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COMMENT

The coherent-state method of evaluating the density matrix for an oscillator in a constant magnetic field

Gong Renshan

Department of Physics, Jiangxi University, Nanchang, Jiangxi, People's Republic of China

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Abstract. The coherent-state method is proposed for evaluating the Bloch density matrix for a charged isotropic oscillator placed in a constant magnetic field. The method first reduces the Bloch equation, satisfied by the density matrix $e^{-\beta\hat{H}}$, to a partial differential equation by means of the coherent-state representation, and then calculates the density matrix. A generalised problem in which a uniform electric field coexists is also discussed.

1. Introduction

Recently considerable interest has arisen in the evaluation of the Bloch density matrix $\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle$ for a three-dimensional charged oscillator placed in a constant magnetic field [1-4]. It is true that all of these treatments have their own merits, but it is also undeniable that they rely more or less on involved manipulations. In this comment, therefore, we develop an alternative method which is much simpler both in principle and in practice. In this method we first focus our attention on the Bloch equation, which is satisfied by the density matrix $e^{-\beta\hat{H}}$, in the coherent-state representation and try to reduce it to a partial differential equation. Once the solutions of this equation are obtained, the evaluation of the Bloch density matrix element is a relatively simple matter. Then the Bloch density matrix for a three-dimensional charged isotropic oscillator placed in a constant magnetic field can be calculated. A generalised problem in which a uniform electric field coexists is also discussed.

2. The Bloch equation in the coherent-state representation

The standard coherent-state $|\mu\rangle$ for N degrees of freedom is defined by [5-7]

$$|\mu\rangle = \exp(-\tfrac{1}{2}|\mu|^2)\sum_{[n]}\frac{(\mu a^{\dagger})^{[n]}}{[n]!}|0\rangle$$
$$= \exp(-\tfrac{1}{2}|\mu|^2)\sum_{[n]}\frac{\mu^{[n]}}{\sqrt{[n]!}}|[n]\rangle \qquad (1a)$$

where

$$[n]=(n_1, n_2, \ldots, n_N) \qquad [n]! = n_1!n_2!\ldots n_N! \qquad (1b)$$

$$\mu = (\mu_1, \mu_2, \ldots, \mu_N) \qquad \mu^{[n]} = \mu_1^{n_1}\mu_2^{n_2}\ldots\mu_N^{n_N} \qquad |\mu|^2 = \sum_{j=1}^{N}|\mu_j|^2 \qquad (1c)$$

$$(\mu a^{\dagger})^{[n]} = (\mu_1 a_1^{\dagger})^{n_1}(\mu_2 a_2^{\dagger})^{n_2}\ldots(\mu_N a_N^{\dagger})^{n_N} \qquad (1d)$$

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while the integration measure is

$$\mathrm{d}m(\mu)=\pi^{-N}\prod_{i=1}^{N}\prod_{j=1}^{N}\mathrm{d}\,\mathrm{Re}\,\mu_i\,\mathrm{d}\,\mathrm{Im}\,\mu_j. \tag{2}$$

Thus the scalar product $\langle\lambda|\mu\rangle$ may be written as

$$\langle\lambda|\mu\rangle=\exp(-\tfrac{1}{2}|\lambda|^2-\tfrac{1}{2}|\mu|^2+\bar{\lambda}\mu) \tag{3}$$

where bar stands for conjugate complex and $\langle\lambda|\lambda\rangle=1$. The completeness relation is

$$\int \mathrm{d}m(\mu)|\mu\rangle\langle\mu|=1. \tag{4}$$

Let us consider a system denoted by $\hat{H}(a_j^\dagger, a_j)$ $(j=1,2,\ldots,N)$, which is in the Wick order. The Bloch density matrix $\rho=\mathrm{e}^{-\beta H}$ $(\beta=1/kT)$ satisfies the following Bloch equation:

$$\frac{\partial}{\partial\beta}\hat{\rho}=-\tfrac{1}{2}[\hat{H}\hat{\rho}+\hat{\rho}\hat{H}]. \tag{5}$$

