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1994 J. Phys. A: Math. Gen. 27 4645

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A path-integral approach to expectation values in time-dependent problems

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Received 26 October 1993, in final form 11 February 1994

Abstract. Within the framework of Feynman path integration, expectation values of quantum mechanical operators may be exactly obtained for a class of time-dependent problems. Attention is focused on the two-dimensional motion of a charged particle in a perpendicular magnetic field with a time-dependent driving force. A harmonic oscillator potential is included to ensure that the corresponding density matrix is properly defined although some expectation values are defined without it. This potential is at least a mathematical convenience. Some discussion concerning the conditions under which steady states may be attained is also included.

1. Introduction

The introduction of the density matrix provides a convenient formalism for expressing the expectation values of quantum mechanical operators [1, 2]. A statistical state is such that a particle may find itself in any quantum state according to a probability distribution. The density matrix contains all the necessary statistical information in such a way that the expectation value of an operator Q is given by

$$\langle Q(\tau) \rangle = \text{Tr } Q(\tau)\rho(\tau). \quad (1.1)$$

In this equation both Q and the density matrix ρ are shown as explicit functions of time τ . They also depend, of course, on the canonical coordinates r and p . We will work in the Schrödinger representation of quantum mechanics in which these coordinates are independent of time. The expectation values are naturally independent of the choice of representation.

The time development of the density matrix is due to the propagator or time evolution operator U . Specifically

$$\rho(\tau) = U(\tau)\rho(0)U(\tau)^\dagger \quad (1.2)$$

where the propagator is the solution of the Schrödinger equation

$$i\hbar\dot{U}(\tau) = H(\tau)U(\tau). \quad (1.3)$$

The formal solution can be written as

$$U(\tau) = T \exp\left(-\frac{i}{\hbar} \int_0^\tau d\sigma H(\sigma)\right) \quad (1.4)$$

where T is the time ordering operator. The matrix elements of the propagator in the position basis set can be written as Feynman path integrals. In the case that the Hamiltonian is a quadratic form in the canonical coordinates we can write [3, 4]

$$U(r, t; r') = G(t) \exp\left(\frac{i}{\hbar} S(r, t; r')\right). \quad (1.5)$$

The matrix element represents an integration over all paths starting at time zero from r' and ending at time t at r . The path integral depends on the classical action S and the prefactor G which is independent of the end points of the paths.

In this article we are interested in Hamiltonians having the form

$$H(\tau) = H_0 + H_1(\tau) \quad (1.6)$$

where H_1 is non-zero only for positive times and H_0 does not depend on time. Before H_1 is switched on the density matrix may be modelled according to a Boltzmann distribution. We may choose

$$\rho_0 = Z^{-1} U_0(-i\hbar\beta) \quad (1.7)$$

where β is the inverse temperature,

$$Z = \int dr U_0(r, -i\hbar\beta; r) \quad (1.8)$$

and U_0 is the propagator corresponding to H_0 . The essential idea is that, once ρ_0 is determined, the density matrix at a later positive time t is given by

$$\rho(t) = U(t)\rho_0 U(t)^\dagger. \quad (1.9)$$

If the entire Hamiltonian is a quadratic form in the canonical coordinates it is a straightforward exercise to obtain suitable expressions for the propagators U_0 and U . It is then possible to obtain expressions for the expectation values of operators for the time-dependent problem. Concerning our choice of density matrix ρ_0 , it will be noticed that the expectation values of the canonical coordinates are independent of the inverse temperature β .

This type of path-integral approach has been used before to study the problem of polaron mobility [5-7]. The principal quantity of interest was the expectation value of the velocity of a slow electron in a polar crystal, however, this velocity was not explicitly calculated. Also, the details as to how the electron-phonon interaction was turned on were left vague. The polaron was considered to be moving under the influence of applied electromagnetic fields in a steady state. This article will also discuss the conditions under which a steady state may be attained.

