COULOMB GREEN'S FUNCTION IN CLOSED FORM*

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Recently one of us (L.H.) has obtained an expression in closed form for the nonrelativistic Coulomb Green's function.[1] Knowing the form of this expression, we wish to outline here a simple derivation of the Green's function and summarize some further results.

The Green's function is the solution $G(\vec{r}_2, \vec{r}_1, \omega)$ of the differential equation

$$\{\nabla_2{}^2 + (2k\nu)/r_2 + k^2\}G(\vec{r}_2, \vec{r}_1, \omega) = \delta^3(\vec{r}_2 - \vec{r}_1);$$
$$\nu = (ka_1)^{-1}; \quad a_1 = 4\pi\hbar^2/mZe^2; \quad k = (2m\omega/\hbar)^{1/2},$$
$$\mathrm{Im}(k) > 0; \tag{1}$$

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

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

$$\left.\begin{array}{l} r_2 G(\vec{r}_2, \vec{r}_1, \omega) \to 0 \\ \vec{r}_2\cdot\vec{\nabla}_2 G(\vec{r}_2, \vec{r}_1, \omega) \to 0 \end{array}\right\} \text{for } r_2 \to \infty. \tag{2}$$

Here $\hbar\omega$ is a complex number not in the eigenvalue spectrum of the Hamiltonian of the system. The Green's function as defined by (1) and (2) is unique.[2]

The retarded (advanced) "physical" Green's function, defined for real $\hbar\omega$, is obtained from $G(\vec{r}_2, \vec{r}_1, \omega)$ by taking the limit as $\hbar\omega$ approaches the real axis from above (below). For $\hbar\omega > 0$ the physical Green's functions so obtained have an oscillatory behavior as $r_2 \to \infty$, the retarded Green's function consisting of only outgoing spherical waves and the advanced Green's function consisting of only incoming spherical waves. For $\hbar\omega < 0$ the retarded and advanced Green's functions coincide, and both agree with the "general" Green's function as defined by (1) and (2). These $\hbar\omega$ values are "nonpropagating" in the sense that the Green's functions decay exponentially as $r_2 \to \infty$.

Rotational invariance and uniqueness require that $G(\vec{r}_2, \vec{r}_1, \omega)$ depend on $\vec{r}_1$ and $\vec{r}_2$ only in the forms r_1, r_2, and $|\vec{r}_2 - \vec{r}_1|$. It is natural to factor out $|\vec{r}_2 - \vec{r}_1|^{-1}$ from G. If we let $F(r_2, r_1, |\vec{r}_2 - \vec{r}_1|) = -4\pi|\vec{r}_2 - \vec{r}_1|G$, then F satisfies the homogeneous equation

$$\{\nabla_2{}^2 - 2|\vec{r}_2 - \vec{r}_1|^{-2}(\vec{r}_2 - \vec{r}_1)\cdot\vec{\nabla}_2 + 2k\nu/r_2 + k^2\} \times F(r_2, r_1, |\vec{r}_2 - \vec{r}_1|) = 0, \tag{3}$$

together with the normalization condition $F(\vec{r}_2 = \vec{r}_1) = 1$. Now the striking feature of the solution[1] for G is that $F(r_2, r_1, |\vec{r}_2 - \vec{r}_1|)$ is a function of only the two variables $x \equiv r_1 + r_2 + |\vec{r}_2 - \vec{r}_1|$ and $y \equiv r_1 + r_2 - |\vec{r}_2 - \vec{r}_1|$ and is of the form

$$F(r_2, r_1, |\vec{r}_2 - \vec{r}_1|) \propto (\partial/\partial x - \partial/\partial y)f_1(x)f_2(y). \tag{4}$$

