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LETTER TO THE EDITOR

The Bloch density matrix for a localised oscillator in a magnetic field

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Abstract. A closed analytic form is obtained for the Bloch or canonical density matrix of a localised oscillator in a magnetic field of arbitrary strength, by solving the Bloch equation with the completeness boundary condition.

In recent work on the melting of a Wigner electron crystal (1934, 1938) in an applied magnetic field, we noticed that it was possible to calculate the full canonical or Bloch density matrix for one localised Wigner oscillator. The purpose of this letter is to derive the explicit form of this density matrix $C(\boldsymbol{r}_0\boldsymbol{r}\beta)$ defined by

$$C(\boldsymbol{r}_0\boldsymbol{r}\beta)=\sum_i \psi_i^*(\boldsymbol{r}_0)\psi_i(\boldsymbol{r})\exp(-\beta\varepsilon_i) \tag{1}$$

where the ψ_i's and the corresponding one-electron energies ε_i are solutions of the Schrödinger equation

$$H\psi_i=\varepsilon_i\psi_i \tag{2}$$

while $\beta=(k_{\mathrm{B}}T)^{-1}$. In (2), the specific Hamiltonian we work with is

$$H=\frac{(\boldsymbol{p}-e\boldsymbol{A}/c)^2}{2m}+\tfrac{1}{2}k(x^2+y^2) \tag{3}$$

where the magnetic field $\mathscr{H}$ is applied along the z axis and the gauge is chosen such that the vector potential $\boldsymbol{A}$ is given by

$$\boldsymbol{A}=(-\tfrac{1}{2}\mathscr{H}y,\tfrac{1}{2}\mathscr{H}x,0). \tag{4}$$

The Bloch equation

$$H_r C(\boldsymbol{r}_0\boldsymbol{r}\beta)=-\partial C(\boldsymbol{r}_0\boldsymbol{r}\beta)/\partial\beta \tag{5}$$

is then explicitly of the form

$$\frac{\partial C}{\partial\beta}=\left[\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\mathrm{i}\hbar\omega\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)-\left(\tfrac{1}{2}k+\frac{e^2\mathscr{H}^2}{8mc^2}\right)(x^2+y^2)\right]C, \tag{6}$$

where $\omega=e\mathscr{H}/2mc$ is the Larmor frequency. Equation (6) must be solved subject

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to the initial condition

$$C(\boldsymbol{r}_0\boldsymbol{r}0)=\delta(\boldsymbol{r}_0-\boldsymbol{r}), \tag{7}$$

which follows immediately from (1) by completeness.

In the case when the force constant k is put equal to zero, Sondheimer and Wilson (1951) have given $C(\boldsymbol{r}_0\boldsymbol{r}\beta)$ explicitly. Our purpose here is to generalise their result to include the linear restoring force on the electron. To do so, we first generalise their assumptions to express the general structure of the density matrix as

$$\begin{aligned}C(\boldsymbol{r}_0\boldsymbol{r}\beta)=f(\beta)\exp\{&-\mathrm{i}(x_0y-y_0x)\phi(\beta)-[(x-x_0)^2+(y-y_0)^2]g(\beta)\\&-[(x+x_0)^2+(y+y_0)^2]h(\beta)\}.\end{aligned} \tag{8}$$

Given this structure, the four functions f, ϕ, g and h have been determined by substituting (8) into the Bloch equation (6) and requiring that the resulting equation is satisfied for all values of $\boldsymbol{r}_0$ and $\boldsymbol{r}$. Five equations result, namely

$$\partial(g+h)/\partial\beta=-(2\hbar^2/m)(g+h)^2+\tfrac{1}{2}m\omega^2b^2 \tag{9}$$

$$\partial(g+h)/\partial\beta=-(2\hbar^2/m)(g-h)^2+(\hbar^2/2m)\phi^2 \tag{10}$$

$$\partial(g-h)/\partial\beta=-(2\hbar^2/m)(g^2-h^2)+\tfrac{1}{2}\hbar\omega\phi \tag{11}$$

$$\partial\phi/\partial\beta=-(2\hbar^2/m)(g+h)\phi+2\hbar\omega(g-h) \tag{12}$$

and

$$\partial\ln f/\partial\beta=-(2\hbar^2/m)(g+h), \tag{13}$$

where b is defined by

$$b=(1+k/m\omega^2)^{1/2}. \tag{14}$$

We note first that one can immediately integrate (9) and (13) to yield, with $\alpha=\hbar\omega\beta$,

$$g+h=(m\omega b/2\hbar)\coth(b\alpha+a) \tag{15}$$

and

$$f=B/\sinh(b\alpha+a), \tag{16}$$

where a and B are 'constants' of integration, i.e. independent of β but dependent on magnetic field and force constant.

At this point, it is very helpful to invoke the work of Darwin (1931) who was concerned with the calculation of the diamagnetism of a free electron by means of the device of letting the force constant k vanish. In the course of that work, Darwin obtained the ψ_i's and ε_i's from the Schrödinger equation (2) and in particular from the ε_i's he calculated the partition function $Q=\Sigma_i\exp(-\beta\varepsilon_i)$ as

$$Q=\frac{\exp\alpha}{\{\exp[(b+1)\alpha]-1\}\{1-\exp[-(b-1)\alpha]\}}. \tag{17}$$

From (1) it is clear that since the ψ_i's there are normalised we can write

$$\int C(\boldsymbol{r}\boldsymbol{r}\beta)\,\mathrm{d}\boldsymbol{r}=Q \tag{18}$$

and using the diagonal form of (8) in (18) we find that f and h are related by

$$f(\beta)/h(\beta) = (4/\pi)Q. \tag{19}$$

Hence combining (19) with (15) and (16), and using (17), we find

$$h(\beta) = \frac{\pi B}{2}\left(\coth(b\alpha) - \frac{\cosh \alpha}{\sinh(b\alpha)}\right) \tag{20}$$

and

$$g(\beta) = \left(\frac{m\omega b}{2\hbar} - \frac{\pi}{2}B\right)\coth(b\alpha) + \frac{\pi}{2}B\frac{\cosh \alpha}{\sinh(b\alpha)}. \tag{21}$$

The function a has had to be put equal to zero to satisfy the delta function boundary condition (7).

The next step is to use (10)-(12) to determine the phase $\phi(\beta)$ and the function B depending on the force constant and magnetic field. We substitute therefore (20) and (21) into (10)-(12), to find

$$\phi(\beta) = 2\pi B\frac{\sinh \alpha}{\sinh(b\alpha)} \tag{22}$$

and

$$B = m\omega b/2\pi\hbar. \tag{23}$$

Thus, the Bloch density matrix is given explicitly by substituting the above results for g, h, ϕ and f (with $a = 0$) into (8). It is readily verified that in the case of a free electron in a magnetic field, i.e. b tends to unity, the result of Sondheimer and Wilson (1951) is recovered, apart from a trivial factor describing free motion in the z direction. Switching off the magnetic field, the known diagonal form of $C(\boldsymbol{r}_0\boldsymbol{r}\beta)$ (see, e.g., Stephen and Zalewski 1962) is readily regained.

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