The system of interest here is that of a particle of mass m and charge q moving in two dimensions under the influence of a perpendicular constant magnetic field B and a harmonic oscillator potential. For positive times, the particle is also influenced by a driving force F . This force has two components in the plane of motion which are uniform in space but depend arbitrarily on time. This system is described by the Lagrangian

$$L(r, \dot{r}, \tau) = \frac{1}{2}m\dot{r}^2 - \frac{1}{2}m\omega^2 r^2 + \frac{1}{2}m\Omega\dot{r}^\dagger J\tau + F(\tau) \cdot r \quad (1.10)$$

where r is the two-dimensional position vector. The vector potential is given according to the symmetric gauge by

$$A = \frac{1}{2}B(-y, x, 0). \quad (1.11)$$

The 2×2 matrix J [8] is given by

$$J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad (1.12)$$

so that, working in Gaussian electromagnetic units

$$\frac{q}{c} \dot{r} \cdot A = \frac{1}{2} m \Omega \dot{r}^+ J r \quad (1.13)$$

with the cyclotron frequency Ω defined by $\Omega = qB/mc$. For clarity \dot{r} is written as a row vector.

To conclude this introduction a word of caution is necessary. In order to obtain an expression for the density matrix ρ_0 it is essential that the trace in (1.8) be defined. To understand this we can write the matrix elements of the propagator U_0 in terms of the eigenfunctions ψ_λ of the stationary-state Schrödinger equation. If the eigenfunctions can be labelled discretely then [2, 3]

$$U_0(r, -i\hbar\beta; r') = \sum_\lambda \exp(-\beta E_\lambda) \psi_\lambda(r) \psi_\lambda(r')^* \quad (1.14)$$

where E_λ is the eigenvalue corresponding to ψ_λ . The trace of U_0 is given simply by

$$Z = \sum_\lambda \exp(-\beta E_\lambda). \quad (1.15)$$

If however the labels are not discrete

$$U_0(r, -i\hbar\beta; r') = \int d\lambda \exp(-\beta E_\lambda) \psi_\lambda(r) \psi_\lambda(r')^* \quad (1.16)$$

and the eigenfunctions are normalized according to

$$\int dr \psi_\lambda(r) \psi_{\lambda'}(r)^* = \delta(\lambda - \lambda'). \quad (1.17)$$

Clearly the trace of U_0 is not defined in this case. For a charged particle moving in a constant magnetic field the labels are not entirely discrete [9]. These problems are avoided by the inclusion of the harmonic oscillator potential. It will, however, be noticed that the expectation values of the canonical coordinates are defined in the limit of zero ω .

2. The density matrix

The expression for the path integral corresponding to the Lagrangian (1.10) is given by standard techniques [3, 4] and reads

$$U(r, t; r') = \frac{m\Delta}{4\pi i \hbar \sin \frac{1}{2} \Delta t} \exp\left(\frac{i}{\hbar} S(r, t; r')\right) \quad (2.1)$$

with the classical action S given by

$$\begin{aligned}
 S(r, t; r') &= \frac{1}{4}m\Delta \cot \frac{1}{2}\Delta t (r^2 + r'^2) - \frac{1}{2}m\Delta r^+ \frac{\exp(-\frac{1}{2}J\Omega t)}{\sin \frac{1}{2}\Delta t} r' \\
 &+ \frac{1}{\sin \frac{1}{2}\Delta t} \int_0^t d\tau (r^+ \sin \frac{1}{2}\Delta\tau \exp(-\frac{1}{2}J\Omega(t-\tau)) \\
 &+ r'^+ \sin \frac{1}{2}\Delta(t-\tau) \exp(\frac{1}{2}J\Omega\tau))F(\tau) \\
 &- \frac{2}{m\Delta \sin \frac{1}{2}\Delta t} \int_0^t d\tau \int_0^\tau d\sigma \sin \frac{1}{2}\Delta(t-\tau) \sin \frac{1}{2}\Delta\sigma F(\tau)^+ \\
 &\times \exp(-\frac{1}{2}J\Omega(\tau-\sigma))F(\sigma) \tag{2.2}
 \end{aligned}$$

and $\Delta^2 = \Omega^2 + 4\omega^2$. This result is actually valid for any driving force $F(\tau)$, however, in what follows it will be switched on only for positive times.

