SCHRÖDINGER EQUATION FOR A DIRAC BUBBLE POTENTIAL

S.M. BLINDER
Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, USA

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The quantum-mechanical problem of a particle moving in a "Dirac bubble potential" $U(r) = (\lambda/r_0)\delta(r - r_0)$ is solved exactly for both bound and continuum states by making use of partial wave Green's functions $G_l(r, r_0, k)$. Phase shifts are expressed in a compact form related to those for an impenetrable sphere.

Recently I worked out a closed-form solution to the Schrödinger equation for a hydrogen atom perturbed by a modification of the Fermi contact interaction [1]. Specifically, the perturbation added to the Coulomb potential is

$$\mathcal{H}' = \alpha\delta(r - r_0)/4\pi r_0^2, \quad \alpha \equiv \tfrac{8}{3}\pi \boldsymbol{\mu}_S \cdot \boldsymbol{\mu}_I, \tag{1}$$

in which $\boldsymbol{\mu}_S$ and $\boldsymbol{\mu}_I$ are, respectively, electron spin and nuclear spin magnetic moment operators. The nuclear moment in this model is idealized as a magnetic shell (or bubble) of radius r_0. As r_0 is decreased to zero, the nucleus approaches a point magnetic dipole and eq. (1) reduces to the conventional Fermi contact interaction operator $\mathcal{H}' = \alpha\delta^3(\boldsymbol{r})$.

We shall consider in this paper a simpler version of the problem *without* the Coulomb potential. The results will add another to the small number of exactly soluble quantum-mechanical problems. The Schrödinger equation for a particle in a Dirac bubble potential is written:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{\alpha}{4\pi r_0^2}\delta(r - r_0)\right]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}). \tag{2}$$

Spherical symmetry allows the factorization $\psi(\boldsymbol{r}) = R_{kl}(r)Y_{lm}(\theta,\phi)$. The radial equation can be arranged to

$$\left[k^2 + \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right]R_{kl}(r)$$
$$= (\lambda/r_0)R_{kl}(r_0)\delta(r - r_0), \tag{3}$$

having defined

$$E \equiv \hbar^2k^2/2m, \quad \lambda \equiv m\alpha/2\pi\hbar^2 r_0. \tag{4}$$

We observe that eq. (3) is isomorphous with the defining relation for the lth partial wave Green's function

$$\left[k^2 + \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right]G_l(r, r_0, k) = \delta(r - r_0)/r_0^2. \tag{5}$$

In standard Sturm–Liouville form:

$$\left[\frac{\partial}{\partial z}z^2\frac{\partial}{\partial z} + z^2 - l(l+1)\right]G_l = k\delta(z - z_0), \quad z \equiv kr. \tag{6}$$

The solution to (6) regular at $z = 0$ with outgoing wave behavior as $z \to \infty$ is a product of spherical Bessel functions:

$$G_l(r, r_0, k) = -ikj_l(kr_<)h_l^{(1)}(kr_>), \tag{7}$$

in which $r_>$ and $r_<$ are, respectively, the larger and smaller of r, r_0.

Outgoing wave solutions to the Schrödinger equation (3) with $E > 0$ can accordingly be represented in the form

$$R_{kl}(r) = Aj_l(kr) - i\lambda kr_0 R_{kl}(r_0)j_l(kr_<)h_l^{(1)}(kr_>). \tag{8}$$

The first term (complementary function) is a solution of the free-particle equation regular at $r = 0$. For consistency at $r = r_0$, the constant A must fulfil the condition

$$A j_l(kr_0) = R_{kl}(r_0)[1 + i\lambda k r_0 j_l(kr_0) h_l^{(1)}(kr_0)]. \quad (9)$$

The magnitude of $R_{kl}(r_0)$ determines the normalization of the wavefunction.

