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The propagator for a charged particle in a constant magnetic field and with a quadratic potential

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Abstract. We obtain the propagator for a charged particle in the presence of a constant magnetic field and any positive definite quadratic potential. We then calculate the trace and obtain the eigenvalues of the Hamiltonian concerned.

1. Introduction

In recent years there has been an increase in the number of papers devoted to the calculation of exact propagators for quantum mechanical systems. Whilst this is a good thing, there has perhaps been a tendency to follow the direct line of approach too closely. If one wishes to calculate the propagator for a charged particle in the presence of a magnetic field and a quadratic potential, the direct approach leads to history dependent path integrals which are extremely difficult to evaluate [1, 2]. The method of summing over quantal states is also very difficult. An alternative approach is taken in (3) where the memory dependent term is replaced by a time dependent potential which is somewhat simpler to handle. The method of approach adopted herein has been developed from its beginnings in [3]. The propagator is given for a constant magnetic field and any positive definite quadratic potential and from it we obtain the eigenvalues of the quantum mechanical Hamiltonian.

2. The propagator

Let $H(\hbar, \boldsymbol{B})$ be the quantum mechanical Hamiltonian

$$H(\hbar, \boldsymbol{B}) = \tfrac{1}{2}(\mathrm{i}\hbar\nabla_y + \tfrac{1}{2}\boldsymbol{B}\wedge \boldsymbol{y})^2 + \tfrac{1}{2}\boldsymbol{y}^{\mathrm{T}}A^2\boldsymbol{y}$$

where A^2 is a positive definite quadratic form and $\boldsymbol{B}\in\mathbb{R}^3$. Let $H(\boldsymbol{p}, \boldsymbol{q})$ and $L(\dot{\boldsymbol{q}}, \boldsymbol{q})$ be the corresponding classical Hamiltonian and Lagrangian respectively, namely

$$H(\boldsymbol{p}, \boldsymbol{q}) = \tfrac{1}{2}(-\boldsymbol{p} + \tfrac{1}{2}\boldsymbol{B}\wedge \boldsymbol{q})^2 + \tfrac{1}{2}\boldsymbol{q}^{\mathrm{T}}A^2\boldsymbol{q},$$

$$L(\dot{\boldsymbol{q}}, \boldsymbol{q}) = \tfrac{1}{2}\dot{\boldsymbol{q}}^2 + \tfrac{1}{2}\boldsymbol{B}\wedge \boldsymbol{q}\cdot\dot{\boldsymbol{q}} - \tfrac{1}{2}\boldsymbol{q}^{\mathrm{T}}A^2\boldsymbol{q}.$$

We have set $e = m = c = 1$ for the sake of clarity. The classical equation of motion inherent in the above system is

$$-\ddot{\boldsymbol{q}} = \boldsymbol{B}\wedge\dot{\boldsymbol{q}} + A^2\boldsymbol{q}.$$

Letting $\boldsymbol{q}_c$ be a solution of the above with the initial and final conditions $\boldsymbol{q}_c(0)=\boldsymbol{x}$ and $\boldsymbol{q}_c(t)=\boldsymbol{y}$, define $S(\boldsymbol{y},\boldsymbol{x},t)$ by

$$S(\boldsymbol{y},\boldsymbol{x},t)=\int_0^t L(\dot{\boldsymbol{q}}_c(s),\boldsymbol{q}_c(s))\,\mathrm{d}s.$$

If $G(\boldsymbol{y},\boldsymbol{x},t)$ is the propagator of the Schrödinger equation

$$[\mathrm{i}\hbar\,\partial/\partial t-H(\hbar,\boldsymbol{B})]\psi=0$$

then

$$G(\boldsymbol{y},\boldsymbol{x},t)=(2\pi\mathrm{i}\hbar)^{-3/2}|-\partial^2 S(\boldsymbol{y},\boldsymbol{x},t)/\partial y_j\,\partial x_k|^{1/2}\exp[\mathrm{i}S(\boldsymbol{y},\boldsymbol{x},t)/\hbar].$$

This is just the propagator which you would expect to obtain by using a semiclassical method or by formally using a Feynman path integral approach. This in itself is hardly surprising but the specific form for $G(\boldsymbol{y},\boldsymbol{x},t)$ will enable one to compute the trace and spectrum for any $\boldsymbol{B}$ and any positive definite A^2. Once we obtain the form of $G(\boldsymbol{y},\boldsymbol{x},t)$ we will check the following three conditions

