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On the spectra of atoms and hadrons

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For relativistic closed systems, an operator is explained which has as stationary eigenvalues the squares of the total cms energies, while the wave function has only half as many components as the corresponding Dirac wave function. The operator's time dependence is generalized to a Klein-Gordon equation. It ensures relativistic kinematics in radiative decays. The new operator is not hermitian.

Energy levels of bound states are calculated by a variety of methods, which include relativity at least approximately. In atomic theory, the equation $H\psi_D = E\psi_D$ is used, where H is the n-body Dirac-Breit Hamiltonian, and ψ_D is an n-electron Dirac spinor with 4^n components. For half a century, great hopes were attached to the Bethe-Salpeter equation, for example in the calculation of positronium spectra [1]. Most of these methods have been adapted to hadrons, namely to mesons as quark-antiquark bound states and baryons as three-quark bound states. New methods such as nonrelativistic quantum electrodynamics (NRQED) and numerical calculations on a space-time lattice have been added. In this note, the recent extension of another new method to radiative decays is presented. Its time-independent form is similar to $H\psi_D = E\psi_D$, namely $M^2\psi = E^2\psi$, but ψ has only half as many components as ψ_D. It applies only to closed systems, where E denotes the total cms energy. For atoms, this implies a relativistic inclusion of the nucleus, which is of little practical importance. It is relativistically exact, which does not mean that it is exact. Rather, relativity ensures a symmetry which is lost if only one of the constituents is treated nonrelativistically. It is most important for the lighter mesons and baryons which have so far resisted any quantitative treatment. If one will ever find a reliable M^2 for mesons and baryons, it will automatically contain the relativistic kinematics of radiative decays. This kinemetics is very simple: In the emission of a photon of energy $\hbar\omega$, momentum conservation endows the system with a recoil momentum $\boldsymbol{P} = -\hbar\boldsymbol{k}$ opposite to the photon momentum, with $k = \omega/c$. The resulting photon energy is

$$\hbar\omega = (E^2 - E'^2)/2E, \tag{1}$$

where E' is the total energy of the final state in its own cms. The photon spectrum calculated from Dirac's time-dependent perturbation theory, $i\hbar\partial\psi_D/\partial t = H\psi_D$, disagrees with (1), with the single exception of the radiation from Landau levels in a constant magnetic field. The amount of disagreement depends on the number of relativistic recoil corrections in H. Via dispersion relations, the photon spectrum also affects the Lamb shift of energy levels.

For two-body atoms such as muonium ($e^-\mu^+$) or positronium (e^-e^+), M^2 was first derived approximately from the Dirac-Breit equation [2], later directly from the two-body S-matrix of perturbative QED [3]. It is discussed extensively in [4], with the notation $M^2 = 2h$. For the eigenvalues of M^2, particle theorists sometimes use the symbol of one of the three Mandelstam variables, $s = E^2$. The E^2 -form has recently been derived from the Dirac-Breit equation for arbitrary n [5].

In the following, units $\hbar = c = 1$ will be used, and $i\hbar\partial/\partial t$ will be abbreviated as ∂_t. The time-dependent version of M^2 was first found empirically by noting that

$$i\partial_\tau \psi(\tau) = M^2(\tau)\psi(\tau), \quad \tau = t/E \tag{2}$$

does reproduce (1) [6]. Trusting Lorentz invariance, this equation is extended in a forthcoming review [7] to a Klein-Gordon equation,

$$\Box\psi = M^2\psi, \quad \Box = \nabla^2 - \partial^2_{t,lab}, \tag{3}$$

where t_{lab} is the lab time of the moving atom or hadron. The eigenvalue of ∇^2 is $-\boldsymbol{P}^2$, which by definition vanishes in the cms (the atomic rest system). There, one has $t_{lab} = t,\ -\partial_t^2\psi = M^2\psi$. In first-order perturbation theory, (2) follows from (3) by the ansatz $\psi = exp\{-iEt\}\psi(\tau)$. For a free stable atom or hadron of energy E_{lab} and momentum $\boldsymbol{P}$, (3) is the quantum version of the Einstein relation,

$$E^2_{lab} - c^2\boldsymbol{P}^2 = E^2 \equiv M^2c^4. \tag{4}$$

Here c is re-inserted in order to display the form $E = Mc^2$, even though the relevant operator is M^2. It is the mass-square operator. In relativity, the mass itself appears only in nonrelativistic expansions.