Introducing the distribution function $F(\bar{\lambda},\mu;\beta)$ defined by

$$F(\bar{\lambda},\mu;\beta)=\exp(\tfrac{1}{2}|\lambda|^2+\tfrac{1}{2}|\mu|^2)\langle\lambda|\hat{\rho}|\mu\rangle \tag{6}$$

and with the help of the following formulae

$$\int \mathrm{d}m(z')\exp(-|z'|^2+z\bar{z}')\varphi(\bar{z}')f(z')=\varphi\left(\frac{\mathrm{d}}{\mathrm{d}z}\right)f(z) \tag{7}$$

$$\int \mathrm{d}m(z')\exp(-|z'|^2+\bar{z}z')\varphi(z')f(\bar{z}')=\varphi\left(\frac{\mathrm{d}}{\mathrm{d}\bar{z}}\right)f(\bar{z}) \tag{8}$$

we can obtain

$$\exp(\tfrac{1}{2}|\lambda|^2+|\mu|^2)\int \mathrm{d}m(\nu)\langle\lambda|\hat{H}|\nu\rangle\langle\nu|\hat{\rho}|\mu\rangle=L^*(\bar{\lambda})F(\bar{\lambda},\mu;\beta) \tag{9}$$

$$\exp(\tfrac{1}{2}|\lambda|^2+\tfrac{1}{2}|\mu|^2)\int \mathrm{d}m(\nu)\langle\lambda|\hat{\rho}|\nu\rangle\langle\nu|\hat{H}|\mu\rangle=L(\mu)F(\bar{\lambda},\mu;\beta) \tag{10}$$

where the operators $L^*(\bar{\lambda})$ and $L(\mu)$ are defined by

$$L^*(\bar{\lambda})f(\bar{\lambda})=\hat{H}\left(\bar{\lambda},\frac{\mathrm{d}}{\mathrm{d}\bar{\lambda}'}\right)f(\bar{\lambda}')|_{\bar{\lambda}'=\bar{\lambda}} \tag{11}$$

$$L(\mu)f(\mu)=\hat{H}\left(\frac{\mathrm{d}}{\mathrm{d}\mu'},\mu\right)f(\mu')|_{\mu'=\mu} \tag{12}$$

and the fact that $\hat{H}(a_j^\dagger, a_j)$ is a Hermitian operator leads to

$$\overline{L^*(\bar{\lambda})}=L(\lambda). \tag{13}$$

Thus the Bloch equation (5) can be converted into a partial differential equation

$$\frac{\partial}{\partial\beta}F(\bar{\lambda},\mu;\beta)=-\tfrac{1}{2}[L^*(\bar{\lambda})+L(\mu)]F(\bar{\lambda},\mu;\beta). \tag{14}$$

It is clear from (6) that the 'initial' condition at $\beta = 0$ $(T \to \infty)$ is

$$\lim_{\beta \to 0} F(\bar{\lambda}, \mu; \beta) \equiv F_0(\bar{\lambda}, \mu) = e^{\bar{\lambda}\mu}. \tag{15}$$

Therefore, the formal solution of (14) is given with the help of (15) by

$$F(\bar{\lambda}, \mu; \beta) = \exp\{-\tfrac{1}{2}\beta[L^*(\bar{\lambda}) + L(\mu)]\}F_0(\bar{\lambda}, \mu). \tag{16}$$

If we find a set of orthonormal eigenfunctions of $L(\mu)$ which is denoted by $\{\varphi_l(\mu)\}$

$$L(\mu)\varphi_l(\mu) = \Lambda_l \varphi_l(\mu) \tag{17}$$

$$\sum_l \bar{\varphi}_l(\lambda)\varphi_l(\mu) = F_0(\bar{\lambda}, \mu) = e^{\bar{\lambda}\mu} \tag{18}$$

$$\int dm(\mu)\, e^{-|\mu|^2} \bar{\varphi}_l(\mu)\varphi_k(\mu) = \delta_{lk} \tag{19}$$

where Λ_l, which is the lth eigenvalue of $L(\mu)$, is real by nature and $\varphi_l(\mu)$ is an entire analytical function of respective arguments μ_j, then the distribution function $F(\bar{\lambda}, \mu; \beta)$ can be written as

$$F(\bar{\lambda}, \mu; \beta) = \sum_l e^{-\Lambda_l \beta} \bar{\varphi}_l(\lambda)\varphi_l(\mu). \tag{20}$$

