Energy-dependent Hamiltonians, charge densities, and recoil effects*

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Two recent papers are shown to be related, and the unifying ingredient is an energy-dependent Hamiltonian.

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Recently Dress *et al.*[1] have measured the two-photon capture rate of subthermal neutrons on protons. Their results are 10^{+3}– 10^{4} bigger than expected and have an unusual spectral distribution. This experiment was performed in response to the calculations of Adler,[2] who suggested that non-orthogonality of initial and final states could lead to a much larger result than one would normally expect. This suggestion, revolutionary though it may seem, was prompted by the remarks of Breit and Rustgi,[3] who noted that energy-dependent potentials caused by meson exchanges in the nucleus could modify the conventional orthogonality relationship. Recently Riska[4] has pointed out that the energy-dependent potentials do produce orthogonal wave functions, but the conventional orthogonality relationship is modified and depends on the potential, in agreement with deForest.[5]

This problem, as emphasized by Riska, is reducible to the two-channel problem. The two channels for simplicity may be taken to be the "bare" nucleus and nucleus plus one pion, respectively, with the channel coupling potential creating and destroying a meson, which is virtual for the problem under discussion. As shown by Riska, the orthogonality problem arises when the equations of motion for the two channels are reduced to effective one-channel equations. However, since the original wave functions were orthonormal, *some* orthonormality relations must hold for the reduced wave functions.

Intimately related to this problem are the contributions of meson exchanges to nuclear charge and current operators. We follow the nomenclature used in the pioneering work of Chemtob and Rho[6] (CR) and illustrate in Fig. 1(a) the "recoil" contribution and in Fig. 1(b) the disconnected diagram which leads in perturbation theory to the "normalization" correction. The meson exchange in Fig. 1(b) is, of course, responsible for the nuclear force. Chemtob and Rho demonstrated in an appendix of their classic paper that the nuclear wave functions of their model were not normalized in the conventional manner and a normalization factor was introduced to account for this. It is clear from their derivation that their wave functions correspond to an energy-dependent potential and it is inappropriate to approximate these wave functions with ordinary Schrödinger wave functions obtained from energy-independent potentials. Recently, it has been shown[7] that Fig. 1(b), when renormalized according to the conventional methods of time-dependent perturbation theory, cancels that part of the recoil term of Chemtob and Rho which necessitated the normalization factor. This procedure can be shown to be precisely in accordance with the requirement that the nuclear

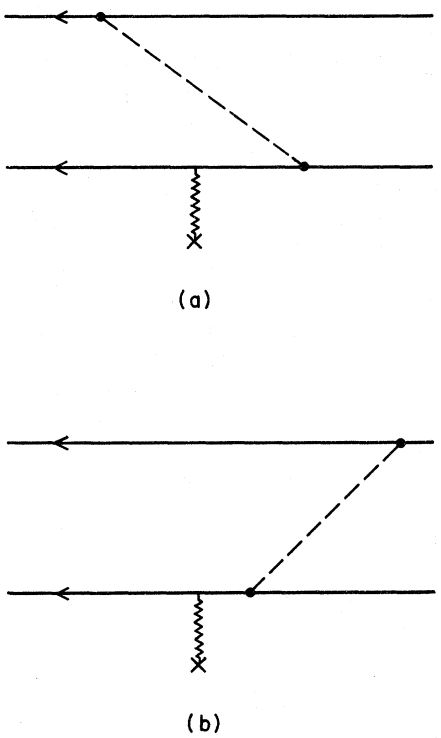

FIG. 1. Recoil graph contribution to meson-exchange charge or current operator (a) and disconnected graph (b) which leads to renormalization.

potentials be energy independent. Since the method of CR was used recently by Jackson, Landé, and Riska[8] to calculate corrections to the deuteron charge form factor, it is worthwhile to demonstrate, using a model whose physics is not in doubt, that the cancellation does indeed take place.

Also related to these problems is the work of McGee,[9] who investigated inelastic scattering of electrons from deuterons. McGee's procedure in developing the effective electromagnetic interaction between nucleons in a nucleus resulted in a momentum-dependent charge distribution. We will show that the definition of the charge density is not unique and may be chosen to have a momentum dependence similar to McGee's. We will also show that the form the charge density takes is intimately related to the possible energy dependence of the potential.

