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Coulomb Green function with a definite value of L_z†

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Abstract. An integral representation is obtained for the Coulomb Green function belonging to a definite value of L_z.

The purpose of this paper is to write down the Coulomb Green function which corresponds to a definite value of the operator

$$L_z = (\boldsymbol{r} \times \boldsymbol{p})_z.$$

According to Hostler and Pratt (1963) the Green function $G(\boldsymbol{r}_2, \boldsymbol{r}_1, \omega)$, which is a solution of the differential equation:

$$[\nabla_2^2 + (2k\nu/r_2) + k^2]G(\boldsymbol{r}_2, \boldsymbol{r}_1, \omega) = \delta^3(\boldsymbol{r}_2 - \boldsymbol{r}_1)$$

$$\nu = (ka_1)^{-1}; \qquad a_1 = 4\pi\hbar^2(mze^2)^{-1}; \qquad k = (2m\omega/\hbar)^{1/2} \qquad \text{Im}\, k > 0 \tag{1}$$

is given by:

$$G(\boldsymbol{r}_2, \boldsymbol{r}_1, \omega) = -\frac{\Gamma(1-\mathrm{i}\nu)}{4\pi|\boldsymbol{r}_2 - \boldsymbol{r}_1|}\frac{1}{\mathrm{i}k}\left(-\frac{\partial}{\partial y} + \frac{\partial}{\partial x}\right) W_{\mathrm{i}\nu;1/2}(-\mathrm{i}kx)M_{\mathrm{i}\nu;1/2}(-\mathrm{i}ky) \tag{2}$$

which satisfies the following boundary conditions at the origin and at infinity:

$$\left.\begin{array}{l} r_2^{1/2}G(\boldsymbol{r}_2, \boldsymbol{r}_1, \omega) \to 0 \\ r_2^{1/2}\boldsymbol{r}_2 \cdot \nabla_2 G(\boldsymbol{r}_2, \boldsymbol{r}_1, \omega) \to 0 \end{array}\right\} \quad \text{as } r_2 \to 0$$

$$\left.\begin{array}{l} r_2 G(\boldsymbol{r}_2, \boldsymbol{r}_1, \omega) \to 0 \\ \boldsymbol{r}_2 \cdot \nabla_2 G(\boldsymbol{r}_2, \boldsymbol{r}_1, \omega) \to 0 \end{array}\right\} \quad \text{for } r_2 \to \infty$$

with

$$x = r_1 + r_2 + |\boldsymbol{r}_2 - \boldsymbol{r}_1|, \qquad y = r_1 + r_2 - |\boldsymbol{r}_2 - \boldsymbol{r}_1|.$$

Now let us write the above expression in cylindrical coordinates:

$$G(\boldsymbol{r}_2, \boldsymbol{r}_1, \omega) = \frac{1}{2\pi}\sum_{m=-\infty}^{+\infty} G^m(\rho_2 z_2, \rho_1 z_1, \omega)\exp[\mathrm{i}m(\phi_2 - \phi_1)]. \tag{3}$$

Introducing:

$$\lambda = \phi_2 - \phi_1 \tag{4}$$

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we have:

$$\frac{\mathrm{d}x}{\mathrm{d}\lambda}=\frac{\rho_1\rho_2\sin\lambda}{|\boldsymbol{r}_2-\boldsymbol{r}_1|}=-\frac{\mathrm{d}y}{\mathrm{d}\lambda} \tag{5}$$

and therefore equation (2) can be written as:

$$G(\boldsymbol{r}_2,\boldsymbol{r}_1,\omega)=-\frac{\Gamma(1-\mathrm{i}\nu)}{4\pi\rho_1\rho_2}\frac{1}{\mathrm{i}k}\frac{1}{\sin\lambda}\frac{\mathrm{d}}{\mathrm{d}\lambda}[W_{\mathrm{i}\nu;1/2}(-\mathrm{i}kx)M_{\mathrm{i}\nu;1/2}(-\mathrm{i}ky)]. \tag{6}$$

As $x>y$ we can use the following representation for the product of two Whittaker functions (Buchholz 1969, equation (50)):

$$W_{\mathrm{i}\nu;1/2}(a_1t)M_{\mathrm{i}\nu;1/2}(a_2t)$$
$$=\frac{t\sqrt{a_1a_2}}{\Gamma(1-\mathrm{i}\nu)}\int_0^\infty\exp[-\tfrac{1}{2}(a_1+a_2)t\cosh v]\coth^{2\mathrm{i}\nu}(\tfrac{1}{2}v)I_1(t\sqrt{a_1a_2}\sinh v)\,\mathrm{d}v \tag{7}$$

with $t=-\mathrm{i}k$; $a_1=x$; $a_2=y$.

