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1987 J. Phys. A: Math. Gen. 20 5549

(http://iopscience.iop.org/0305-4470/20/16/029)

J. Phys. A: Math. Gen. 20 (1987) 5549-5554. Printed in the UK

Evaluation of the Bloch density matrix for a charged oscillator in a magnetic field by canonical transformations

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Received 30 March 1987

Abstract. The problem of a charged particle moving in an anisotropic harmonic oscillator potential in the presence of a constant external magnetic field is reduced to that of a particle in an anisotropic oscillator by using canonical transformations. The Bloch density matrix for the original problem is then exactly evaluated by transforming the well known result for the anisotropic oscillator with the aid of the integral kernel corresponding to the canonical transformation under consideration.

1. Introduction

The problem of a charged particle moving in an anisotropic three-dimensional harmonic oscillator potential in the presence of a constant external magnetic field has received much attention in recent years. This may be attributed to the fact that this problem can be considered as a model representing different situations in physics. For example, electrons in an anisotropic metal lattice subjected to an external constant magnetic field can be represented by such a model. Hence, the quantum-mechanical analogue of the problem above is expected to have many applications.

One of the quantities of importance for performing calculations with this model is the full canonical or Bloch density matrix. In the past, calculations of this quantity have been carried out for a free electron in a magnetic field by Sondheimer and Wilson (1951) and for the anisotropic harmonic oscillator by Feynman and Hibbs (1965). Recently, March and Tosi (1985) obtained a closed analytic expression for the Bloch density matrix for an electron in an isotropic harmonic oscillator potential in the presence of a constant external magnetic field of arbitrary strength by extending the method of solving the Bloch equation for the system developed earlier by Sondheimer and Wilson (1951). More recently, the Bloch density matrix for the same problem was obtained directly from the analytical evaluation in polar coordinates of the corresponding path integral expression for the non-relativistic propagator of the system (Manoyan 1986). However as has been noted by Manoyan (1986), the applicability of this method is restricted to the special case of an isotropic harmonic oscillator. Also, we have found that the method of March and Tosi (1985) leads to coupled differential equations which are difficult to solve when extended to the general anisotropic case.

In the present work, it is our intention to present an alternative method for exactly evaluating the Bloch density matrix for the general anisotropic case. This is achieved by exploiting the analogy between the present problem and that of a particle in a cranked harmonic oscillator potential well known in nuclear physics (Glas *et al* 1978, Habeeb 1987a). This allows us to use the method of canonical transformations, as for

0305-4470/87/165549+06$02.50

the cranked harmonic oscillator, to transform the present problem to that of a particle moving in an anisotropic oscillator potential for which the Bloch density matrix is already known (Feynman and Hibbs 1965). The Bloch density matrix for the original problem is then exactly evaluated by transforming the expression for the anisotropic oscillator with the aid of the integral kernel corresponding to the canonical transformation under consideration.

2. The canonical transformation method

The Hamiltonian operator of the system under consideration is

$$\hat{H} = (1/2m)[(\hat{p}_1 + \tfrac{1}{2}m\omega_c x_2)^2 + (\hat{p}_2 - \tfrac{1}{2}m\omega_c x_1)^2 + \hat{p}_3^2] + \tfrac{1}{2}m(\omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2) \tag{1}$$

where $\omega_c = |q|B/mc$ is the cyclotron frequency associated with the particle of charge q and mass m, and we have chosen the symmetric gauge, $\boldsymbol{A} = (-\tfrac{1}{2}Bx_2, \tfrac{1}{2}Bx_1, 0)$, for the vector potential associated with the constant external magnetic field $\boldsymbol{B}$ directed along the 3-axis. It can easily be shown that (1) may salso be written as

$$\hat{H} = (\hat{\boldsymbol{p}}^2/2m) + \tfrac{1}{2}m(\omega_1'^2 x_1^2 + \omega_2'^2 x_2^2 + \omega_3'^2 x_3^2) - \omega\hat{L}_3 \tag{2}$$