3. Oscillator placed in a constant magnetic field

The Hamiltonian of the system is given (in the natural units $\hbar = c = 1$) by

$$\hat{H} = \frac{1}{2m}(\boldsymbol{p} - e\boldsymbol{A})^2 + \tfrac{1}{2}mf^2\boldsymbol{r}^2 \tag{21}$$

where $f > 0$ is a constant. Assuming that the direction of the magnetic field is parallel to the x_3 axis and the strength is denoted by $\mathscr{H}$, the vector potential may be taken as $\boldsymbol{A} = (-\tfrac{1}{2}\mathscr{H}x_2, \tfrac{1}{2}\mathscr{H}x_1, 0)$. Introducing the oscillator operators

$$a_j = \sqrt{\frac{m\omega_j}{2}}\left(x_j + \frac{i}{m\omega_j}p_j\right) \qquad a_j^\dagger = \sqrt{\frac{m\omega_j}{2}}\left(x_j - \frac{i}{m\omega_j}p_j\right) \qquad (j = 1, 2, 3) \tag{22}$$

where $\omega_j = \sqrt{f^2 + \omega^2} \equiv \omega_0$ $(j = 1, 2)$, $\omega_3 = f$ and $\omega = e\mathscr{H}/2m$, the Hamiltonian (21) may be written as

$$\hat{H} = \sum_{j=1,2,3} a_j^\dagger \omega_j a_j + i\omega(a_1^\dagger a_2 - a_2^\dagger a_1) + \varepsilon_0 \tag{23}$$

where $\varepsilon_0 = \tfrac{1}{2}(\omega_1 + \omega_2 + \omega_3)$. It is clear that the operator $L(\mu)$ in (17) is

$$L(\mu) = \varepsilon_0 + \omega_0\mu_1\frac{\partial}{\partial\mu_1} + \omega_0\mu_2\frac{\partial}{\partial\mu_2} + \omega_3\mu_3\frac{\partial}{\partial\mu_3} + i\omega\mu_2\frac{\partial}{\partial\mu_1} - i\omega\mu_1\frac{\partial}{\partial\mu_2} \tag{24}$$

and in this case, the eigenfunctions and eigenvalues of (17) are

$$\varphi_{lmn}(\mu) = \frac{1}{\sqrt{l!\,m!\,n!}}\left(\frac{\mu_1 + i\mu_2}{\sqrt{2}}\right)^l \left(\frac{\mu_1 - i\mu_2}{\sqrt{2}}\right)^m \mu_3^n \qquad (l, m, n = 0, 1, 2, \ldots) \tag{25}$$

$$\Lambda_{lmn} = \varepsilon_0 + (\omega_0 + \omega)l + (\omega_0 - \omega)m + \omega_3 n \qquad (l, m, n = 0, 1, 2, \ldots). \tag{26}$$

Therefore, the distribution function $F(\bar{\lambda}, \mu; \beta)$ can be directly obtained from (20)

$$F(\bar{\lambda}, \mu; \beta) = e^{-\beta\varepsilon_0} \exp\{\tfrac{1}{2} e^{-\beta(\omega_0+\omega)}(\bar{\lambda}_1 - i\bar{\lambda}_2)(\mu_1 + i\mu_2) + \tfrac{1}{2} e^{-\beta(\omega_0-\omega)}(\bar{\lambda}_1 + i\bar{\lambda}_2)(\mu_1 - i\mu_2) + e^{-\beta\omega_3}\bar{\lambda}_3\mu_3\}. \tag{27}$$

Furthermore, using the explicit expression for the coherent-state in the coordinate representation

$$\langle \boldsymbol{r}|\lambda\rangle = \left(\frac{m}{\pi}\right)^{3/4} (\omega_1\omega_2\omega_3)^{1/4} \times \exp\left\{\sum_j [-\tfrac{1}{2}\xi_j^2 + \sqrt{2}\lambda_j\xi_j - \tfrac{1}{2}\lambda_j^2 - \tfrac{1}{2}\bar{\lambda}_j\lambda_j]\right\} \qquad (\xi_j = \sqrt{m\omega_j}\, x_j) \tag{28}$$

and the integration formula

$$\int dm(z) \exp(a|z|^2 + bz + c\bar{z} + fz^2 + g\bar{z}^2) = \frac{1}{\sqrt{a^2 - 4fg}} \exp\left[\frac{-abc + b^2g + c^2f}{a^2 - 4fg}\right]$$
$$(\mathrm{Re}(a+f+g) < 0,\ \mathrm{Re}(a^2 - 4fg) > 0 \text{ or } \mathrm{Re}(a-f-g) < 0,\ \mathrm{Re}(a^2 - 4fg) > 0) \tag{29}$$

the elements of the density matrix in the coordinate representation may be easily obtained