An expression for the elements of the density matrix ρ_0 can be obtained by consideration of (2.1) for the situation in which there is no driving force. We first observe that

$$U_0(r, t; r') = \frac{m\Delta}{4\pi i\hbar \sin \frac{1}{2}\Delta t} \exp\left(\frac{i}{\hbar} S_0(r, t; r')\right) \tag{2.3}$$

where

$$S_0(r, t; r') = \frac{1}{4}m\Delta \cot \frac{1}{2}\Delta t (r^2 + r'^2) - \frac{1}{2}m\Delta r^+ \frac{\exp(-\frac{1}{2}J\Omega t)}{\sin \frac{1}{2}\Delta t} r'. \tag{2.4}$$

The trace of the propagator $U_0(t)$ is then given by

$$\text{Tr } U_0(t) = \frac{1}{2(\cos \frac{1}{2}\Delta t - \cos \frac{1}{2}\Omega t)} \tag{2.5}$$

and, replacing t with $-i\hbar\beta$, it is found that

$$\begin{aligned}
 \rho_0(r, r') &= \frac{U_0(r, -i\hbar\beta; r')}{\text{Tr } U_0(-i\hbar\beta)} \\
 &= \frac{m\Delta(\cosh \frac{1}{2}\beta\hbar\Delta - \cosh \frac{1}{2}\beta\hbar\Omega)}{2\pi\hbar \sinh \frac{1}{2}\beta\hbar\Delta} \\
 &\times \exp\left(-\frac{m\Delta}{4\hbar} \coth \frac{1}{2}\beta\hbar\Delta (r^2 + r'^2) + \frac{m\Delta}{2\hbar} r^+ \frac{\exp(\frac{1}{2}iJ\beta\hbar\Omega)}{\sinh \frac{1}{2}\beta\hbar\Delta} r'\right). \tag{2.6}
 \end{aligned}$$

The elements of the density matrix $\rho(t)$ are given by

$$\rho(r, t; r') = \int dx \int dx' U(r, t; x) \rho_0(x, x') U(r', t; x')^* \tag{2.7}$$

where we have used the fact that the propagator U is Hermitian. After substitution from (2.1) and (2.2) and performance of tedious but straightforward Gaussian integrations it is found that

$$\rho(r, t; r') = \rho_0(r, r') \exp(C(r, t; r')) \tag{2.8}$$

where

$$\begin{aligned}
 C(r, t; r') &= \frac{i}{\hbar} (r-r')^+ \int_0^t d\tau \cos \frac{1}{2}\Delta(t-\tau) \exp(-\frac{1}{2}J\Omega(t-\tau))F(\tau) \\
 &\quad - \frac{i}{\hbar} \frac{\sinh \frac{1}{2}\beta\hbar\Omega}{\sinh \frac{1}{2}\beta\hbar\Delta} (r-r')^+ JR(t) \\
 &\quad + \frac{1}{\hbar} \left(\coth \frac{1}{2}\beta\hbar\Delta - \frac{\cosh \frac{1}{2}\beta\hbar\Omega}{\sinh \frac{1}{2}\beta\hbar\Delta} \right) \left(r+r' - \frac{2}{m\Delta} R(t) \right) \cdot R(t)
 \end{aligned} \tag{2.9}$$

with

$$R(t) = \int_0^t d\tau \sin \frac{1}{2}\Delta(t-\tau) \exp(-\frac{1}{2}J\Omega(t-\tau))F(\tau). \tag{2.10}$$

The expectation values of the canonical coordinates are given by [2]

$$\langle r \rangle = \int dr r \rho(r, t; r) \tag{2.11}$$

and

$$\langle p \rangle = i\hbar \int dr \int dr' \delta(r-r') \frac{\partial}{\partial r'} \rho(r, t; r'). \tag{2.12}$$

Substitution of the explicit expression for the density matrix then yields

$$\langle r \rangle = \frac{2}{m\Delta} \int_0^t d\tau \sin \frac{1}{2}\Delta(t-\tau) \exp(-\frac{1}{2}J\Omega(t-\tau))F(\tau) \tag{2.13}$$

and

$$\langle p \rangle = \int_0^t d\tau \cos \frac{1}{2}\Delta(t-\tau) \exp(-\frac{1}{2}J\Omega(t-\tau))F(\tau). \tag{2.14}$$

A check on consistency is provided by the equation of motion

$$m\langle \dot{r} \rangle = \langle p \rangle - \frac{1}{2}m\Omega J \langle r \rangle \tag{2.15}$$

which is easily shown to be satisfied.