The essential point is of course to construct M^2. However, before going into details, it may be adequate to mention a property which is unusual and even embarrassing, at least for physicists: M^2 is not hermitian. There are in fact two equivalent stationary versions,

$$M^2\psi = E^2\psi, \quad (M^2)^\dagger\chi = E^2\chi. \tag{5}$$

It is of course known that also non-hermitian operators may have real eigenvalues, but in the past this has been regarded as an avoidable complication. Decomposing M^2 into its hermitian and antihermitian components,

$$M^2 = M_h^2 + M_a^2, \quad (M^2)^\dagger = M_h^2 - M_a^2, \tag{6}$$

it is clear that the real eigenvalue E^2 cannot depend on the sign of M_a^2. If one of the two equations applies, the other applies as well.

The construction of M^2 is best explained by using Dirac spinors, with a separate set of Dirac gamma-matrices for each particle (the nucleus is also treated like a Dirac particle). From the individual chiral matrices γ_i^5 (with eigenvalues ± 1), one constructs a total chirality matrix, $\gamma^5_{tot} = \gamma^5_1 \dots \gamma^5_n$, which also has eigenvalues ± 1. The corresponding components of ψ_D are called ψ and χ, respectively:

$$\gamma^5_{tot}\psi = \psi, \quad \gamma^5_{tot}\chi = -\chi. \tag{7}$$

As γ^5_{tot} is not conserved, the Dirac-Breit equation couples components of opposite total chiralities, but one component is easily eliminated in terms of the other, resulting in (5).

Obviously, the elimination of components turns the original hermitian operator into a nonhermitian one in the subspace.

The appearance of E^2 follows from a coordinate transformation and the subsequent elimination of components. The substitutions $\boldsymbol{r}_i = E\boldsymbol{r}_{i,E}$ and the definition $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$ allow one to rewrite $V_{ij} = q_i q_j / r_{ij} = EV_{ij,E}$, and correspondingly for the momentum operators. A factor E may be extracted from the whole Dirac-Breit operator (provided one refrains from "positive-energy projectors"). Elimination of half of the components transforms the factor E into E^2.

For two fermions, the approximate construction of M^2 from the Dirac-Breit operator leads to amazing cancellations. The Dirac-Breit operator is linear in the particle momenta $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$. With $\boldsymbol{p}_1 = -\boldsymbol{p}_2 \equiv \boldsymbol{p}$ in the cms, the expected bilinear terms cancel out. A somewhat tricky transformation $\psi = C_1\psi_1$ eliminates the kinetic energy of particle 2 altogether. The final result is an effective Dirac equation similar to that of hydrogen, with four components for the effective electron, and another factor of two for the hyperfine interaction from the spin of the effective proton. It remains valid for positronium, apart from the virtual annihilation interaction.

In general, eigenstates of chirality are not parity eigenstates. The parity transformation contains the product of the Dirac matrices $\gamma_i^0 = \beta_i$, $\beta_{tot} = \beta_1 \ldots \beta_n$. For even n, however, β_{tot} commutes with γ_{tot}^5, and common eigenstates do exist. In this case, each equation (5) is separately parity invariant. For $n = 2$, the nonhermiticity of M^2 is restricted to the hyperfine operator, which also contains a factor E^{-2}.

Other operators expected from the Dirac-Breit equation for $n = 2$ are V^2 and retardation operators, which are part of the Breit operators. They all disappear from M^2. A more precise derivation of M^2 uses the S-matrix of QED, which must be reduced from its standard 16×16-form to 8×8 before the interaction is abstracted as the Fourier transform of the T-matrix. If one restricts oneself to the one-photon exchange, the absence of V^2 is trivial. If on the other hand one works with the traditional 16-component formalism, one also obtains an operator V^2 at some stage of the calculation. This operator is cancelled by a two-photon exchange contribution at a later stage.

When the S-matrix for three fermions is constructed from two-fermion submatrices, one finds that also the case $n = 3$ has some cancellations. Otherwise, $n = 3$ is infinitely more complicated than $n = 2$. The cms condition $\boldsymbol{p}_1 + \boldsymbol{p}_2 + \boldsymbol{p}_3 = 0$ is not nearly as helpful as $\boldsymbol{p}_1 + \boldsymbol{p}_2 = 0$. β_{tot} and γ_{tot}^5 anticommute for $n = 3$, and β_{tot} exchanges ψ with χ. This creates a rather strange situation: The two separate equations (5) are coupled by the parity transformation and by nothing else.

The absence of odd powers of E can be traced back to the CPT theorem of quantum field theory. According to Feynman, a plane wave $exp\{-ik_0t + i\boldsymbol{kr}\}$ is associated not only with a particle of energy k_0 moving forward in time, but also with an antiparticle of energy $-k_0$ moving backwards. A formalism which reproduces the S-matrix of QED and QCD includes automatically antiatoms and antihadrons as solutions of energies $-E$ of closed systems.

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