where $\omega_i'^2 = \omega_i^2 + \omega^2$; $(i = 1, 2, 3)$, $\omega = \tfrac{1}{2}\omega_c$ is the Larmor frequency and $\hat{L}_3 = x_1\hat{p}_2 - x_2\hat{p}_1$ is the component of the angular momentum operator along the 3-axis. The Hamiltonian operator (2) is equivalent to that of a particle moving in an anisotropic harmonic oscillator potential with frequencies ω_i'; $(i = 1, 2, 3)$ cranked about the 3-axis with the Larmor frequency ω (Glas *et al* 1978). Hence, the method of canonical transformations as applied for the latter problem (Glas *et al* 1978, Habeeb 1987a) should also be applicable to the present one. Since some of the formulae of Glas *et al* (1978) are also needed in the present work, we briefly review their work in the rest of this section with emphasis on the main results that are needed here.

First we note that (2) can be separated as

$$\hat{H} = \hat{H}_\omega + \hat{H}_3 \tag{3}$$

where

$$\hat{H}_\omega = \tfrac{1}{2}\sum_{i=1,2}[(\hat{p}_i^2/m) + m\omega_i'^2 x_i^2] - \omega\hat{L}_3. \tag{4}$$

It follows that the eigenfunctions of $\hat{H}$ can be factorised in the form

$$\Psi(\boldsymbol{r}) = \psi(x_1, x_2)\phi(x_3) \tag{5}$$

where $\phi(x_3)$ is the well known eigenfunction of the one-dimensional oscillator Hamiltonian $\hat{H}_3$ and $\psi(x_1, x_2)$ is the eigenfunction of $\hat{H}_\omega$ to be determined. Now, we perform the canonical transformation

$$x_i' = Ax_i + B\hat{p}_j' \qquad \hat{p}_i' = \hat{p}_i + Cx_j \qquad i, j = 1, 2;\ j \neq i. \tag{6}$$

Requiring that the transformed operator $\hat{H}_\omega'(x_1', x_2', \hat{p}_1', \hat{p}_2')$ takes the form of the Hamiltonian operator for two uncoupled harmonic oscillators, or

$$\hat{H}_\omega' = \tfrac{1}{2}\sum_{i=1,2}[(\hat{p}_i'^2/m_i) + m_i\Omega_i^2 x_i'^2] \tag{7}$$

and that the transformation (6) is unitary, we obtain three equations for the three unknowns A, B and C whose solution gives (Glas *et al* 1978)

$$A=\tfrac{1}{2}[1+(\omega_2'^2-\omega_1'^2)/S]$$
$$B=2\omega/mS \tag{8}$$
$$C=(m/4\omega)(\omega_2'^2-\omega_1'^2-S)$$

where

$$S=\operatorname{sign}(\omega_2'-\omega_1')[(\omega_2'^2-\omega_1'^2)^2+8\omega^2(\omega_1'^2+\omega_2'^2)]^{1/2}. \tag{9}$$

After some lengthy manipulations, the new oscillator frequencies Ω_1, Ω_2 and masses m_1, m_2 can be shown to be (Glas *et al* 1978)

$$\Omega_1^2=\tfrac{1}{2}(\omega_1'^2+\omega_2'^2)+\omega^2-\tfrac{1}{2}S$$
$$\Omega_2^2=\tfrac{1}{2}(\omega_1'^2+\omega_2'^2)+\omega^2+\tfrac{1}{2}S$$
$$m_1=m\left(\frac{\Omega_1^2-\Omega_2^2}{\Omega_1^2-\omega_2'^2+\omega^2}\right) \tag{10}$$
$$m_2=m\left(\frac{\Omega_2^2-\Omega_1^2}{\Omega_2^2-\omega_1'^2+\omega^2}\right).$$

In deriving (10), the helpful formula

$$(\Omega_i^2-\omega_1'^2+\omega^2)(\Omega_i^2-\omega_2'^2+\omega^2)=4\omega^2\Omega_i^2 \qquad i=1,2 \tag{11}$$

which has also proved to be useful in the present work, has been used. Creation and annihilation operators can be introduced for $\hat{H}'_\omega$ in the usual manner. In terms of these operators the excited states $\psi_{n_1n_2}(x_1, x_2)$ can be constructed and an integral representation for them can also be derived in the form

$$\psi_{n_1n_2}(x_1,x_2)=\int_{-\infty}^{\infty}\mathrm{d}x_1'\int_{-\infty}^{\infty}\mathrm{d}x_2'\langle x_1x_2|x_1'x_2'\rangle\langle x_1'x_2'|n_1n_2\rangle. \tag{12}$$