(i) $$[\mathrm{i}\hbar\,\partial/\partial t-H(\hbar,\boldsymbol{B})]G(\boldsymbol{y},\boldsymbol{x},t)=0,$$

(ii) $$G(\boldsymbol{y},\boldsymbol{x},t+s)=\int G(\boldsymbol{y},\boldsymbol{z},t)G(\boldsymbol{z},\boldsymbol{x},s)\,\mathrm{d}\boldsymbol{z},$$

(iii) $$\lim_{t\to 0^+}\int G(\boldsymbol{y},\boldsymbol{x},t)f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}=f(\boldsymbol{y}).$$

Define the matrix B by $B\boldsymbol{z}=\boldsymbol{B}\wedge\boldsymbol{z}$ for any $\boldsymbol{z}\in\mathbb{R}^3$. A solution $\boldsymbol{q}_c$ of the classical equations of motion is obtained from the solutions of

$$\dot{\boldsymbol{\xi}}(s)=\begin{bmatrix}0 & I\\ -A^2 & -B\end{bmatrix}\boldsymbol{\xi}(s)$$

where

$$\boldsymbol{\xi}(s)=\begin{bmatrix}\boldsymbol{q}_c(s)\\ \dot{\boldsymbol{q}}_c(s)\end{bmatrix}.$$

$\boldsymbol{\xi}(s)$ is no more than

$$\boldsymbol{\xi}(s)=\exp\left\{s\begin{bmatrix}0 & I\\ -A^2 & -B\end{bmatrix}\right\}\boldsymbol{\xi}(0).$$

Define the 3×3 matrices $E(s)$, $F(s)$, $G(s)$ and $H(s)$ by

$$\begin{bmatrix}\dot{E} & \dot{F}\\ \dot{G} & \dot{H}\end{bmatrix}=\begin{bmatrix}0 & I\\ -A^2 & -B\end{bmatrix}\begin{bmatrix}E & F\\ G & H\end{bmatrix},$$

$$\begin{bmatrix}E(0) & F(0)\\ G(0) & H(0)\end{bmatrix}=\begin{bmatrix}I & 0\\ 0 & I\end{bmatrix}.$$

Thus

$$\boldsymbol{\xi}(s)=\begin{bmatrix}E(s) & F(s)\\ G(s) & H(s)\end{bmatrix}\boldsymbol{\xi}(0).$$

We may simplify the integration of $L(\dot{\boldsymbol{q}}_c, \boldsymbol{q}_c)$ by use of the equation of motion to get

$$S(\boldsymbol{y}, \boldsymbol{x}, t) = \tfrac{1}{2}[\boldsymbol{q}_c(t) \cdot \dot{\boldsymbol{q}}_c(t) - \boldsymbol{q}_c(0) \cdot \dot{\boldsymbol{q}}_c(0)].$$

Making use of $\boldsymbol{\xi}(s)$ we have

$$S(\boldsymbol{y}, \boldsymbol{x}, t) = \tfrac{1}{2}\{\boldsymbol{y}^{\mathrm{T}}H(t)F^{-1}(t)\boldsymbol{y} + \boldsymbol{x}^{\mathrm{T}}F^{-1}(t)E(t)\boldsymbol{x} + \boldsymbol{y}^{\mathrm{T}}(-2F^{-1}(t))^{\mathrm{T}}\boldsymbol{x}\}$$

where $t>0$ is small enough to ensure that $F^{-1}(t)$ exists. For example, if $A^2 = \mathrm{diag}(\lambda^2, \lambda^2, \mu^2)$ and $\boldsymbol{B} = (0, 0, B)$ then $F(t)$ has an eigenvalue proportional to $\sin \mu t$. Clearly $F^{-1}(t)$ is not defined for $t = \pi/\mu$. We have used the equalities

$$F^{\mathrm{T}}(t) = -F(-t)$$

and

$$G(t) - H(t)F^{-1}(t)E(t) = -(F^{-1}(t))^{\mathrm{T}}.$$

The first of these equalities is obtained by showing that $F^{\mathrm{T}}(t)$ and $-F(-t)$ are solutions of a second-order differential equation with the same initial data and the second equality follows from

$$\begin{bmatrix} E(s) & F(s) \\ G(s) & H(s) \end{bmatrix}^{-1} = \exp\left\{-s\begin{bmatrix} 0 & I \\ -A^2 & -B \end{bmatrix}\right\}.$$

The determinant $|-\partial^2 S(\boldsymbol{y}, \boldsymbol{x}, t)/\partial y_j\, \partial x_k|$ is just $|F^{-1}(t)|$.