Although the two-channel problem is not unfamiliar, detailed properties of its solution are probably unfamilar to most physicists, so we resort to a two-channel problem which is familiar. The insight we are seeking does not depend on the details of the two-channel problem, but on the basic structure of the problem itself. The Dirac equation may be regarded as a two-channel problem which connects positive energy states of the nucleon (or other fermion) to the negative energy states. The gap between these sets of states is $2m$, where m is the nucleon mass, and this is sufficiently large that an expansion in powers of $(1/m)$ is efficacious for most applications in atomic and nuclear physics. The expansion procedure eliminates the lower two components of the four-component spinors, which are necessary for a description of the negative energy states, in terms of the upper two components, which are large for the positive energy solutions we will treat. Equivalently, "pair" contributions[6] are eliminated in terms of effective operators. The conventional approach to this reduction is the Foldy-Wouthuysen (FW) transformation[10] which produces a two-component wave function and energy-independent effective Hamiltonian. Our procedure will yield the same results, and thus constitutes a novel derivation of previously obtained results, but at the same time will shed light on the three problems discussed above.

We write the Dirac equation for a particle of mass m interacting with a scalar potential V_S and a vector potential V_V in terms of the upper component wave function ψ_1 and lower component wave function ψ_2 for an energy $E \equiv m+\epsilon$:

$$(m+V_S+V_V)\psi_1 = E\psi_1 - \vec{\sigma}\cdot\vec{p}\,\psi_2, \tag{1a}$$

$$(E+m+V_S-V_V)\psi_2 = \vec{\sigma}\cdot\vec{p}\,\psi_1. \tag{1b}$$

The lower equation may be inverted to produce

$$\psi_2 = \frac{1}{E+m+V_S-V_V}\,\vec{\sigma}\cdot\vec{p}\,\psi_1, \tag{2a}$$

$$(V_S+V_V)\psi_1 + \vec{\sigma}\cdot\vec{p}\left[\frac{1}{E+m+V_S-V_V}\right]\vec{\sigma}\cdot\vec{p}\,\psi_1 = \epsilon\psi_1. \tag{2b}$$

The second term in Eq. (2b) is an energy-dependent contribution to the Hamiltonian, $\Delta H(\epsilon)$. A natural, though inadequate, approximation is to assume $\epsilon, V_S, V_V \ll m$ and replace the bracketed factor by $2m$, resulting in the nonrelativistic Schrödinger equation for ψ_1. We wish to work to order $(v/c)^2$ past the nonrelativistic approximation, and to do this it is necessary to expand the denominator to first order, which yields after some algebra

$$\Delta H(\epsilon) = \frac{\vec{p}^2}{2m} - \frac{\vec{p}^4}{8m^3} + \frac{\vec{\nabla}^2 V_V}{8m^2} + \frac{\vec{\sigma}\cdot\vec{\nabla}(V_V - V_S)\times\vec{p}}{4m^2} - \frac{\{\vec{p}\,;\{\vec{p}, V_S\}\}}{8m^2} - \{\epsilon - H_0, \vec{p}^2/8m^2\}, \tag{3}$$

where $H_0 = \vec{p}^2/2m + V_v + V_s$ is the nonrelativistic Hamiltonian. All the terms except the first and last define the relativistic corrections to H_0 of lowest order (ΔH) and are precisely the same as those derived using the FW transformation in Ref. 11. Defining $H = H_0 + \Delta H$, we can write Eq. (2b) in the approximate form

$$\left\{\epsilon - H, \frac{1}{2} + \frac{\vec{p}^2}{8m^2}\right\}\psi_1 = 0, \tag{4}$$

which is not the Schrödinger equation. It may be manipulated into Schrödinger form by defining

$$\psi^S = (1+\vec{p}^{\,2}/8m^2)\psi_1, \tag{5}$$

so that we obtain finally

$$(\epsilon - H)\psi_S = 0. \tag{6}$$

The definition (5) for the Schrödinger wave function was obtained from the FW transformation in Ref. 12. The charge density may also be obtained in the same way. For convenience, we examine the matrix element of an arbitrary "even" operator, $O(x)$, which does not mix upper and lower components. These parts of O are O_1 and O_2, respectively. Using Eq. (2a) the matrix element of O between states m and n has the form

$$\begin{aligned}\langle m\,|\,O\,|\,n\rangle &= \psi_{1m}^{\dagger}O_1\psi_{1n} + \psi_{2m}^{\dagger}O_2\psi_{2n} \\ &= \psi_{1m}^{\dagger}\Bigg(O_1 + \vec{\sigma}\cdot\vec{p}\,\frac{1}{E_m+m+V_S-V_V} \\ &\quad \times O_2\,\frac{1}{E_n+m+V_S-V_V}\,\vec{\sigma}\cdot\vec{p}\Bigg)\psi_{1n}.\end{aligned} \tag{7}$$

