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Path integral evaluation of the Bloch density matrix for an oscillator in a magnetic field

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Abstract. The non-relativistic propagator for a localised oscillator in a magnetic field of arbitrary strength is evaluated analytically by performing the path integral in polar coordinates. The result is then used to obtain the Bloch density matrix for the system as well as the eigenvalues of the Hamiltonian concerned.

1. Introduction

It has been recently shown by March and Tosi (1985) that it is possible to calculate the full canonical or Bloch density matrix for a localised oscillator in a magnetic field of arbitrary strength by solving the Bloch equation subject to a completeness boundary condition. In order to do so, they generalise the assumptions of Sondheimer and Wilson (1951) about the functional form of the density matrix and obtain five first-order differential equations through which the desired result is derived.

We would like to show that this result follows directly from the analytical evaluation in polar coordinates of the corresponding path integral expression for the non-relativistic propagator of the system.

The Schrödinger equation

$$H\Psi(\boldsymbol{r}, t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r}, t) \tag{1}$$

containing H, the Hamiltonian of the system, as a differential operator can be replaced by an integral equation

$$\Psi(\boldsymbol{r}, t) = \int K(\boldsymbol{r}, \boldsymbol{r}_0; t)\Psi(\boldsymbol{r}_0, 0)\,\mathrm{d}\boldsymbol{r}_0 \tag{2}$$

subject to the initial condition $K(\boldsymbol{r}, \boldsymbol{r}_0; 0) = \delta(\boldsymbol{r} - \boldsymbol{r}_0)$. The kernel of equation (2) corresponds to the propagator of the wavefunction Ψ from the point $\boldsymbol{r}_0$ to $\boldsymbol{r}$ in time t.

In Feynman's formulation of quantum mechanics (1948), the propagator is given by the path integral

$$K(\boldsymbol{r}, \boldsymbol{r}_0; t) = \int \exp[\mathrm{i}S(\boldsymbol{r}, \boldsymbol{r}_0; t)/\hbar]\,\mathrm{D}\boldsymbol{x} \tag{3}$$

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where integrations are over all possible paths starting at $\boldsymbol{r}_0=\boldsymbol{x}(0)$ and terminating at $\boldsymbol{r}=\boldsymbol{x}(t)$. The function $S(\boldsymbol{r}, \boldsymbol{r}_0; t)$ in the integrand is the classical action

$$S(\boldsymbol{r}, \boldsymbol{r}_0; t)=\int_0^t L(\dot{\boldsymbol{x}}, \boldsymbol{x})\,\mathrm{d}\tau \tag{4}$$

and $L(\dot{\boldsymbol{x}}, \boldsymbol{x})$ is the Lagrangian of the system in question.

Alternatively, we can also express the propagator of the system in terms of the eigenfunctions Ψ_i and eigenvalues ε_i of the Hamiltonian as

$$K(\boldsymbol{r}, \boldsymbol{r}_0; t)=\sum_i \Psi_i^*(\boldsymbol{r}_0)\Psi_i(\boldsymbol{r})\exp(-\mathrm{i}\varepsilon_i t/\hbar). \tag{5}$$

2. The propagator

The specific Hamiltonian we work with is

$$H=\frac{(\boldsymbol{p}-\frac{1}{2}e\boldsymbol{B}\times\boldsymbol{r})^2}{2m}+\tfrac{1}{2}\kappa r^2 \tag{6}$$

where the magnetic field $\boldsymbol{B}$ is applied along the z axis, and the gauge is chosen such that the vector potential $\boldsymbol{A}$ is given by $\frac{1}{2}c\boldsymbol{B}\times\boldsymbol{r}$.

The corresponding Lagrangian in cylindrical coordinates (r, θ, z) is

$$L=\tfrac{1}{2}m(\dot{r}^2+r^2\dot{\theta}^2+2\omega r^2\dot{\theta})-\tfrac{1}{2}\kappa r^2+(\tfrac{1}{2}m\dot{z}^2-\tfrac{1}{2}\kappa z^2) \tag{7}$$

where $\omega=eB/2m$ is the Larmor frequency.