Condition (i) is satisfied since $S(\boldsymbol{y}, \boldsymbol{x}, t)$ is a solution of the Hamilton–Jacobi equation

$$-\partial S/\partial t = H(\nabla_y S, \boldsymbol{y}),$$

H being the classical Hamiltonian, and since $\dot{F}(s) \equiv H(s)$.

In order to check condition (ii) one has to grind out the integration. This, however, is quite instructive. The term in the exponent of $G(\boldsymbol{y}, \boldsymbol{z}, t)G(\boldsymbol{z}, \boldsymbol{x}, s)$ which only involves $\boldsymbol{z}$ is

$$(\mathrm{i}/2\hbar)\boldsymbol{z}^{\mathrm{T}}(F^{-1}(t)E(t) + H(s)F^{-1}(s))\boldsymbol{z} = (\mathrm{i}/2\hbar)\boldsymbol{z}^{\mathrm{T}}(F^{-1}(t)F(t+s)F^{-1}(s))\boldsymbol{z}$$

and upon integration this leads to the correct amplitude for $G(\boldsymbol{y}, \boldsymbol{x}, t+s)$ assuming that $t+s$ is small enough to ensure that $F^{-1}(t+s)$ exists and that $F^{-1}(t)F(t+s)F^{-1}(s)$ is symmetric. Let $D = F^{-1}(t)F(t+s)F^{-1}(s)$ for convenience. Then

$$\begin{aligned} D^{\mathrm{T}} &= (F^{-1}(t)F(t+s)F^{-1}(s))^{\mathrm{T}} \\ &= F^{-1}(s)^{\mathrm{T}}F(t+s)^{\mathrm{T}}F^{-1}(t)^{\mathrm{T}} \\ &= -F^{-1}(-s)F(-t-s)F^{-1}(-t) \\ &= -F^{-1}(-s)[E(-s)F(-t) + F(-s)H(-t)]F^{-1}(-t) \\ &= -F^{-1}(-s)E(-s) - H(-t)F^{-1}(-t) \\ &= H(s)F^{-1}(s) + F^{-1}(t)E(t) \\ &= D, \end{aligned}$$

proving that D is indeed symmetric. We are left with the exponent

$$\boldsymbol{y}^{\mathrm{T}}H(t)F^{-1}(t)\boldsymbol{y} + \boldsymbol{x}^{\mathrm{T}}F^{-1}(s)E(s)\boldsymbol{x} \\ \qquad -\tfrac{1}{4}\{[\boldsymbol{y}^{\mathrm{T}}(-2F^{-1}(t))^{\mathrm{T}} + \boldsymbol{x}^{\mathrm{T}}(-2F^{-1}(s))]D^{-1/2}\}^2$$

to simplify. Upon expanding this we get

$$y^{\mathrm{T}}[H(t)F^{-1}(t)+F^{-1}(t)^{\mathrm{T}}F(s)F^{-1}(t+s)]y$$
$$+x^{\mathrm{T}}[F^{-1}(s)E(s)+F^{-1}(t+s)F(t)F^{-1}(s)^{\mathrm{T}}]x+y^{\mathrm{T}}(-2F^{-1}(t+s))^{\mathrm{T}}x.$$

The term in both y and x is already in its final form and the other two terms take on their correct forms after some simple algebra involving the F matrices. For example

$$\begin{aligned}
F^{-1}(s)E(s)&+F^{-1}(t+s)F(t)F^{-1}(s)^{\mathrm{T}}\\
&=F^{-1}(t+s)[F(t+s)F^{-1}(s)E(s)+F(t)(G(s)-H(s)F^{-1}(s)E(s))]\\
&=F^{-1}(t+s)[(E(t)F(s)+F(t)H(s))F^{-1}(s)E(s)\\
&\quad+F(t)(G(s)-H(s)F^{-1}(s)E(s))]\\
&=F^{-1}(t+s)[E(t)E(s)+F(t)G(s)]\\
&=F^{-1}(t+s)E(t+s).
\end{aligned}$$

Thus condition (ii) is satisfied.