The functions $\langle x_1'x_2'|n_1n_2\rangle$ are the well known oscillator eigenfunctions of $\hat{H}'_\omega$ in the x_1x_2 representation and the integral kernel in (12) is given by

$$\langle x_1x_2|x_1'x_2'\rangle=(2\pi\hbar|B|)^{-1}\exp[(\mathrm{i}/\hbar B)(-\mathrm{i}Ax_1x_2+x_1x_2'+x_1'x_2-x_1'x_2')]. \tag{13}$$

For more details about these solutions, their properties and recurrence relations the reader is referred to Glas *et al* (1978).

3. Evaluation of the Bloch density matrix

The Bloch density matrix $C(\boldsymbol{r}, \boldsymbol{r}_0; \beta)$ for the problem described by Hamiltonian (1) is defined by

$$C(\boldsymbol{r},\boldsymbol{r}_0;\beta)=\sum_{n_1n_2n_3}\Psi_{n_1n_2n_3}(\boldsymbol{r})\Psi^*_{n_1n_2n_3}(\boldsymbol{r}_0)\exp(-\beta\varepsilon_{n_1n_2n_3}) \tag{14}$$

where the $\Psi_{n_1n_2n_3}$ are the solutions of the Schrödinger equation

$$\hat{H}\Psi_{n_1n_2n_3}=\varepsilon_{n_1n_2n_3}\Psi_{n_1n_2n_3} \tag{15}$$

and the $\varepsilon_{n_1n_2n_3}$ are their corresponding single-particle energies, while $\beta=(k_B T)^{-1}$. Using (3) and (5), (14) can be written as

$$C(\boldsymbol{r},\boldsymbol{r}_0;\beta)=C_1(x_1,x_2,x_{10},x_{20};\beta)C_2(x_3,x_{30};\beta) \tag{16}$$

where

$$C_1(x_1,x_2,x_{10},x_{20};\beta)=\sum_{n_1n_2}\psi_{n_1n_2}(x_1,x_2)\psi^*_{n_1n_2}(x_{10},x_{20})\exp(-\beta\varepsilon_{n_1n_2}) \tag{17}$$

$$C_2(x_3,x_{30};\beta)=\sum_{n_3}\phi_{n_3}(x_3)\phi^*_{n_3}(x_{30})\exp(-\beta\varepsilon_{n_3}) \tag{18}$$

$$\varepsilon_{n_1n_2n_3}=\varepsilon_{n_1n_2}+\varepsilon_{n_3} \tag{19}$$

and the ϕ_{n_3} are one-dimensional harmonic oscillator eigenfunctions with corresponding eigenvalues $\varepsilon_{n_3}=(n_3+\frac{1}{2})\hbar\omega_3$. The expression for $C_2(x_3,x_{30};\beta)$ is the well known Bloch density matrix for a one-dimensional oscillator and does not concern us here. Using (12), (17) can be written as

$$\begin{aligned}C_1(x_1,x_2,x_{10},x_{20};\beta)&\\ &=\int_{-\infty}^{\infty}\mathrm{d}x_1'\int_{-\infty}^{\infty}\mathrm{d}x_2'\int_{-\infty}^{\infty}\mathrm{d}x_{10}'\int_{-\infty}^{\infty}\mathrm{d}x_{20}'\langle x_1x_2|x_1'x_2'\rangle\\ &\quad\times\langle x_{10}x_{20}|x_{10}'x_{20}'\rangle C_1'(x_1',x_2',x_{10}',x_{20}';\beta)\end{aligned} \tag{20}$$

where

$$C_1'(x_1',x_2',x_{10}',x_{20}';\beta)=\sum_{n_1n_2}\langle x_1'x_2'|n_1n_2\rangle\langle n_1n_2|x_{10}'x_{20}'\rangle\exp(-\beta\varepsilon_{n_1n_2}). \tag{21}$$

