UWThPh-1982-18

SPECTRAL CONCENTRATION IN THE NONRELATIVISTIC LIMIT

F. Gesztesy
Institut für Theoretische Physik (2860000 AT)
Universität Graz
A-8010 Graz, Austria

H. Grosse and B. Thaller
Institut für Theoretische Physik (6711000 AT)
Universität Wien
A-1090 Wien, Austria

Abstract

First order relativistic corrections to the Schrödinger operator according to Foldy and Wouthuysen are rigorously discussed in the framework of singular perturbation theory. For Coulomb plus short-range interactions we investigate the corresponding spectral properties and prove spectral concentration and existence of first order pseudoeigenvalues in the nonrelativistic limit.

The Foldy-Wouthuysen method [1-3] of studying the nonrelativistic limit played an important role for the interpretation of the Dirac equation. This formal procedure is of interest because it leads to the definition of relativistic corrections to Schrödinger operators for a spin 1/2 particle in external fields. Similar corrections are also used to calculate relativistic effects in two electron atoms [3]. Thus it is worthwhile to investigate rigorously the effects of these strongly singular perturbations, and to show how one has to deal with them. For spherically symmetric potentials V(r) the first order relativistic correction obtained from the partial wave Dirac operator reads in $L^2((0,\infty);dr)$ [2,3]

$$h_{\ell,\kappa}(c) = h_\ell + V + \frac{1}{c^2} k_{\ell,\kappa} \tag{1}$$

where ($\hbar = 2m = e = 1$)

$$h_\ell = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} = -\frac{d^2}{dr^2} + \frac{\kappa(\kappa+1)}{r^2} \tag{2}$$

$$k_{\ell,\kappa} = -h_\ell^2 - \frac{\kappa}{r}\frac{dV}{dr} + \frac{1}{2}\frac{d^2V}{dr^2} \tag{3}$$

and $\kappa = \pm 1, \pm 2, \ldots \pm(j+1/2), \ldots$ for $j = \ell \mp 1/2$ is the Dirac quantum number (eigenvalue of $-(\vec{\sigma}\cdot\vec{L}+1)$). j is the total angular momentum. For each ℓ except $\ell = 0$ there are two values of κ, namely ℓ, $-\ell-1$, according to the two possibilities of adding orbital and spin angular momentum [2,3]. Typically we consider interactions of the form

$$V(r) = \frac{\gamma}{r} + V_s(r), \qquad \gamma \in \mathbb{R}, \tag{4}$$

where the short-range part V_s is twice continuously differentiable and vanishes together with its first and second derivatives at infinity.

The terms in (3) are just the familiar kinetic energy correction, the spin-orbit term, and the so-called Darwin term. Due to the Coulomb part γ/r of V(r) the spin-orbit term contains $\gamma(\kappa+1)/r^3$. For $\ell \neq 0$ (i.e. $\kappa \neq -1$) this term is strongly singular at the origin and would destroy self-adjointness when added to the Schrödinger operators $h_\ell + V$. The situation is improved by the presence of $-h_\ell^2/c^2$ because the inequality

$$\int \frac{|\psi(r)|^2}{r^4}\,dr \leq \frac{1}{(-\frac{3}{4}+\ell(\ell+1))^2}\int |(h_\ell\psi)(r)|^2 dr, \quad \ell \geq 1, \qquad (5)$$

allows one to define $-h_\ell^2 + \gamma(\kappa+1)/r^3$, $\ell \geq 1$, as a self-adjoint operator by interpreting the sum in the sense of quadratic forms ($h_\ell + V$ is then infinitesimally bounded relativ to this operator). For $\gamma \neq 0$ and $\ell = 0$ part of the Darwin term reduces formally to a δ-interaction centered at the origin. The correct way to define $h_{\ell=0,\kappa=-1}(c)$ in that case is to choose a particular self-adjoint extension of

$$-\frac{d^2}{dr^2} + \frac{\gamma}{r} - \frac{1}{c^2}\frac{d^4}{dr^4}$$

(different from the Friedrichs extension) by imposing boundary conditions at the origin [5,6]. Due to the point-like nature of this δ-interaction it is only present for $\ell = 0$ ($\kappa = -1$), i.e. for impact parameter equal to zero. Thus, if $\gamma \neq 0$, the treatment of the case $\ell = 0$ is considerably different [5] and for simplicity we assume in the following $\ell \geq 1$ as long as $\gamma \neq 0$.