$$\begin{aligned}\langle \boldsymbol{r}|\hat{\rho}|\boldsymbol{r}'\rangle &= \int dm(\lambda)\, dm(\mu) \langle \boldsymbol{r}|\lambda\rangle\langle\lambda|\hat{\rho}|\mu\rangle\langle\mu|\boldsymbol{r}'\rangle \\ &= \left(\frac{m}{2\pi}\right)^{3/2} \left(\frac{\omega_0^2\omega_3}{\sinh^2\beta\omega_0 \sinh\beta\omega_3}\right)^{1/2} \\ &\quad \times \exp\left\{\frac{m\omega_3}{2\sinh\beta\omega_3}[-(x_3^2 + x_3'^2)\cosh\beta\omega_3 + 2x_3x_3'] \right. \\ &\quad + \frac{m\omega_0}{2\sinh\beta\omega_0}[-(x_1^2 + x_2^2 + x_1'^2 + x_2'^2)\cosh\beta\omega_0 + 2(x_1x_1' + x_2x_2')\cosh\beta\omega \\ &\quad \left. + i2(x_1'x_2 + x_2'x_1)\sinh\beta\omega]\right\}\end{aligned} \tag{30}$$

which is in agreement with [2].

4. The case when a uniform electric field coexists

With a slight modification the same method can also be applicable to a generalised case in which a uniform electric field $\boldsymbol{E} = (E_1, E_2, E_3)$ coexists. The Hamiltonian now becomes

$$\begin{aligned}\hat{H}^e &= \frac{1}{2m}(\boldsymbol{p} - e\boldsymbol{A})^2 + \tfrac{1}{2}mf^2\boldsymbol{r}^2 + e\boldsymbol{E}\cdot\boldsymbol{r} \\ &= \sum_{j=1,2,3} (a_j^\dagger\omega_j a_j + f_j a_j^\dagger + f_j a_j) + i\omega(a_1^\dagger a_2 - a_2^\dagger a_1) + \varepsilon_0\end{aligned} \tag{31}$$

where $f_j = eE_j/\sqrt{2m\omega_j}$ $(j=1,2,3)$. With this Hamiltonian, the operator in (17) may be written as

$$L^{e}(\mu)=\varepsilon_0+\sum_{j=1,2,3}\left(\omega_j\mu_j\frac{\partial}{\partial\mu_j}+f_j\frac{\partial}{\partial\mu_j}+f_j\mu_j\right)+\mathrm{i}\omega\left(\mu_2\frac{\partial}{\partial\mu_1}-\mu_1\frac{\partial}{\partial\mu_2}\right). \tag{32}$$

Accordingly, the eigenfunctions and eigenvalues of $L^{e}(\mu)$ can be easily obtained

$$\begin{aligned}\varphi^{e}_{lmn}(\mu)=\frac{2^{-1/2(l+m)}}{\sqrt{l!m!n!}}&\left(\mu_1+\mathrm{i}\mu_2+\frac{f_1+\mathrm{i}f_2}{\omega_0+\omega}\right)^{l}\left(\mu_1-\mathrm{i}\mu_2+\frac{f_1-\mathrm{i}f_2}{\omega_0-\omega}\right)^{m}\left(\mu_3+\frac{f_3}{\omega_3}\right)^{n}\\ &\times\exp\left\{-\frac{(f_1-\mathrm{i}f_2)(\mu_1+\mathrm{i}\mu_2)}{2(\omega_0+\omega)}-\frac{(f_1+\mathrm{i}f_2)(\mu_1-\mathrm{i}\mu_2)}{2(\omega_0-\omega)}\right.\\ &\left.-\frac{f_3\mu_3}{\omega_3}-\frac{f_1^2+f_2^2}{2(\omega_0+\omega)^2}-\frac{f_1^2+f_2^2}{2(\omega_0-\omega)^2}-\frac{f_3^2}{\omega_3^2}\right\}\end{aligned} \tag{33}$$

$$\Lambda^{e}_{lmn}=\varepsilon_0'+(\omega_0+\omega)l+(\omega_0-\omega)m+\omega_3 n \tag{34}$$

where

$$\varepsilon_0'=\varepsilon_0-\frac{f_1^2+f_2^2}{2(\omega_0+\omega)}-\frac{f_1^2+f_2^2}{2(\omega_0-\omega)}-\frac{f_3^2}{\omega_3}. \tag{35}$$

The calculations of $F^{e}(\bar{\lambda},\mu;\beta)$ and $\langle \boldsymbol{r}|\hat{\rho}^{e}|\boldsymbol{r}'\rangle$ are trivial, so we omit them here.

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