In order to see that condition (iii) holds first note that $tF^{-1}(t)$ is well behaved as $t\to 0^+$. If one now applies the method of stationary phase to

$$\int G(y,x,t)f(y)\,\mathrm{d}y$$

the limit is easily obtained.

3. The trace and eigenvalues

The trace is

$$\int_{\mathbf{R}^3} G(x,x,t)\,\mathrm{d}x$$

where $G(x,x,t)$ is simply

$$(2\pi\mathrm{i}\hbar)^{-3/2}|F(t)|^{-1/2}\exp\{(\mathrm{i}/2\hbar)[x^{\mathrm{T}}(H(t)F^{-1}(t)+F^{-1}(t)E(t)-2(F^{-1}(t))^{\mathrm{T}})x]\}.$$

We have previously shown that both $H(t)F^{-1}(t)$ and $F^{-1}(t)E(t)$ are symmetric and so we only have to consider the symmetric part of $(F^{-1}(t))^{\mathrm{T}}$. We are left to calculate the determinant of

$$\begin{aligned}
H(t)F^{-1}(t)&+F^{-1}(t)E(t)-F^{-1}(t)-(F^{-1}(t))^{\mathrm{T}}\\
&=G(t)+(H(t)-I)F^{-1}(t)(I-E(t)).
\end{aligned}$$

One may show that

$$|G(t)+(H(t)-I)F^{-1}(t)(I-E(t))|=-|F^{-1}(t)|\begin{vmatrix}E(t)-I & F(t)\\ G(t) & H(t)-I\end{vmatrix}.$$

Thus

$$\int_{\mathbf{R}^3} G(x,x,t)\,\mathrm{d}x=-\mathrm{i}\begin{vmatrix}E(t)-I & F(t)\\ G(t) & H(t)-I\end{vmatrix}^{-1/2}.$$

The eigenvalues of $\left[\begin{smallmatrix} E(t)-I & F(t) \\ G(t) & H(t)-I \end{smallmatrix}\right]$ are simply $(e^{i\alpha_j t}-1)$ where $i\alpha_j$, $j=1,\ldots,6$, are the eigenvalues of $\left[\begin{smallmatrix} 0 & I \\ -A^2 & -B \end{smallmatrix}\right]$. If we choose our coordinate axes to be the eigenvectors of A^2 we may represent A^2 and B by

$$A^2=\begin{bmatrix} a^2 & 0 & 0 \\ 0 & b^2 & 0 \\ 0 & 0 & c^2 \end{bmatrix} \qquad B=\begin{bmatrix} 0 & -B_3 & B_2 \\ B_3 & 0 & -B_1 \\ -B_2 & B_1 & 0 \end{bmatrix}.$$

This enables the eigenvalues $i\alpha_j$ to be written as $\pm i\lambda$ where λ is the positive square root of one of the three real roots of the cubic equation

$$(\lambda^2-a^2)(\lambda^2-b^2)(\lambda^2-c^2)=\lambda^2[\lambda^2|\boldsymbol{B}|^2-(a^2B_1^2+b^2B_2^2+c^2B_3^2)].$$

Let the roots of the above equation be α_1^2, α_2^2 and α_3^2. Then

$$\int_{\mathbb{R}^3} G(x,x,t)\,\mathrm{d}x=-\prod_{j=1}^{3}[(e^{i\alpha_j t}-1)(1-e^{-i\alpha_j t})]^{-1/2}.$$

One may formally expand the above expression in powers of $e^{i\alpha_j t}$ or calculate its Fourier transform to obtain the eigenvalues of $H(\hbar,\boldsymbol{B})$. These are

$$E_{lmn}=\hbar[(l+\tfrac{1}{2})\alpha_1+(m+\tfrac{1}{2})\alpha_2+(n+\tfrac{1}{2})\alpha_3]$$

for l, m, $n\in\mathbb{Z}^+$.

4. Conclusion

The propagator is

$$G(y,x,t)=(2\pi i\hbar)^{-3/2}|F(t)|^{-1/2}$$
$$\times\exp\{(i/2\hbar)[y^{\mathrm{T}}H(t)F^{-1}(t)y+x^{\mathrm{T}}F^{-1}(t)E(t)x-2x^{\mathrm{T}}F^{-1}(t)y]\}$$

where E, F and H are easily calculable. From this we have obtained the trace in terms of t and thus the spectrum. As one usually obtains the propagator for particles in the presence of a magnetic field by calculating history dependent path integrals one will be able to use the propagator above to gain information about such path integrals.

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