\\&=\sum_{i=1}^{N}\left\{\frac{1}{2}m\frac{(x_i-x_i')^2}{\tau-\tau'}\right.\\&\quad+\int_{\tau'}^{\tau}dt\,F_i(t)\left(x_i\frac{t-\tau'}{\tau-\tau'}+x_i'\frac{\tau-t}{\tau-\tau'}\right)\\&\quad\left.+\frac{1}{2m}\int_{\tau'}^{\tau}dt\int_{\tau'}^{\tau}dt'\,F_i(t)G_0(t,t')F_i(t')\right\}.\end{aligned} \tag{14}$$

The double integral in Eq. (14) can be rewritten in the following form once the step functions in $G_0(t,t')$, defined in Eq. (10), are evaluated analytically:

$$\frac{1}{2m}\int_{\tau'}^{\tau}dt\int_{\tau'}^{\tau}dt'\,F_i(t)G_0(t,t')F_i(t') =-\frac{1}{m}\int_{\tau'}^{\tau}dt\int_{\tau'}^{t}dt'\,F_i(t)F_i(t')\frac{(\tau-t)(t'-\tau')}{\tau-\tau'}. \tag{15}$$

We note that the one-dimensional case of Eq. (14), i.e., $N=1$, is well known. For example, it is equal to the $\omega\to 0$ limit of Eq. (3-66) of Ref. 2. It is presented also in Ref. 9, where it is identified as the characteristic functional of the conditional Wiener measure. The integrals in Eq. (14) may in general, however, be difficult and tedious to evaluate, particularly for a complicated $\mathbf{F}(t)$. Therefore we have programed the evaluation of this action in Mathematica code. The result may then be used in Eq. (2) to get the kernel or Green's function for the process. The final Mathematica output for this kernel may have tens or hundreds of terms, which may not be arranged in a transparent order. The best way to use our program is to let Mathematica generate the kernel in terms of C code or Fortran code by using the Mathematica internal function Cform or FortranForm, and to then use it in one's own C or Fortran program for further calculations.

II. SPECIAL CASES

We present four important special cases of an electron interacting with an electric field, where $\mathbf{F}(t)=-|e|\mathbf{E}(t)$. To confirm the validity of our program, we indicate briefly how our results for the first two special cases may be compared with published results elsewhere. Our results for the third and fourth special cases have not been presented elsewhere; we indicate, however, how in some limiting cases they reduce to results of others. The Green's functions we obtain in these cases are being used to calculate laser detachment cross sections for H^- in the presence of static electric fields.[10] In the following inputs and outputs, m is the electron mass, $-e$ is the electron charge, and hbar is Planck's constant divided by 2π. (Note that some authors in the references given below denote the electron charge as

$e=-|e|$.) For each special case we give the input statement and our program's output result. We then discuss the relation of our result to results of others. A brief description of our code, of the meaning of the input and output statements, and our source code are given in the Appendix.

In every case, one needs first to load our program, FeynmanPathIntegral, into Mathematica by entering the following command:

```
In[1]:=<<FeynmanPathIntegral
```

Then one may proceed to evaluate the path integrals for particular cases.

A. Green's function for an electron in a one-dimensional constant electric field ($E=E_S\hat{i}$; $F_S=-eE_S\hat{i}=F_S\hat{i}$)

```
In[2]:=FeynmanPathIntegral[{FS},1]
Out[2]:=Power[E,(I((FS^2(-t+tp)^3)/(24m)+(FS(t-tp)x[1])/2+
(m(x[1]-xp[1])^2)/(2(t-tp))+(FS(t-tp)xp[1])/2))/hbar]
Sqrt[-I m/2/(hbar Pi(t-tp))]
```

This input considers the case of a constant electric field in one dimension. Our result is identical to Eq. (6.40) on p. 38 of Ref. 5. Equation (3.62) on p. 64 of Ref. 2 also treats this case; however, there is a factor (f/m) missing from the third term. (Reference 5 has pointed out this misprint in Ref. 2.)

B. Volkov Green's function for an electron in a monochromatic, linearly polarized electric field [$E=E_L\cos\omega t\,\hat{i}$; $F(t)=-eE_L\cos\omega t\,\hat{i}=F_L\cos\omega t\,\hat{i}$]

```
In[3]:=FeynmanPathIntegral[{FL Cos[w t],0,0},3]
Out[3]:=Power[E,(I(-(FL^2(-4+2t^2w^2-4t tp w^2+2 tp^2 w^2-
2 Cos[2t w]+4 Cos[(t-tp)w]-2 Cos[2 tp w]+
4 Cos[(t+tp)w]-t w Sin[2t w]+tp w Sin[2t w]+
t w Sin[2 tp w]-tp w Sin[2 tp w]))/(8m(t-tp)w^4)+
(FL(Cos[t w]-Cos[tp w]+t w Sin[t w]-tp w Sin[t w])x[1])/
((t-tp)^2w)+(FL(-Cos[t w]+Cos[tp w]-t w Sin[tp w]+tp w
Sin[tp w])xp[1])/((t-tp)w^2)+(m((x[1]-xp[1])^2+(x[2]-xp[2])^2
+(x[3]-xp[3])^2))/(2(t-tp))))/hbar](-I m/2/(hbar Pi(t-tp)))^(3/2)
```

