

An Exactly Solvable Model for the Fermi Contact Interaction

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A model for the Fermi contact interaction is proposed in which the nuclear moment is represented as a magnetized spherical shell of radius r_0 . For a hydrogen-like system thus perturbed, the Schrödinger equation is solvable without perturbation theory by use of the Coulomb Green's function. Approximation formulas are derived in terms of a quantum defect in the Coulombic energy formula. It is shown that the usual Fermi potential cannot be applied beyond first-order perturbation theory.

Key words: Fermi contact interaction

Atomic hyperfine interactions involving s -electrons are well accounted for by the Fermi contact operator [1, 2]

$$\begin{aligned}\mathcal{H}' &= \lambda \pi a^3 \mathbf{s} \cdot \mathbf{I} \delta^3(\mathbf{r}) \\ \lambda &\equiv \frac{8}{3} g g_I \mu_B \mu_N / a^3, \quad \delta^3(\mathbf{r}) = \delta(r) / 4\pi r^2.\end{aligned}\quad (1)$$

Additionally, nuclear spin-spin coupling in NMR can be attributed predominantly to a second-order mechanism involving the Fermi contact interaction [3]. An unfortunate concomitant to this mechanism is the appearance of divergent nuclear magnetic self-interactions [4]. These divergences are unphysical. The problem shows up in fact even when (1) is applied to the second-order perturbation energy of a hydrogen atom [5]. An extensive literature exists on attempts to circumvent this difficulty in calculations of spin-spin coupling constants in molecules, notably HD [6].

We should like to propose as an alternative, a model for the contact interaction which leads to an exactly solvable atomic problem. Thereby, spin-spin coupling can be treated as a *first-order* perturbation and divergences are avoided entirely. In

physical terms, the point nuclear magnetic dipole implied by the Fermi Hamiltonian (1) is to be replaced by a uniformly magnetized spherical shell of radius r_0 . This is effected simply by the substitution in Eq. (1):

$$\delta(r) \rightarrow \delta(r - r_0). \quad (2)$$

We designate the resultant operator as the *modified Fermi potential* [7].

A hydrogen-like system perturbed by a modified Fermi potential is represented by the Schrödinger equation (for s -states):

$$\left\{ -\frac{\hbar^2}{2\mu} \nabla^2 - \frac{Ze^2}{r} + \frac{8\pi}{3} gg_I \mu_B \mu_N \mathbf{s} \cdot \mathbf{I} \frac{\delta(r - r_0)}{4\pi r_0^2} \right\} \psi(r) = E\psi(r). \quad (3)$$

We adopt the modified atomic units

$$\hbar = c = \mu = 1, \quad \mu = m(1 + m/M)^{-1}, \quad a \equiv \hbar^2/\mu e^2 = 1 \quad (4)$$

and introduce the radial function $P(r)$ such that

$$\psi(r) = P(r)/(4\pi r^2)^{1/2} \quad (5)$$

and the wavenumber k where

$$E = k^2/2. \quad (6)$$

The Schrödinger equation then reduces to the form

$$\left(k^2 + \frac{\partial^2}{\partial r^2} + \frac{2Z}{r} \right) P(r) = \frac{\lambda_F}{2r_0^2} P(r_0) \delta(r - r_0) \quad (7)$$

where

$$\lambda_F \equiv (\mathbf{s} \cdot \mathbf{I})_F \lambda, \quad (\mathbf{s} \cdot \mathbf{I})_F = \frac{1}{2}[F(F+1) - s(s+1) - I(I+1)], \quad F = I \pm \frac{1}{2}. \quad (8)$$

For atomic hydrogen ($Z = 1$, $I = \frac{1}{2}$), using the experimental free-electron g -factor $g = 2.0023193134$,

$$\lambda = 2.1600 \times 10^{-7}, \quad \lambda_1 = \frac{1}{4}\lambda, \quad \lambda_0 = -\frac{3}{4}\lambda.$$