We may make some observations concerning the results (2.13) and (2.14). First, they are independent of the inverse temperature β . In physical terms this, of course, is not unexpected since the system of interest involves the motion of a single particle. Other expectation values do, however, depend on the inverse temperature. In particular the expectation value of the Hamiltonian can be shown to be given by

$$\langle H \rangle = \frac{1}{2}m\langle \dot{r} \rangle^2 + \frac{1}{2}m\omega^2 \langle r \rangle^2 - F(t) \cdot \langle r \rangle + \frac{\hbar}{2} \frac{\Delta \sinh \frac{1}{2}\beta\hbar\Delta - \Omega \sinh \frac{1}{2}\beta\hbar\Omega}{\cosh \frac{1}{2}\beta\hbar\Delta - \cosh \frac{1}{2}\beta\hbar\Omega}. \tag{2.16}$$

Our second observation is that the expressions for $\langle r \rangle$ and $\langle p \rangle$ are defined in the limit of zero ω in spite of the fact that the density matrix is not. The expressions are

$$\langle r \rangle = \frac{J}{m\Omega} \int_0^t d\tau (\exp(-J\Omega(t-\tau)) - 1)F(\tau) \tag{2.17}$$

and

$$\langle p \rangle = \frac{1}{2} \int_0^t d\tau (\exp(-J\Omega(t-\tau)) + 1) F(\tau). \quad (2.18)$$

In general some expectation values are defined in the limit of zero ω and some, such as $\langle r^2 \rangle$, are not. The expectation value of the Hamiltonian is of course defined.

3. Steady states

A particle is said to be in a steady state if the expectation value of its acceleration is zero. This must be the case of the system under consideration before the driving force is turned on. Without this force, the expectation value $\langle r \rangle$ and all its time derivatives are equal to zero. The question that now arises concerns the conditions under which a steady state may be attained after the force is turned on.

Differentiation twice of (2.13) with respect to t yields

$$m\langle \ddot{r} \rangle = F(t) + \frac{J}{4\Delta} \int_0^t d\tau ((\Delta - \Omega)^2 \exp(\frac{1}{2}J(\Delta - \Omega)(t - \tau)) - (\Delta + \Omega)^2 \exp(-\frac{1}{2}J(\Delta + \Omega)(t - \tau))) F(\tau). \quad (3.1)$$

This result may be simplified by an integration by parts. Since $F(0) = 0$, an alternative expression is

$$m\langle \ddot{r} \rangle = \frac{1}{2\Delta} \int_0^t d\tau ((\Delta - \Omega) \exp(\frac{1}{2}J(\Delta - \Omega)(t - \tau)) + (\Delta + \Omega) \exp(-\frac{1}{2}J(\Delta + \Omega)(t - \tau))) \dot{F}(\tau). \quad (3.2)$$

By equating this result with zero, the following condition for a steady state is obtained:

$$\int_0^t d\tau ((\Delta - \Omega) \exp(\frac{1}{2}J(\Delta - \Omega)(t - \tau)) + (\Delta + \Omega) \exp(-\frac{1}{2}J(\Delta + \Omega)(t - \tau))) \dot{F}(\tau) = 0. \quad (3.3)$$

The simplest way to satisfy this condition is by adiabatic switching [9]. The driving force is modelled according to

$$F(\tau) = \Theta(\tau)(1 - \exp(-\eta\tau))F_0 \quad (3.4)$$

where η is a positive infinitesimal quantity and F_0 is a constant vector which the driving force becomes after a very long time t . This time is chosen so that ηt tends to infinity. Clearly $\dot{F}(\tau)$ is zero and (3.3) is satisfied. The driving force is switched on so slowly that the steady state is undisturbed. In fact the system after an infinite time is the same as the time-independent case where a constant driving force F_0 is present for all times. The density matrix for this situation may be obtained by two methods. First, a constant force may be substituted into the classical action (2.2). Second, the expression (3.4) for the driving force may be substituted into (2.9) with $\eta t \rightarrow \infty$. This is of course consistent with the theorem of Gell-Mann and Low [10].