In view of this result, we write the dependence on $\vec{r}_2$ in terms of the variables $\sigma \equiv r_1 + r_2$ and $\rho \equiv |\vec{r}_2 - \vec{r}_1|$, where in principle F could still have a further dependence on r_1:

$$\left\{\frac{\partial^2}{\partial\rho^2} + \frac{\partial^2}{\partial\sigma^2} + \frac{\rho^2 + \sigma^2 - 2\sigma r_1}{\rho(\sigma - r_1)}\frac{\partial^2}{\partial\rho\partial\sigma} + \frac{\rho^2 - \sigma^2 + 2\sigma r_1}{\rho^2(\sigma - r_1)}\frac{\partial}{\partial\sigma} + \frac{2k\nu}{\sigma - r_1} + k^2\right\}F(\sigma, \rho, r_1) = 0. \tag{5}$$

The significance of the partial derivatives in (4) now becomes apparent: If we let $F(\sigma, \rho, r_1) = (\partial/\partial\rho)D(\sigma, \rho, r_1)$, then the term in (5) linear in the differential operators can be eliminated from the equation. We find $(\partial/\partial\rho)MD(\sigma, \rho, r_1) = 0$, where

$$M = \left\{\frac{\partial^2}{\partial\rho^2} + \frac{\partial^2}{\partial\sigma^2} + \frac{\rho^2 + \sigma^2 - 2\sigma r_1}{\rho(\sigma - r_1)}\frac{\partial^2}{\partial\rho\partial\sigma} + \frac{2k\nu}{\sigma - r_1} + k^2\right\}. \tag{6}$$

Thus MD is a function of σ and r_1 only. However, note that D is not determined uniquely: If D' is an acceptable solution, then so is $D = D' - D_0(\sigma, r_1)$, where D_0 is an arbitrary function of σ and r_1. We may choose D_0 such that $MD = 0$.

The significance of the transformation to the variables x and y now also becomes apparent: When M is expressed in terms of these variables, no mixed derivatives occur. So far we have made no use of the fact that we are dealing with the pure Coulomb potential $V(r_2) = -Ze^2/4\pi r_2$ rather than a general potential $V(r_2)$. Now the special feature of the pure Coulomb case is that M is separable in x and y. We may rewrite the equation $MD = 0$ in the form

$$\{(x^2 - 2xr_1)O(x) - (y^2 - 2yr_1)O(y)\}D(x, y, r_1) = 0,$$

$$O(z) = \left(\frac{\partial^2}{\partial z^2} + \frac{k^2}{4} + \frac{k\nu}{z}\right). \tag{7}$$

Any solution of the equation $O(z)f(z) = 0$ can be written as a linear combination of the two Whittaker functions $W_{i\nu;\,1/2}(-ikz)$ and $\mathfrak{M}_{i\nu;\,1/2}(-ikz)$.[3] A solution for D is hence $D = \text{constant} \times [f_1(x)f_2(y)]$, where f_1 and f_2 are Whittaker functions. The choice of Whittaker functions follows from the boundary conditions (2) and the choice of constant from the normalization requirement $F(\vec{r}_2 = \vec{r}_1) = 1$. We finally have for the Green's function

$$G(\vec{r}_2, \vec{r}_1, \omega) = -\frac{\Gamma(1-i\nu)}{4\pi|\vec{r}_2 - \vec{r}_1|}\frac{1}{ik}\left(-\frac{\partial}{\partial y} + \frac{\partial}{\partial x}\right)W_{i\nu;\,1/2}(-ikx) \times \mathfrak{M}_{i\nu;\,1/2}(-iky), \tag{8}$$

in agreement with the result previously obtained.[1]

Although some integral representations are known for G,[1,4] we are not aware that the result (8) has previously been obtained. Meixner[2] has given the expression for the Green's function for the special case $\vec{r}_1 = 0$. His result agrees with that obtained from (8):

$$G(\vec{r}_2, 0, \omega) = -(4\pi r_2)^{-1}\Gamma(1-i\nu)W_{i\nu;\,1/2}(-2ikr_2). \tag{9}$$