Now Eq. (7) is isomorphous with the defining equation for the S -wave Coulomb Green's function [8]

$$\left(k^2 + \frac{\partial^2}{\partial r^2} + \frac{2Z}{r} \right) g(r, r_0, k) = \delta(r - r_0) \quad (9)$$

having defined

$$g(r, r_0, k) \equiv rr_0 G_0(r, r_0, k). \quad (10)$$

The appropriate boundary conditions are

$$r^{-1/2} g(r, r_0, k) \rightarrow 0, \quad r^{1/2} \partial g / \partial r \rightarrow 0 \quad \text{as } r \rightarrow 0 \quad (11)$$

and

$$g(r, r_0, k) \rightarrow 0, \quad \partial g / \partial r \rightarrow 0 \quad \text{as } r \rightarrow \infty \quad (12)$$

which are applicable as well to the Schrödinger equation (7). Thus the latter must possess solutions of the form

$$P_\nu(r) = \frac{\lambda_F}{2r_0^2} P_\nu(r_0) g(r, r_0, k) \quad (13)$$

provided that k does not lie in the unperturbed Coulomb eigenvalue spectrum. The Green's function is given by [8]

$$g(r, r_0, k) = (2ik)^{-1} \Gamma(1 - i\nu) M_{i\nu}^{1/2}(-2ikr_<) W_{i\nu}^{1/2}(-2ikr_>) \quad (14)$$

where $\nu \equiv Z/k$, $\text{Im } k > 0$, M and W are Whittaker functions as defined by Buchholz [9]. Since we shall be concerned with bound states, it is expedient to make the substitutions

$$i\nu \rightarrow \nu, \quad -ik \rightarrow k.$$

Accordingly

$$g(r, r_0, k) = -(2k)^{-1} \Gamma(1 - \nu) M_\nu(2kr_<) W_\nu(2kr_>). \quad (15)$$

We have in addition dropped the second index on the Whittaker functions since it will have the value $\frac{1}{2}$ throughout. In place of (6) we have now

$$E_\nu = -k^2/2 = -Z^2/2\nu^2 \quad (16)$$

which has the same form as for Coulomb eigenvalues but with *non-integral* values of the quantum number ν . For $\lambda \ll 1$ ($\lambda \sim 10^{-7}$ for hydrogen) it can be anticipated that the bound state energies given by (16) will differ only minutely from the values $E_n = -Z^2/2n^2$. It is convenient to introduce a quantum defect such that

$$\nu = n + \delta, \quad n = 1, 2, \dots \quad (17)$$

Then

$$E_\nu = -\frac{Z^2}{2n^2} + \frac{Z^2}{n^3} \delta + O(\delta^2). \quad (18)$$

A consistency condition on the eigenfunctions (13), obtained by setting $r = r_0$, gives a transcendental equation determining the bound state eigenvalues, viz.,

$$\frac{\lambda_F}{2r_0^2} g(r_0, r_0, k) = 1. \quad (19)$$

Now the S -wave Coulomb Green's function defined by (9) has the spectral representation

$$g(r, r_0, \epsilon) = \sum_n \frac{P_n(r) P_n(r_0)}{\epsilon - \epsilon_n}, \quad \epsilon \equiv -Z^2/\nu^2 \quad (20)$$

in terms of the unperturbed s -state radial functions $P_n(r)$. In the discrete spectrum,

$$P_n(r) = (Z/n)^{1/2} M_n(2Zr/n), \quad \epsilon_n = -Z^2/n^2. \quad (21)$$

For the perturbed state $n = N$, $\nu = N + \delta$, the Green's function expanded in powers of the quantum defect takes the form

$$g(r, r_0, \varepsilon) = \left(\frac{N^3}{2Z^2\delta} + \frac{3N^2}{4Z^2} \right) P_N(r)P_N(r_0) + k(r, r_0, \varepsilon_N) + O(\delta) \quad (22)$$

where $k(r, r_0, \varepsilon_N)$ is the reduced Coulomb Green's function [10, 11]

$$k(r, r_0, \varepsilon_N) \equiv \sum_{n \neq N} \frac{P_n(r)P_n(r_0)}{\varepsilon_N - \varepsilon_n} \quad (23)$$