Then equation (6) gives

$$G(\boldsymbol{r}_2,\boldsymbol{r}_1,\omega=\frac{1}{4\pi}\frac{1}{\rho_1\rho_2}\frac{1}{\sin\lambda}\frac{\mathrm{d}}{\mathrm{d}\lambda}$$
$$\times\int_0^\infty\exp[\tfrac{1}{2}\mathrm{i}k(x+y)\cosh v]\sqrt{xy}I_1(-\mathrm{i}k\sqrt{xy}\sinh v)\coth^{2\mathrm{i}\nu}(\tfrac{1}{2}v)\,\mathrm{d}v. \tag{8}$$

Let us recall that:

$$xy=2r_1r_2+2z_1z_2+2\rho_1\rho_2\cos\lambda$$
$$x+y=2(r_1+r_2) \tag{9}$$

and therefore it follows that (see also Hostler 1964):

$$G(\boldsymbol{r}_2,\boldsymbol{r}_1,\omega)=\frac{1}{4\pi}\int_0^\infty\mathrm{d}v\coth^{2\mathrm{i}\nu}(\tfrac{1}{2}v)(\mathrm{i}k\sinh v)$$
$$\times\exp[\mathrm{i}k(r_1+r_2)\cosh v]I_0(-\mathrm{i}k\sqrt{xy}\sinh v). \tag{10}$$

Now, as we have:

$$I_0(z)=J_0(\mathrm{i}z)$$

and also, by Graf's addition theorem (Erdélyi 1953, equation (5)),

$$J_0(\sigma)=\sum_{m=-\infty}^{+\infty}J_m(\xi_1)J_m(\xi_2)\exp(\mathrm{i}m\lambda) \tag{11}$$

with:

$$\sigma=(\xi_1^2+\xi_2^2-2\xi_1\xi_2\cos\lambda)^{1/2}=(xyk^2\sinh v)^{1/2}.$$

Equation (10) can be written as:

$$G(\boldsymbol{r}_2, \boldsymbol{r}_1, \omega) = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \exp(\mathrm{i}m\lambda)$$

$$\times \frac{1}{2} \int_0^\infty \mathrm{d}v \coth^{2\mathrm{i}\nu}(\tfrac{1}{2}v)(\mathrm{i}k \sinh v) \exp[\mathrm{i}k(r_1 + r_2)\cosh v] J_m(\xi_1) J_m(\xi_2) \quad (12)$$

$$|\xi_1| > |\xi_2|$$

Comparison with equation (3) gives:

$$G^m(\rho_2 z_2, \rho_1 z_1, \omega)$$

$$= \frac{1}{2} \int_0^\infty \mathrm{d}v \exp[\mathrm{i}k(r_1 + r_2)\cosh v] \coth^{2\mathrm{i}\nu}(\tfrac{1}{2}v)(\mathrm{i}k \sinh v) J_m(\xi_1) J_m(\xi_2) \quad (13)$$

where:

$$\xi_1 = 2^{-1/2} k \sinh v[(r_1 r_2 + z_1 z_2 + \rho_1 \rho_2)^{1/2} + (r_1 r_2 + z_1 z_2 - \rho_1 \rho_2)^{1/2}]$$

$$\xi_2 = 2^{-1/2} k \sinh v[(r_1 r_2 + z_1 z_2 + \rho_1 \rho_2)^{1/2} - (r_1 r_2 + z_1 z_2 - \rho_1 \rho_2)^{1/2}].$$

This Green function can have some applications. For instance by writing down the integral equation for the wavefunction of an hydrogen atom in an external uniform magnetic field, with the help of the Green function equation (12), the bound state energies and the corresponding wavefunctions can be obtained by solving numerically the corresponding homogeneous integral equation.

In similar kinds of problem which involve only one variable this is easily handled and we obtain rather accurate energies as well as wavefunctions, at least for the lowest states (Byron and Fuller 1970).

In our present case, from the computational point of view the problem is more difficult since the corresponding wavefunctions ψ_m depend on two variables ρ_2 and z_2.

Similar considerations hold if we take as the Green function that corresponding to a free electron in an uniform magnetic field (Bellandi and Zimerman 1975).

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