This input considers the case of an electron moving in a monochromatic, linearly polarized electric field.[11] Our result may be compared with the result obtained from Eqs. (2.9)–(2.12) of Becker *et al.*[12] Our result, which is in the length gauge, may also be compared with the velocity gauge result obtained from Eq. (2) of Manakov and Fainshtein.[13] The Green's function operators in these two gauges (denoted by L and V, respectively) are related by[14–16]

$$G_L=TG_VT^{\dagger}, \tag{16}$$

where

$$T\equiv\exp\left(\frac{i}{\hbar}\frac{|e|}{c}\,\mathbf{r}\cdot\mathbf{A}(t)\right), \tag{17}$$

where $\mathbf{A}(t)$ is the vector potential in the velocity gauge, i.e.,

$$\mathbf{E}(t)=-\frac{1}{c}\frac{\partial}{\partial t}\mathbf{A}(t).$$

C. Green's function for an electron in a circularly polarized, monochromatic electric field and a static electric field [$E=E_L\cos\omega t\,\hat{i}+E_L\sin\omega t\,\hat{j}+E_S$; $F(t)=-eE=F_L\cos\omega t\,\hat{i}+F_L\sin\omega t\,\hat{j}+F_S\hat{k}$]

```
In[4]:=FeynmanPathIntegral[{FL Cos[w t],FL Sin[w t],FS},3]
```

This input considers the case of an electron in a circularly polarized, monochromatic electric field and a static electric field. Our length gauge result may be compared once again to the velocity gauge result obtained from the general formula in Eq. (2) of Ref. 13, provided one chooses the integration constant for the z component of the vector potential properly by using $A_z(\tau)=-cE_S(\tau+C)$, where $C=-(t+t')/2$. In the limit that $\mathbf{r}=\mathbf{r}'=\mathbf{0}$, our result may be compared with Eq. (5) of Ref. 13. In the limit that $E_S=0$, our result may be compared with Eqs. (2.9)–(2.12) of Ref. 12.

The output from the above input is fairly complex. Various Mathematica commands such as Expand, Factor, Collect, Trig→True, etc., should be used a few times in order to obtain the following simplified form of output:

```
Power[E,(I/hbar)(-FS^2(t-tp)^3)/(24m)-FL^2(t-tp)/(2mw^2)+

FL^2(1-Cos[w(t-tp)])/(m(t-tp)w^4)+(FL/w)(x[1]-xp[1])

((Cos[t w]-Cos[tp w])/((t-tp)w)+Sin[t w]-Sin[tp w])+

(FL/w)(x[2]-xp[2])((Sin[t w]-Sin[tp w])/((t-tp)w)

-(Cos[t w]-Cos[tp w]))+FS(x[3]-xp[3])(t-tp)/2+

(m((x[1]-xp[1])^2+(x[2]-xp[2])^2+(x[3]-xp[3])^2))/(2(t-tp))]

(-I m/2 / (hbar Pi(t-tp)))^3/2
```

D. Green's function for an electron in a linearly polarized, monochromatic electric field and a static electric field [$E=E_X \cos \omega t\,\hat{i}+E_Y \cos \omega t\,\hat{j}+(E_Z \cos \omega t+E_S)\hat{k}$; $F(t)=-eE=F_X \cos \omega t\,\hat{i}+F_Y \cos \omega t\,\hat{j}+(F_Z \cos \omega t+F_S)\hat{k}$]

```
In[5]:=FeynmanPathIntegral[{FX Cos[w t], FY Cos[w t], FZ Cos[w t] + FS}, 3,
       FortranForm]
```

This input considers the case of an electron in a linearly polarized, monochromatic electric field and a static electric field. The result may be compared to the results of the same references as in Sec. II C above. However, the long Fortran code output is not presented here, but is available, by ftp over the Internet, along with all other codes in this paper. To connect to our ftp service via the World Wide Web, point your browser to ⟨`ftp://www.aip.org/cip/cip_sourcecode`⟩. We emphasize that our Mathematica output might not be in the simplest possible form even after some steps of manipulation. Hence the C or Fortran code converted from the output may possibly involve repetitive numerical computations. Thus, additional efforts might be needed to analyze and simplify the output before it is used. However, as the developer of Mathematica, Stepfen Wolfram, has pointed out, Mathematica shows its advantage when human time is much more expensive than computer (CPU) time. Thus, one needs to balance one's efforts and computing resources carefully in this particular case.

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APPENDIX

A. Description of the program Feynman Path Integral

This program is a Mathematica package, which must be loaded while running the Mathematica software. The package should work with any version of Mathematica above 2.0 on any kind of machine, without modification.