Putting (22) into (19), with neglect of contributions $O(\delta)$, and solving for the quantum defect, we obtain

$$\delta_{N,F} \approx \frac{\frac{\lambda_F N^3}{4Z^2 r_0^2} |P_N(r_0)|^2}{1 - \frac{\lambda_F}{2r_0^2} \left[\frac{3N^2}{4Z^2} |P_N(r_0)|^2 + k(r_0, r_0, \varepsilon_N) \right]} \quad (24)$$

Explicitly for the $1s$ state, $N = 1$,

$$P_1(r) = 2Z^{3/2} r e^{-Zr} \quad (25)$$

and from formulas given by Hameka [10] and Hostler [11]

$$k(r_0, r_0, \varepsilon_1) = 2Zr_0^2 e^{-2Zr_0} \left[-\frac{1}{2Zr_0} + \ln(2Zr_0) - 2Zr_0 - f(2Zr_0) + \gamma - \frac{5}{2} \right] \quad (26)$$

where

$$\begin{aligned} f(\rho) &\equiv \int_0^\rho \frac{e^x - 1 - x}{x^2} dx \\ &= -\left(\frac{e^\rho - 1 - \rho}{\rho^2} \right) + \text{Ei}(\rho) - \ln \rho - \gamma. \end{aligned} \quad (27)$$

The $1s$ quantum defect is thus given by

$$\delta_{1,F} \approx \frac{\lambda_F Z e^{-2Zr_0}}{1 + \lambda_F Z e^{-2Zr_0} \left[\frac{1}{2Zr_0} - \ln(2Zr_0) + 2Zr_0 + f(2Zr_0) - \gamma + 1 \right]} \quad (28)$$

Under the further approximation that $r_0 \ll 1$ (bohr)

$$\delta_{1,F} \approx \frac{\lambda_F Z (1 - 2Zr_0)}{1 + \lambda_F / 2r_0} \quad (29)$$

In the more detailed derivation given elsewhere [7], it was shown that Eq. (29) applies more generally to *all* bound hydrogen-like s -states.

For $\lambda_F > 0$, say the $F = 1$ state of hydrogen, the quantum defect (29) converges uniformly to zero as $r_0 \rightarrow 0$. Thus for a repulsive deltafunction potential, the energy reverts to its unperturbed Coulomb value. For $\lambda_F < 0$, say the $F = 0$ state of hydrogen, Eq. (29) remains valid so long as $|\lambda_F|/2r_0 \ll 1$. The quantum defect

goes through "resonance" near $r_0 = |\lambda_F|/2$. The condition $|\delta| \ll 1$ is violated so that the entire derivation becomes invalid. The desired limit can however be obtained by considering the asymptotic forms of Eqs. (15) and (19) as $k \rightarrow \infty$ (or $\nu \rightarrow 0$). From formulas given in Buchholz [9]

$$\Gamma(1 - \nu)M_\nu(2kr_0)W_\nu(2kr_0) \rightarrow 1 \quad \text{as } k \rightarrow \infty. \quad (30)$$

Thus

$$-\frac{\lambda_F}{4kr_0^2} \approx 1 \quad (31)$$

or

$$k \approx |\lambda_F|/4r_0^2. \quad (32)$$

The limit $k \rightarrow \infty$ does indeed correspond to $r_0 \rightarrow 0$ for negative λ_F . By virtue of (16), $E_\nu \rightarrow -\infty$ as $r_0 \rightarrow 0$, showing that all bound states are pulled down to $-\infty$ by an attractive Fermi potential. Velenik *et al.* [12], using variational arguments, arrived at the same conclusions with regard to repulsive and attractive deltafunction potentials added to a Coulombic system.

By expanding the quantum defect (29) in powers of λ_F and substituting into (18), one obtains a perturbation expansion of the hyperfine interaction energy. As shown in Ref. [7], in the limit $r_0 \rightarrow 0$, the first-order term approaches the Fermi formula

$$E^{(1)} = \lambda_F |\psi_n(0)|^2 \quad (33)$$

while all higher-order perturbation contributions diverge.

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