For our purposes we may replace each denominator in Eq. (7) by $2m$, while higher-order terms may be obtained by expanding these factors if desired:

$$\langle m|O|n\rangle \cong \psi_{1m}^{\dagger}(O_1 + \{\vec{p}^2/8m^2, O_2\} + [\vec{\sigma}\cdot\vec{p}, [O_2/8m^2, \vec{\sigma}\cdot\vec{p}]])\psi_{1n} . \tag{8}$$

The charge density is a special case with $O_1 = O_2 = \rho(x)$, with ρ a δ function. Performing the commutators in Eq. (8), the resulting terms are the usual Darwin-Foldy and spin-orbit contributions to the density.[10] The FW procedure also produces these terms, but *not* the second term. The reason is the definition in Eq. (5). If we replace ψ_1 by ψ^S the extra term disappears to order $(v/c)^2$. The orthogonality relationship is deduced by taking $O = 1$:

$$\langle m|n\rangle = \delta_{mn} = \int \psi_{1m}^{\dagger}(1 + \vec{p}^2/4m^2)\psi_{1n} = \int \psi_m^{S\dagger}\psi_n^S , \tag{9}$$

which shows that the conventional orthonormality relation is satisfied by ψ^s and the complete wave function ψ, while ψ_1 satisfies a modified relationship. Indeed, the reason for this behavior is that ψ_1 satisfies an energy-dependent Hamiltonian problem, while ψ and ψ^S satisfy an ordinary one. While it is true that if ψ is normalized in the ordinary way, ψ_1 is not so normalized, it is not sufficient to account for this by multiplying ψ_1 by an appropriate constant,[6] since the orthogonality relationship cannot be changed by this device.

This model problem has a one-to-one correspondence to problems involving meson exchanges. The meson exchange in Fig. 1(b) involves a propagator while the meson is "in the air" and this leads to an energy-dependent potential. Similarly, the recoil contribution in Fig. 1(a) involves two propagators while the meson is in the air and is identical in form to the second term in Eq. (7). The formalism with the energy-dependent potential has, of course, the same difficulties we saw in Eq. (9), and a recoil term (the Z operator of CR) analogous to the $\vec{p}^2$ term in Eq. (8). Switching to an energy-independent potential, which is necessary if we wish to use Schrödinger wave functions in the calculation, is accomplished by an identity similar to Eq. (5), which, upon substituting into the recoil matrix element, cancels the Z-operator term of CR and Ref. 8. The new representation, unlike the old, has conventionally orthonormal wave functions. Isotopic considerations plus other approximations eliminated the analog of the last term in Eq. (8) in Ref. 8. Thus, their entire recoil contribution should be dropped. Finally, we have the novel interpretation of the Darwin-Foldy and spin-orbit contributions to the density as recoil corrections.

We also note that if we perform a nonunitary transformation which reintroduces momentum dependence into the charge density (i.e., $\vec{p}^2$ terms), we will automatically change the wave function which will then correspond to an energy-dependent Hamiltonian. The charge density of McGee,[9] which contains $\vec{p}^2$ terms, therefore requires an energy-dependent nuclear Hamiltonian, and does not correspond to ordinary Schrödinger wave functions.

In summary, we have solved the nonrelativistic reduction of the Dirac equation in a novel way which allowed us to identify the recoil and normalization terms of Chemtob and Rho. The major part of the recoil term, used in the calculation of Jackson, Landé, and Riska, cancels if we insist on using energy-independent potentials in calculating wave functions. The remaining terms are the well-known contributions obtained by the FW procedure. The transformation from an energy-dependent Hamiltonian to an energy-independent one restores the orthonormality relationship from an unconventional one to the usual one. Finally, the form the charge density takes depends intimately on the form the dynamics takes. All of our conclusions are consistent with the previous work of Feldman,[13] Blomqvist,[14] and others[15] on the meson exchange problem.

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