For $r > r_0$, the eigenfunctions (8) can be expressed in terms of phase shifts δ_l as follows:

$$R_{kl}(r) = \text{const}\,[j_l(kr)\cos\delta_l - n_l(kr)\sin\delta_l]. \quad (10)$$

With use of (9) it is shown that

$$\operatorname{ctn}\delta_l = \frac{n_l(kr_0)}{j_l(kr_0)} - \frac{1}{\lambda k r_0 [j_l(kr_0)]^2}. \quad (11)$$

As $\lambda \to \infty$, the bubble becomes opaque and (11) reduces to the well-known result for scattering by an impenetrable sphere [2, p. 38]:

$$\operatorname{ctn}\xi_l = n_l(kr_0)/j_l(kr_0). \quad (12)$$

In the limit $\lambda \to 0$, on the other hand, one obtains the Born approximation phase shifts [2, p. 89]

$$\eta_l = -\frac{2mk}{\hbar^2}\int_0^\infty V(r)[j_l(kr)]^2 r^2 \mathrm{d}r = -\lambda k r_0 [j_l(kr_0)]^2. \quad (13)$$

Putting (12) and (13) into (11), one can express the phase shifts δ_l in the compact form

$$\operatorname{ctn}\delta_l = \operatorname{ctn}\xi_l + \eta_l^{-1}. \quad (14)$$

For consideration of the $E < 0$ bound states of a bubble potential, it is convenient to introduce the variable

$$\kappa \equiv -ik, \quad E = -\hbar^2\kappa^2/2m. \quad (15)$$

The Green's function (7) can be written

$$G_l(r, r_0, \kappa) = -\kappa\, \mathcal{I}_l(\kappa r_<)\mathcal{K}_l(\kappa r_>) \quad (16)$$

in terms of modified spherical Bessel functions defined as follows:

$$\mathcal{I}_l(z) \equiv (\pi/2z)^{1/2} I_{l+1/2}(z) = i^{-l} j_l(iz),$$

$$\mathcal{K}_l(z) \equiv (2/\pi z)^{1/2} K_{l+1/2}(z) = -i^l h_l^{(1)}(iz). \quad (17)$$

Specifically, the first three functions of each type are [3]

$$\mathcal{I}_0(z) = z^{-1}\sinh z,$$

$$\mathcal{I}_1(z) = z^{-1}\cosh z - z^{-2}\sinh z,$$

$$\mathcal{I}_2(z) = (z^{-1} + 3z^{-3})\sinh z - 3z^{-2}\cosh z \quad (18)$$

and

$$\mathcal{K}_0(z) = z^{-1}\,\mathrm{e}^{-z}$$

$$\mathcal{K}_1(z) = (z^{-1} + z^{-2})\mathrm{e}^{-z}$$

$$\mathcal{K}_3(z) = (z^{-1} + 3z^{-2} + 3z^{-3})\mathrm{e}^{-z}. \quad (19)$$

For bound states the Schrödinger equation (3) has the solutions

$$R_{\kappa l}(r) = -\lambda\kappa r_0 R_{\kappa l}(r_0)\mathcal{I}_l(\kappa r_<)\mathcal{K}_l(\kappa r_>), \quad (20)$$

there being no complementary function for $E < 0$. For $r = r_0$, the consistency condition on eq. (20),

$$-\lambda\kappa r_0 \mathcal{I}_l(\kappa r_0)\mathcal{K}_l(\kappa r_0) = 1 \quad (21)$$

provides a transcendental equation determining the eigenvalues of the problem.

For $z \geqslant 0$, both $\mathcal{I}_l(z)$ and $\mathcal{K}_l(z)$ are positive definite. Thus (21) has real solutions corresponding to bound states only when $\lambda < 0$. This is physically reasonable since the latter condition implies an *attractive* potential. Eq. (21) can be cast in the form

$$z\mathcal{I}_l(z)\mathcal{K}_l(z) = |\lambda|^{-1}, \quad z \equiv \kappa r_0. \quad (22)$$

From formulas given in ref. [3], the left-hand side is verified to be a monotonically-decreasing function of z (for $z \geqslant 0$) with a maximum value $(2l+1)^{-1}$ at $z = 0$. As $z \to \infty$, $z\mathcal{I}_l(z)\mathcal{K}_l(z) \sim 1/2z$.

It follows that there exists one bound state for each angular momentum, so long as

$$|\lambda| > 2l + 1. \quad (23)$$

For $|\lambda| < 2l + 1$, eq. (22) has no solution with $z > 0$, hence no bound states will exist above some critical value of l.

For $l = 0$, eq. (21) reduces to the simple form

$$(1 - \mathrm{e}^{-2\kappa r_0})/2\kappa r_0 = |\lambda|^{-1}. \quad (24)$$

References

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[3] M. Abramowitz and I.A. Stegun, eds., Handbook of mathematical functions (Natl. Bur. Std., Washington, 1972) p. 443.