It is easily seen that, since the brackets in (21) are two-dimensional oscillator eigenfunctions of $\hat{H}_\omega'$ and the $\varepsilon_{n_1n_2}$ are their corresponding eigenvalues, then $C_1'(x_1',x_2',x_{10}',x_{20}';\beta)$ of (21) is the well known Bloch density matrix for a two-dimensional oscillator (Feynman and Hibbs 1965). Using this result, together with (13), in (20) the four-dimensional integral can be reduced to the evaluation of Gaussian integrals, giving

$$\begin{aligned}C_1(x_1,x_2,x_{10},x_{20};\beta)&\\ &=N(\beta)\exp\{(m/2\hbar D(\beta))[\alpha_1(x_1^2+x_{10}^2)+\alpha_2(x_2^2+x_{20}^2)\\ &\quad+\alpha_3x_1x_{10}+\alpha_4x_2x_{20}+\alpha_5(x_2x_{10}-x_1x_{20})+\alpha_6(x_1x_2-x_{10}x_{20})]\}\end{aligned} \tag{22}$$

where the α are functions of β. The expressions for $N(\beta)$, $D(\beta)$ and the α can be greatly simplified after some manipulations in which (11) is used, with the results

$$N(\beta)=(m/2\pi\mathrm{i}\hbar)(1/\omega D^{1/2}(\beta))(\Omega_2^2-\Omega_1^2) \tag{23}$$

$$\begin{aligned}D(\beta)&=2-2\cosh(\hbar\beta\Omega_1)\cosh(\hbar\beta\Omega_2)\\ &\quad-\{[(\omega_1'^2-\omega_2'^2)^2+\omega_c^2(\omega_1'^2+\omega_2'^2)]/\omega_c^2\omega_1'\omega_2'\}\sinh(\hbar\beta\Omega_1)\sinh(\hbar\beta\Omega_2)\end{aligned} \tag{24}$$

$$\begin{aligned}\alpha_1&=[(\Omega_2^2-\Omega_1^2)/\omega_c^2\omega_2'][(\Omega_2\omega_1'-\Omega_1\omega_2')\cosh(\hbar\beta\Omega_2)\sinh(\hbar\beta\Omega_1)\\ &\quad+(\Omega_2\omega_2'-\Omega_1\omega_1')\cosh(\hbar\beta\Omega_1)\sinh(\hbar\beta\Omega_2)]\\ \alpha_2&=[(\Omega_2^2-\Omega_1^2)/\omega_c^2\omega_1'][(\Omega_2\omega_2'-\Omega_1\omega_1')\cosh(\hbar\beta\Omega_2)\sinh(\hbar\beta\Omega_1)\\ &\quad+(\Omega_2\omega_1'-\Omega_1\omega_2')\cosh(\hbar\beta\Omega_1)\sinh(\hbar\beta\Omega_2)]\\ \alpha_3&=[2(\Omega_2^2-\Omega_1^2)/\omega_c^2\omega_2'][(\Omega_1\omega_1'-\Omega_2\omega_2')\sinh(\hbar\beta\Omega_2)\\ &\quad-(\Omega_2\omega_1'-\Omega_1\omega_2')\sinh(\hbar\beta\Omega_1)]\end{aligned}$$

$$\alpha_4 = [2(\Omega_2^2 - \Omega_1^2)/\omega_c^2\omega_1'][(\Omega_1\omega_2' - \Omega_2\omega_1')\sinh(\hbar\beta\Omega_2) - (\Omega_2\omega_2' - \Omega_1\omega_1')\sinh(\hbar\beta\Omega_1)]$$

$$\alpha_5 = [2\mathrm{i}(\Omega_2^2 - \Omega_1^2)/\omega_c][\cosh(\hbar\beta\Omega_1) - \cosh(\hbar\beta\Omega_2)]$$

$$\alpha_6 = [\mathrm{i}(\Omega_2^2 - \Omega_1^2)/\omega_c]\{2 + [(\omega_c^2 + \omega_1'^2 + \omega_2'^2)/\omega_1'\omega_2'] \times \sinh(\hbar\beta\Omega_1)\sinh(\hbar\beta\Omega_2) - 2\cosh(\hbar\beta\Omega_1)\cosh(\hbar\beta\Omega_2)\}. \quad (25)$$