Notice that we could have just as well considered the potential $\kappa(x^2+y^2)+\lambda z^2$ since we can separate the motion in the z direction from this Lagrangian; this motion is readily solvable and contributes trivial factors corresponding to a one-dimensional harmonic oscillator which can be easily incorporated into any of the equations, if needed. We will thus omit it in the forthcoming analysis. The remaining Lagrangian is then in polar coordinates (r, θ). Letting

$$\phi=\theta+\omega t \tag{8}$$

be a new angular variable, we have

$$\dot{\theta}=\dot{\phi}-\omega \tag{9a}$$

$$\dot{\theta}^2+2\omega\dot{\theta}=\dot{\phi}^2-\omega^2 \tag{9b}$$

and, therefore, we can write (7) as

$$L=\tfrac{1}{2}m(\dot{r}^2+r^2\dot{\phi}^2-\Omega^2r^2) \tag{10}$$

where

$$\Omega^2=\omega^2+\kappa/m. \tag{11}$$

Equation (10) is the Lagrangian of a two-dimensional harmonic oscillator in coordinates (r, ϕ) with basic frequency Ω. The corresponding propagator has been obtained by performing the path integral in polar coordinates (r, ϕ) by Peak and Inomata (1969), resulting in

$$K(r\phi, r_0\phi_0; t)=\frac{m\Omega}{2\pi\mathrm{i}\hbar\sin\Omega t}\exp\left(\frac{\mathrm{i}m\Omega}{2\hbar\sin\Omega t}[(r^2+r_0^2)\cos\Omega t-2rr_0\cos(\phi-\phi_0)]\right). \tag{12}$$

The Bloch density matrix is obtained by substituting t for $-i\hbar\beta$ in the above equation, thus yielding

$$C(r\phi, r_0\phi_0; \beta) = \frac{m\Omega}{2\pi\hbar \sinh(\beta\hbar\Omega)} \times \exp\left(\frac{-m\Omega}{2\hbar \sinh(\beta\hbar\Omega)}[(r^2+r_0^2)\cosh(\beta\hbar\Omega) - 2rr_0\cos(\phi-\phi_0)]\right). \tag{13}$$

We must go back to our original coordinates. Using (8), we substitute

$$\phi - \phi_0 = (\theta - \theta_0) - i\beta\hbar\omega \tag{14}$$

in (13) and finally obtain

$$C(\boldsymbol{r}\boldsymbol{r}_0\beta) = \frac{m\Omega}{2\pi\hbar \sinh(\beta\hbar\Omega)} \exp\left(\frac{-m\Omega}{2\hbar \sinh(\beta\hbar\Omega)}\{(r^2+r_0^2)\cosh(\beta\hbar\Omega) - 2rr_0[\cos(\theta-\theta_0)\cosh(\beta\hbar\omega) + i\sin(\theta-\theta_0)\sinh(\beta\hbar\omega)]\}\right) \tag{15}$$

which is the desired result. Let us check it, reproducing some special cases.

(a) In the limit $\Omega \to 0$ and $\omega \to 0$, we should obtain the free particle density matrix:

$$\lim_{\substack{\Omega\to 0\\ \omega\to 0}} C(\boldsymbol{r}\boldsymbol{r}_0\beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right) \exp\left(-\frac{m}{2\hbar^2\beta}(\boldsymbol{r}-\boldsymbol{r}_0)^2\right) \tag{16}$$

which we do.

