Extremum principles for the determination of relativistic ground-state energies

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The spectrum for the Dirac equation for a particle in a potential $V(\mathbf{r})$ includes, in addition to any bound-state energies, a continuum from mc^2 to ∞ and a continuum from $-mc^2$ to $-\infty$. This renders useless an application of Rayleigh-Ritz theory, where one estimates the energy of the lowest state. Various possibilities exist, including working with matrix elements of H^2 (see ref.2 of [142]) or of $1/H$. [R. M. Hill and C. Krauthauser, Phys. Rev. Lett. **72**, 2151 (1994). See also Z. Chen and S.P. Goldman, Phys. Rev. A **45**, 1722 (1992).] The continuum in the latter case has the desirable feature of running from $-mc^2$ to mc^2. While these approaches can work well for one-body problems, they might well be very difficult to implement for many-body problems.

We considered a different approach for the one-body problem, one which might possibly be generalized to the many-body problem [142]. One introduces the Casimir projection operators Λ_+ and Λ_-, where $\Lambda_+\Psi$ and $\Lambda_-\Psi$ give the positive and negative energy components, respectively, of the Dirac wave function Ψ. We then have $\Psi = \Psi_+ + \Psi_-$. We now consider the Dirac equation with a potential V, with Ψ replaced by $\Psi_+ + \Psi_-$, and with an energy $\mathcal{E}$ which is the bound-state energy of interest. Operating on that equation with Λ_+ gives one equation, operating with Λ_- gives a second. Combining the two equations by formally eliminating Ψ_-, we arrive at

$$\Lambda_+(H_0 + V + VG_-(\mathcal{E})V - \mathcal{E})\Lambda_+\Psi_+ = 0, \tag{1}$$

where $G_-(\mathcal{E})$ is a Green function.

The interpretation of Eq.(1) is straightforward. The particle when in positive energy space is subject to a potential V. In addition it can be perturbed by V to make a transition to negative energy space; it then propagates in that space until, again perturbed by V, it makes a transition back to positive energy space.

(Those of you familiar with nuclear theory will recognize the strong analogy to the Feshbach operator formalism, used in the scattering of a particle by a compound target. We denote the incident particle by A. For simplicity, we assume that A is distinguishable from the target particles, and that its incident energy lies below the lowest threshold for excitation of the target. Λ_+ is replaced by P, and Λ_- by Q; P projects the full scattering wave function on to the ground state of the target and Q on to the excited states. Particle A interacts with the target in its ground state, experiencing a potential V. In addition, the target can be perturbed by A and make a virtual transition to an excited state, with A then propagating differently, until the target is again perturbed by A and returns to its ground state.)

Eq.(1) may be readily interpretable, but we are now faced with the difficulty that $\mathcal{E}$ appears twice, in $G_-(\mathcal{E})$ and in the usual fashion. We must therefore make two calculations. First, we must obtain a variational estimate of $G_-(\mathcal{E})$. This is accomplished using a *maximum* principle (whose origin may be traced to the fact that $\mathcal{E}$ lies above the continuous spectrum of $\Lambda_- H \Lambda_+$).

We must then make a variational estimate of $\mathcal{E}$, which we do by using the standard Rayleigh-Ritz *minimum* principle. Having used both a maximum and a minimum principle, the estimate of $\mathcal{E}$ which is arrived at is neither an upper bound nor a lower bound. However, since each of the calculations is based on an extremum principle, the estimate of $\mathcal{E}$ should be rather accurate. A merit of the approach is that it is not limited to central potentials; the problem might be that of an electron in the field of two nuclei.

(We return now to the Feshbach projection formalism. The objective is to obtain an effective potential, to be used in a study of a non-relativistic scattering problem. If one were to attempt to use the formalism to obtain an estimate of the binding energy of the composite system, one would be in a situation similar to that of determining $\mathcal{E}$ defined by a Dirac equation.)

For an approach which might seem to be very different but is in fact rather similar, see J.D. Talman, Phys. Rev. Lett. **57**, 1091(1986).

In addition to studying the energy of a particle in a potential we also considered two interacting particles, labeled a and b, with no external potential. The analog of Λ_+ is then $\Lambda_{+a}\,\Lambda_{+b}$, the product of two one-particle projection operators.

L. Rosenberg, Phys. Rev. A **47**, 1771 (1993), extended the above approach to two electrons and a nucleus.