It should also be stated here that the calculation of the four-dimensional integral in (20) can be simplified if some care is given to the order of performing the one-dimensional integrals. One can easily check that in the isotropic case, $\omega_1 = \omega_2$, (22) gives

$$\lim_{\omega_1 \to \omega_2} C_1(x_1, x_2, x_{10}, x_{20}; \beta) = f(\beta)\exp\{-\mathrm{i}(x_2x_{10} - x_1x_{20})\phi(\beta) - [(x_1 - x_{10})^2 + (x_2 - x_{20})^2]g(\beta) - [(x_1 + x_{10})^2 + (x_2 + x_{20})^2]h(\beta)\} \quad (26)$$

where $f(\beta)$, $g(\beta)$, $\phi(\beta)$ and $h(\beta)$ are as defined by March and Tosi (1985).

4. Partition function and energy eigenvalues

The partition function for the problem considered here is defined as

$$Z(\beta) = \mathrm{Tr}[C(\boldsymbol{r}, \boldsymbol{r}_0; \beta)] = \mathrm{Tr}[C_1(x_1, x_2, x_{10}, x_{20}; \beta)]\,\mathrm{Tr}[C_2(x_3, x_{30}; \beta)] = Z_1(\beta)Z_2(\beta) \quad (27)$$

where $Z_2(\beta)$ is the well known partition function for a one-dimensional oscillator and

$$Z_1(\beta) = \mathrm{Tr}[C_1(x_1, x_2, x_{10}, x_{20}; \beta)] = \int_{-\infty}^{\infty} \mathrm{d}x_1 \int_{-\infty}^{\infty} \mathrm{d}x_2\, C_1(x_1, x_2, x_1, x_2; \beta). \quad (28)$$

Using (22) we obtain

$$Z_1(\beta) = [4\sinh(\hbar\beta\Omega_1/2)\sinh(\hbar\beta\Omega_2/2)]^{-1}. \quad (29)$$

In the special isotropic case, $\omega_1 = \omega_2 \equiv \omega_0$, (29) reduces to that of Darwin (1931) (see also Manoyan 1986). It is also possible to write (29) in the form

$$Z_1(\beta) = \sum_{n_1} \exp[-(n_1 + \tfrac{1}{2})\hbar\beta\Omega_1] \sum_{n_2} \exp[-(n_2 + \tfrac{1}{2})\hbar\beta\Omega_2] \quad (30)$$

from which the energy eigenvalues can be obtained as

$$\varepsilon_{n_1n_2} = \hbar[(n_1 + \tfrac{1}{2})\Omega_1 + (n_2 + \tfrac{1}{2})\Omega_2]. \quad (31)$$

This result is in agreement with that obtained from the solution of the eigenvalue problem for $\hat{H}'_\omega$ of (7) (see also Glas *et al* 1978). In the special isotropic case, $\omega_1 = \omega_2 \equiv \omega_0$, (31) gives

$$\lim_{\omega_1 \to \omega_2} \varepsilon_{n_1n_2} = \hbar[(n_1 + n_2 + 1)\Omega + (n_1 - n_2)\omega] \quad (32)$$

where $\Omega^2 = \omega_0^2 + \omega^2$, which agrees with the result of Manoyan (1986) if we identify his l and n with our n_1 and n_2 respectively.

5. Discussion and conclusions

The present work shows how the analogy between a charged oscillator in a constant external magnetic field and the cranked harmonic oscillator well known in nuclear physics (Glas *et al* 1987) could be exploited to exactly evaluate the Bloch density matrix for the former case using canonical transformations. This also tempts us to treat other problems associated with a charged oscillator in a magnetic field using the same analogy. For example, the recent construction of coherent states for the cranked harmonic oscillator (Habeeb 1987a) could also be considered, by this analogy, as a construction of coherent states for the problem of a charged oscillator in a constant external magnetic field. Also, since the Bloch density matrix and the non-relativistic propagator are simply related (Feynman and Hibbs 1965) one may consider the present work as an exact evaluation of the latter quantity for an anisotropic charged oscillator in a constant magnetic field (cf Davies 1985).

Motivated by the success of the method of canonical transformations as applied here, we hope to treat more complicated situations, such as that of a charged oscillator in time-dependent electric and magnetic fields, in a future work (Habeeb 1987b).

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