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A modified Mehler formula and the Green function of the free electron in a uniform magnetic field

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Abstract. A closed representation is obtained for the Green function of the stationary Schrödinger equation of a free electron in a uniform magnetic field.

1. Derivation of the Green function

Some time ago Sondheimer and Wilson (1951) obtained a closed representation for the Green function of the time-dependent Schrödinger equation for a free electron in a uniform magnetic field. More recently Dodonov *et al* (1975) obtained the corresponding representation for the stationary two-dimensional Schrödinger equation by using the result of Sondheimer and Wilson. Bellandi and Zimmerman (1975) have also discussed the stationary Green function by solving the inhomogeneous Schrödinger equation for the Green function.

The present note contains a derivation of the stationary Green function using a modified Mehler formula for the product of the two-dimensional harmonic oscillator wavefunctions.

The Hamiltonian operator is

$$H = \frac{1}{2\mu} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2,$$

where μ is the electron mass, $\mathbf{A} = \frac{1}{2}(\mathbf{H} \times \mathbf{r})$ is the vector potential and \mathbf{H} is the uniform magnetic field. The Hamiltonian takes the form

$$H = \frac{p_z^2}{2\mu} + \frac{p_x^2 + p_y^2}{2\mu} + \omega L_z + \frac{\mu\omega^2}{2}(x^2 + y^2), \quad (1)$$

if the magnetic field is taken along the z axis, $\omega = |e|\mathcal{H}/(2\mu c)$ with $\mathcal{H} = |\mathbf{H}|$. As L_z is conserved, the eigenfunctions of the Hamiltonian operator equation (1), with $p_z = 0$, in polar coordinates ρ, ϕ in the x, y plane, are the two-dimensional harmonic oscillator wavefunctions (Powell and Crasemann 1965)

$$\psi_{k,m}(\rho, \phi) = \pi^{-1/2} [k! / (k + |m|)!]^{1/2} \exp(-\frac{1}{2}\rho^2) (\rho^2)^{|m|/2} L_k^{|m|}(\rho^2) \exp(im\phi) \quad (2)$$

and the energy eigenvalues are $E_\nu = 2k + |m| + m + 1 = \nu + 1$ (we have put $\omega = \hbar = \mu = 1$); m is the eigenvalue of L_z and k is the radial quantum number.

We define the Green function of the stationary two-dimensional Schrödinger equation for a free electron in a uniform magnetic field by means of the spectral decomposition

$$G(\mathbf{r}, \mathbf{r}'; \lambda) = \sum_{\nu=0}^{\infty} \frac{1}{E_{\nu} - \lambda} \sum_{2k+|m|+m=\nu} \psi_{k,m}(\rho, \phi) \psi_{k,m}^*(\rho', \phi'). \tag{3}$$

The full SU(2) symmetry of the two-dimensional harmonic oscillator is broken by the L_z operator in the Hamiltonian equation (1) and the Mehler formula (Bellandi and Caetano Neto 1976) cannot be used to calculate $G(\mathbf{r}, \mathbf{r}'; \lambda)$. However, a modified Mehler formula can be written in this case (see appendix)

$$\begin{aligned} \pi \sum_{\nu=0}^{\infty} \xi^{\nu} \sum_{2k+|m|+m=\nu} \psi_{k,m}(\rho, \phi) \psi_{k,m}^*(\rho', \phi') \\ = (1 - \xi^2)^{-1} \exp(i|\mathbf{r} \times \mathbf{r}'| - \frac{1}{2}|\mathbf{r} - \mathbf{r}'|) \exp\{-[\xi^2/(1 - \xi^2)]|\mathbf{r} - \mathbf{r}'|^2\}. \end{aligned} \tag{4}$$

The density matrix elements

$$\rho_{\nu}(\mathbf{r}, \mathbf{r}') = \sum_{2k+|m|+m=\nu} \psi_{k,m}(\rho, \phi) \psi_{k,m}^*(\rho', \phi'). \tag{5}$$

have the following integral representation:

$$\begin{aligned} \rho_{\nu}(\mathbf{r}, \mathbf{r}') = \pi^{-1} \exp(i|\mathbf{r} \times \mathbf{r}'| - \frac{1}{2}|\mathbf{r} - \mathbf{r}'|^2) \\ \times \frac{1}{2\pi i} \oint_{\xi=0} \mathrm{d}\xi \xi^{-\nu-1} (1 - \xi^2)^{-1} \exp\{-[\xi^2/(1 - \xi^2)]|\mathbf{r} - \mathbf{r}'|^2\}. \end{aligned} \tag{6}$$