Once the package is loaded in Mathematica, the program is run as a Mathematica package using the following syntax:

FeynmanPathIntegral[*force*, *dimension*, *form*]

force: The external force should be input in the following form: $\{F_1(t),F_2(t),..,F_N(t)\}$, where the $F_i(t)$'s are the components of the force, which are restricted either to be constants or to depend only on time.

dimension: The dimension of the problem, which is N, an integer.

form: The form of the output is optional (and may be omitted along with the comma in front of it). To obtain a specific form of the output, it should be specified by one of the following alternatives: CForm, FortranForm, TeXForm, TextForm, InputForm, OutputForm. C and Fortran are the usual programming languages. TeX is the word processing language. Text gives ascii output. InputForm and OutputForm are the input and output expressions used by Mathematica. If no form is specified, the default for the output is the TextForm.

B. Source code for program Feynman Path Integral

```
BeginPackage["FeynmanPathIntegral`"];
(* This package is written by MinQi Bao, Department of Physics *)
(* and Astronomy, University of Nebraska-Lincoln, Lincoln, NE  *)
(* 68588-0111, USA. Email address: MINQI@PHYSICS1.UNL.EDU.     *)
(* Thank you for using this package, comments are always welcome!*)
FeynmanPathIntegral::usage =
"FeynmanPathIntegral[force, dimension, form] computes Feynman's
Path Integral expression for the kernel K(x,t; xp,tp)
(cf. Eq. (2)) using Eq. (14) to calculate the action.
The action may be obtained for any N-dimensional
generalized external force that is either constant
or depends only on time. The first argument, force,
should be input in the following form: { F1(t), F2(t), ...,
FN(t) }, where the Fi(t)'s are the components of the force.
The second argument, dimension, is N, an integer. The third
argument, form, is optional. It may be omitted along with
the comma in front of it. However, if the output is desired
in a specific format, then the format should be specified
according to one of the following choices: CForm,
FortranForm, TeXForm, TextForm, InputForm, OutputForm."
Begin["Private`"];
FeynmanPathIntegral[force_,dimension_,form_] :=
(* Initiate two N-dimensional coordinates X and X' *)
 ( ndx = Array[x, dimension];  ndxp = Array[xp, dimension];
(* Change the variable t to integration variables in force *)
  t = Global`t ;  u = Global`u ;  v = Global`v ;  tp = Global`tp ;
  forceu = force /. t -> u;  forcev = force /. t -> v;
(* Evaluate the Action action(x,t; xp,tp) *)
  action = (ndx - ndxp) . (ndx - ndxp) m / 2 / (t - tp)                \
           + Integrate[ (forceu . ndx) (u - tp),{u, tp, t} ] / (t - tp)  \
           + Integrate[ (forceu . ndxp) (t - u),{u, tp, t} ] / (t - tp)  \
```

```
            - Integrate[ Integrate[ (forceu . forcev) (t - u) (v - tp),   \
              {v,tp,u}],{u,tp,t}] / m / (t - tp);
(* Evaluate the Kernel kernel(x,t; xp,tp) *)
  kernel = ( (m/(2 Pi hbar I (t-tp)))^(dimension/2) ) Exp[(I/hbar)   \
           action];
(* Change the variables to Global for simpler output. *)
  m = Global`m;  x = Global`x;  xp = Global`xp;  hbar = Global`hbar ;
  form[Sort[Simplify[kernel]]]
 )
(* This is the same function as the above FeynmanPathIntegral *)
(* but without the optional form. *)
FeynmanPathIntegral[force_,dimension_] :=
(* Initiate two N-dimensional coordinates X and X' *)
 ( ndx = Array[x, dimension];  ndxp = Array[xp, dimension];
(* Change the variable t to integration variables in force *)
  t = Global`t;  u = Global`u;  v = Global`v;  tp = Global`tp;
  forceu = force /. t -> u;  forcev = force /. t -> v;
(* Evaluate the Action action(x,t; xp,tp) *)
  action = (ndx - ndxp) . (ndx - ndxp) m / 2 / (t - tp)              \
           + Integrate[ (forceu . ndx) (u - tp),{u, tp, t} ] / (t - tp)  \
           + Integrate[ (forceu . ndxp) (t - u),{u, tp, t} ] / (t - tp)  \
           - Integrate[ Integrate[ (forceu . forcev) (t - u) (v - tp),   \
             {v,tp,u}],{u,tp,t}] / m / (t - tp);
(* Evaluate the Kernel kernel(x,t; xp,tp) *)
  kernel = ( (m/(2 Pi hbar I (t-tp)))^(dimension/2) ) Exp[(I/hbar)   \
           action];
(* Change the variables to Global for simpler output. *)
  m = Global`m;  x = Global`x;  xp = Global`xp;  hbar = Global`hbar;
  Sort[Simplify[kernel]]
 )
End[]; EndPackage[]
```

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