Similar results may be obtained for the Klein-Gordon and Dirac equations. For the Klein-Gordon equation, the Green's function should satisfy

$$\{\nabla_2^{\,2} + 2k\nu/r_2 + a^2/r_2^{\,2} + k^2\}G_{\mathrm{KG}}(\vec{r}_2, \vec{r}_1, \omega) = \delta^3(\vec{r}_2 - \vec{r}_1);$$
$$a = Ze^2/4\pi\hbar c; \quad \nu = a\omega/ck; \quad k = [(\omega/c)^2 - (mc/\hbar)^2]^{1/2}, \quad \mathrm{Im}(k) > 0. \tag{10}$$

If we neglect the $(a/r_2)^2$ term, this equation agrees with the equation of the nonrelativistic Green's function, excepting only that the meanings of the parameters k and ν are different. Consequently, we obtain the result that the Green's function for the Klein-Gordon equation without the potential squared term is given by the expression (8) with k and ν defined as in (10). For the special case that $\vec{r}_1 = 0$, we obtain (9) again but with k and ν defined as in (10), a result obtained by Martin and Glauber.[5]

Now it has been shown[1] that this neglect of the potential squared term is precisely equivalent to neglecting terms of order $a^2/(l+\frac{1}{2})^2$ in comparison to unity in the lth partial wave of the partial-wave expansion of the exact Klein-Gordon Green's function satisfying (10) – i.e., this neglect of the potential squared term is strictly analogous to the approximation introduced by Furry[6] in connection with the Dirac-Coulomb continuum states.

The Coulomb Green's function $K(\vec{r}_2, \vec{r}_1, \omega)$ for the Dirac equation has also been obtained in closed form in the "Furry" approximation.[1] This Green's function can be expressed in the form

$$K(\vec{r}_2, \vec{r}_1, \omega) = \left\{\gamma^0\left(\frac{\omega}{c} + \frac{a}{r_2}\right) + i\vec{\gamma}\cdot\vec{\nabla}_2 + \frac{mc}{\hbar}\right\} \times G_I(\vec{r}_2, \vec{r}_1, \omega), \tag{11a}$$

$$= G_I(\vec{r}_2, \vec{r}_1, \omega)\left\{\gamma^0\left(\frac{\omega}{c} + \frac{a}{r_1}\right) - i\vec{\gamma}\cdot\overleftarrow{\nabla}_1 + \frac{mc}{\hbar}\right\}, \tag{11b}$$

where G_I is the Green's function of the iterated Dirac equation

$$\left\{\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} + \frac{2ia}{cr}\frac{\partial}{\partial t} - \frac{m^2c^2}{\hbar^2} + \frac{a^2}{r^2} + ia\frac{\vec{\alpha}\cdot\vec{r}}{r^3}\right\}\varphi = 0. \tag{12}$$

The expression for G_I in the "Furry" approximation, $a^2/(J+\frac{1}{2})^2 \ll 1$, is found to be:

$$G_I(\vec{r}_2, \vec{r}_1, \omega) \approx \{1 - (ic/2\omega)\vec{\alpha}\cdot(\overleftarrow{\nabla}_2 + \vec{\nabla}_1)\} \times G_0(\vec{r}_2, \vec{r}_1, \omega), \tag{13}$$

where $G_0(\vec{r}_2, \vec{r}_1, \omega)$ denotes the approximate Klein-Gordon Green's function discussed above. This result is in agreement except for terms of order a^2 with the exact result obtained by Martin and Glauber[7] for the special case $\vec{r}_1 = 0$.

The physical Green's function $G(\vec{r}_2, \vec{r}_1, \omega)$ regarded as a function of $\vec{r}_2$ can be interpreted as the Schrödinger wave function corresponding to a source point or sink point located at $\vec{r}_1$ of particles of frequency ω. When $\hbar\omega$ lies in the continuous spectrum, we obtain the Coulomb wave functions with modified plane-wave behavior at large distances by taking the source point (or sink point) $\vec{r}_1$ infinitely remote from the origin.[2,8] The Furry or Sommerfeld-Maue wave function can be derived by applying this procedure to our approximate Dirac Green's function as obtained from (11b).

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