Of more interest is the case where the driving force is modelled by

$$F(\tau) = (\Theta(\tau - \tau_0) - \Theta(\tau - \tau_1))F_1 \tag{3.5}$$

where $t > \tau_1 > \tau_0 > 0$ and F_1 is a constant vector. In this case the force is switched on at time τ_0 and switched off at a later time τ_1 . The derivative of (3.5) is

$$\dot{F}(\tau) = (\delta(\tau - \tau_0) - \delta(\tau - \tau_1))F_1 \tag{3.6}$$

which leads to the steady-state condition

$$(\Delta - \Omega) \exp(J\Delta(t - \tau_0))(1 - \exp(-\frac{1}{2}J(\Delta - \Omega)(\tau_1 - \tau_0))) + (\Delta + \Omega)(1 - \exp(\frac{1}{2}J(\Delta + \Omega)(\tau_1 - \tau_0))) = 0. \tag{3.7}$$

Since this condition must be independent of t and

$$\exp(Jx) = \cos x + J \sin x \tag{3.8}$$

for any x , a steady state can be attained after the driving force has been switched off only if

$$\tau_1 - \tau_0 = \frac{2\pi n}{\Delta} = \frac{2\pi n'}{\Omega} \tag{3.9}$$

where n and n' are integers. The ratio of Δ and Ω must be a rational number in addition to the first equality holding. If the driving force is switched off at the wrong time the system can never regain a steady state.

The condition (3.3) for a steady state is defined in the limit of zero ω and can be written in the form

$$\int_0^t d\tau \exp(J\Omega\tau)\dot{F}(\tau) = 0. \tag{3.10}$$

Using the expression (3.6) for the force, a steady state is regained only if

$$\tau_1 - \tau_0 = \frac{2\pi n}{\Omega} \tag{3.11}$$

for integer n . If the force is switched on adiabatically, the steady state remains undisturbed and the expectation value of the velocity after a very long time is

$$\langle \dot{r} \rangle = -\frac{J}{m\Omega} F_0 \tag{3.12}$$

which is consistent with the Lorentz force [1, 11] if the force F_0 is replaced by qE_0 where E_0 is a constant electric field.

Without the magnetic field ($\Omega = 0$), the steady-state condition is

$$\int_0^t d\tau \cos \omega(t - \tau)\dot{F}(\tau) = 0. \tag{3.13}$$

Substitution from (3.6) enforces the choice

$$\tau_1 - \tau_0 = \frac{2\pi n}{\omega} \tag{3.14}$$

for integer n . If ω is also zero the only condition to be satisfied is $F(t) = 0$. As long as

the driving force is eventually switched off a steady state is regained although it will be a different steady state from the initial one. For example the expectation value of the momentum will increase to

$$\langle p \rangle = \int_0^t d\tau F(\tau) \quad (3.15)$$

from zero.

4. Concluding remarks

In this article expressions for expectation values have been obtained for a class of time-dependent quantum mechanical problems within the framework of Feynman path integration. The Hamiltonian included a harmonic oscillator potential which causes the entire system to have no translational invariance. Mathematically this local oscillator allows the density matrix and expectation values to be well defined. In many cases the expectation values are defined without the local oscillator, but the density matrix is not.

Some physical problems, such as slow electrons in polar crystals [12] and disordered systems [13], are well suited to the application of path-integral techniques. Many results have been obtained, including the ground-state energy of the polaron [12, 14] and the density of states in disordered systems [4]. The variational methods employed involve the introduction of a non-local trial harmonic oscillator which maintains the translational invariance of the system. It is possible that the addition of a local harmonic oscillator in the formalism may allow problems concerning measurement of particle velocities to be more accessible and better understood.

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