The Green function is given by

$$G(\mathbf{r}, \mathbf{r}'; \lambda) = \sum_{\nu=0}^{\infty} \rho_{\nu}(\mathbf{r}, \mathbf{r}') / (E_{\nu} - \lambda) \tag{7}$$

and for $\text{Re}(1 - \lambda) > 0$ can be cast into the form

$$G(\mathbf{r}, \mathbf{r}'; \lambda) = \pi^{-1} \exp(+i|\mathbf{r} \times \mathbf{r}'| - \frac{1}{2}|\mathbf{r} - \mathbf{r}'|^2) \int_0^1 \mathrm{d}\xi \xi^{-\lambda} (1 - \xi^2)^{-1} \exp\{-[\xi^2/(1 - \xi^2)]|\mathbf{r} - \mathbf{r}'|^2\} \tag{8}$$

which is exactly the expression of Bellandi and Zimmerman (1975). With one variable transformation $\xi^2/(1 - \xi^2) = t|\mathbf{r} - \mathbf{r}'|^2$, $G(\mathbf{r}, \mathbf{r}'; \lambda)$ can be written in terms of the Whittaker function (Dodonov *et al* 1975)

$$G(\mathbf{r}, \mathbf{r}'; \lambda) = \frac{1}{2\pi} \Gamma(\frac{1}{2} - \lambda) \exp(i|\mathbf{r} \times \mathbf{r}'|) |\mathbf{r} - \mathbf{r}'|^{-1} W_{\lambda,0}(|\mathbf{r} - \mathbf{r}'|^2). \tag{9}$$

We can also consider a reduced Green function $G^m(\rho, \rho'; \lambda)$, with a defined value of L_z . We write down $G^m(\rho, \rho'; \lambda)$ by using equation (A.3) of the appendix and perform the sum over the residuum in equation (7) with a fixed value of m . The final expression is

$$\begin{aligned} G^m(\rho, \rho'; \lambda) = \pi^{-1} \exp[-\frac{1}{2}(\rho^2 + \rho'^2)] \\ \times \int_0^1 \mathrm{d}\xi \xi^{-\lambda+m} (1 - \xi^2)^{-1} I_m[2\rho\rho'\xi/(1 - \xi^2)] \exp\{-[\xi^2/(1 - \xi^2)](\rho^2 + \rho'^2)\}. \end{aligned} \tag{10}$$

To incorporate the free motion in the z direction we change $\lambda \rightarrow \lambda - \frac{1}{2}p_z^2$ and perform the Fourier transformation in equation (8) and equation (10). The singularities are the well known ones of the two-dimensional harmonic oscillator Green function in the transverse motion (Berendt and Weimar 1972).

Appendix

To prove the modified Mehler formula we introduce a Kronecker delta function in the energy $\delta(2k + |m| + m; \nu)$ in an integral representation

$$\delta(2k + |m| + m) = \frac{1}{2\pi i} \oint_{\xi=0} d\xi \xi^{\frac{2k+|m|+m}{\nu+1}}, \quad (\text{A.1})$$

$$\begin{aligned} & \sum_{2k+|m|+m=\nu} \psi_{k,m}(\rho, \phi) \psi_{k,m}^*(\rho', \phi') \\ &= \frac{1}{2\pi i} \oint_{\xi=0} d\xi \xi^{-\nu-1} \sum_{m=-\infty}^{+\infty} \xi^{|m|+m} \sum_{k=0}^{\infty} \xi^{2k} \psi_{k,m}(\rho, \phi) \psi_{k,m}^*(\rho', \phi'). \end{aligned} \quad (\text{A.2})$$

Introducing the normalized wavefunctions (equation (2)) in (A.2), the sum over k reproduces the generating function of the product of two Laguerre polynomials (Erdelyi 1953)

$$\begin{aligned} & \sum_{2k+|m|+m} \psi_{k,m}(\rho, \phi) \psi_{k,m}^*(\rho', \phi') \\ &= \pi^{-1} \exp[-\frac{1}{2}(\rho^2 + \rho'^2)] \frac{1}{2\pi i} \oint_{\xi=0} d\xi \xi^{-\nu-1} (1-\xi^2)^{-1} \exp\left(-\frac{\xi^2}{1-\xi^2}(\rho^2 + \rho'^2)\right) \\ & \quad \times \sum_{m=-\infty}^{+\infty} \xi^m \exp[im(\phi - \phi')] I_{|m|}\left(2\rho\rho' \frac{\xi}{1-\xi^2}\right). \end{aligned} \quad (\text{A.3})$$

The sum over m reproduces the generating function of the I_m Bessel function and equation (4) follows easily.

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