(b) In the absence of a magnetic field ($B=0$), we should obtain the harmonic oscillator density matrix:

$$\lim_{\omega\to 0} C(\boldsymbol{r}\boldsymbol{r}_0\beta) = \frac{m\Omega}{2\pi\hbar \sinh(\beta\hbar\Omega)} \times \exp\left(\frac{-m\Omega}{2\hbar \sinh(\beta\hbar\Omega)}[(r^2+r_0^2)\cosh(\beta\hbar\Omega) - 2rr_0\cos(\theta-\theta_0)]\right) \tag{17}$$

which is identical to (13), and therefore correct.

(c) In the limit $\kappa \to 0$, $\Omega = \omega$ and we have a particle in a magnetic field:

$$\lim_{\Omega\to\omega} C(\boldsymbol{r}\boldsymbol{r}_0\beta) = \frac{m\omega}{2\pi\hbar \sinh(\beta\hbar\omega)} \exp\left(-\frac{m\omega}{2\hbar}\{(r^2+r_0^2)\coth(\beta\hbar\omega) - 2rr_0[\cos(\theta-\theta_0)\coth(\beta\hbar\omega) + i\sin(\theta-\theta_0)]\}\right) \tag{18}$$

obtaining the result of Sondheimer and Wilson (1951), as we must.

3. The partition function and the energy eigenvalues

We can obtain the partition function as follows:

$$Z(\beta) = \int_0^\infty \int_0^{2\pi} r\, dr\, d\theta\, C(\boldsymbol{r}\boldsymbol{r}\beta). \tag{19}$$

Using (15), we obtain

$$Z(\beta)=\frac{1}{2[\cosh(\beta\hbar\Omega)-\cosh(\beta\hbar\omega)]}. \tag{20}$$

This result was derived by Darwin (1931) using the eigenenergies obtained from the Schrödinger equation to calculate the sum $\Sigma_i \exp(-\beta\varepsilon_i)$.

We now rewrite (20) as follows:

$$Z(\beta)=\frac{1}{4\sinh[\beta\hbar(\Omega+\omega)/2]\sinh[\beta\hbar(\Omega-\omega)/2]} \tag{21}$$

which easily allows series expansions in powers of exponentials:

$$Z(\beta)=\left(\sum_{l=0}^{\infty}\exp[-(l+\tfrac{1}{2})\beta\hbar(\Omega+\omega)]\right)\left(\sum_{n=0}^{\infty}\exp[-(n+\tfrac{1}{2})\beta\hbar(\Omega-\omega)]\right) \tag{22}$$

and from here we can read the energy eigenvalues as

$$\varepsilon(l,n)=\hbar\Omega+(l+n)\hbar\Omega+(l-n)\hbar\omega \tag{23}$$

which correctly reproduces the harmonic oscillator eigenvalues ($\omega\to 0$) as well as those of a charged particle in a magnetic field ($\Omega\to\omega$).

4. Conclusions

The principal result of this paper is equation (15). Besides being an exact result, its main importance lies in the fact that it has been derived by direct evaluation of the propagator path integral in polar coordinates.

The difficulty of the direct approach in cartesian coordinates is underscored by the fact that March and Tosi (1985), as well as Davies (1985) in an essentially equivalent formulation to that of March and Tosi (1985), obtained complete solutions only through alternative approaches to this problem, given that Cheng (1984) and others, although being able to show the existence of an exact result, could not succeed in obtaining simple, complete and explicit expressions for the propagator.

However, this method is amenable only to specific types of problems, being inadequate to obtain the result of Davies (1985) who considers the most general case.

References

Cheng B K 1984 *J. Phys. A: Math. Gen.* **17** 819
Darwin C G 1931 *Proc. Camb. Phil. Soc.* **27** 86
Davies I M 1985 *J. Phys. A: Math. Gen.* **18** 2737
Feynman R P 1948 *Rev. Mod. Phys.* **20** 367
March N H and Tosi M P 1985 *J. Phys. A: Math. Gen.* **18** L643
Peak D and Inomata A 1969 *J. Math. Phys.* **10** 1422
Sondheimer E H and Wilson A H 1951 *Proc. R. Soc.* A **210** 173