The usual way to treat relativistic corrections for eigenvalues is to apply first order perturbation theory in equation (1). For the pure Coulomb potential $V(r) = \gamma/r$, $\gamma < 0$, the results can be compared with the exact solution of the Dirac equation. In that case first order perturbation theory indeed gives the correct expansion of the Dirac eigenvalue up to the order $1/c^2$ [2,3]. From a mathematical point of view this is surprising at first sight because the relativistic corrections in equation (1) are so singular that regular perturbation theory is not applicable. In fact, it is just the other way round: As we have already mentioned one can prove $h_\ell + V$ to be an infinitesimally small operator perturbation of the self-adjoint operator $-k_{\ell,\kappa}/c^2$ for any finite c [4]. Equation (5) shows that $-h_\ell^2/c^2$ is the dominating term in (1) and since it is negative one concludes that $h_{\ell,\kappa}(c)$ is bounded from above. More precisely, it can be shown [4] that the essential spectrum of $h_{\ell,\kappa}(c)$ is given by

$$\sigma_{ess}(h_{\ell,\kappa}(c)) = \sigma_{ess}(h_\ell - \frac{1}{c^2}h_\ell^2) = (-\infty, \frac{c^2}{4}], \qquad (6)$$

i.e. $h_{\ell,\kappa}(c)$ has no discrete eigenvalues at all in the energy region $(-\infty, c^2/4]$. Instead, there may be eigenvalues in the region

$[c^2/4,\infty)$, their location and number depending on the details of the interaction. (Consider for example $V(r) = \gamma/r$, then there are intinitely many eigenvalues accumulating at $c^2/4$ if $\gamma > 0$. For $\gamma < 0$ there may be eigenvalues if $\kappa+1 \leq 0$, but no eigenvalues occur for $\kappa+1 > 0$.) All these eigenvalues escape like $c^2/4 + o(c^2)$ to $+\infty$ in the nonrelativistic limit.

Thus one gets the feeling that the spectrum of $h_{\ell,\kappa}(c)$ has no physical meaning. Discrete eigenvalues have energies $E \geq c^2/4$ for which relativistic $(1/c^2)$-corrections are by no means small, and the addition of higher order corrections would change the spectrum again considerably. Also the kinetic energy correction is only meaningful for energies small compared with $c^2/2$, but the continuous energy spectrum (5) arises from the fact that at high energies, no matter how large c may be, the term $-h_\ell^2/c^2$ will ultimately dominate h_ℓ. On the other hand, for the usual nonrelativistic atomic bound states the expectation value $\langle h_\ell \rangle$ of the kinetic energy is small compared to the rest mass of electrons (some eV versus 0.5 MeV), so that $-\langle h_\ell^2 \rangle/c^2$ indeed will be a small correction in units of the rest energy. In the following we want to show that something like a "trace" of the bound states of $h_\ell + V$ remains when the relativistic correction $-k_{\ell,\kappa}/c^2$ is "switched on", and we investigate in what sense first order perturbation theory has tc be interpreted. The mathematical concepts to describe these facts are found to be spectral concentration and pseudoeigenvalues [7-12].

First of all we have to state in what sense $h_{\ell,\kappa}(c)$ approaches $h_\ell + V$ when c tends to infinity. It turns out that [4]

$$(h_{\ell,\kappa}(c) - i)^{-1}\phi \xrightarrow[c\to\infty]{s} (h_\ell + V - i)^{-1}\phi \qquad (7)$$

for all $\phi \in L^2((0,\infty);dr)$. This strong resolvent convergence implies that all bounded continuous functions of $h_{\ell,\kappa}(c)$ converge strongly.

Now, let H_ε, $\varepsilon \geq 0$, be a family of self-adjoint operators in some Hilbert space H converging for $\varepsilon \to 0$ in the strong resolvent sense to H_0 and let E_0 be an isolated, nondegenerate eigenvalue of H_0 with associated eigenvector ψ_0. $E_0 + \varepsilon E_1$ is called a first order pseudoeigenvalue of H_ε if and only if there exists ψ_ε with

$$\psi_\varepsilon \xrightarrow[\varepsilon\to 0]{s} \psi_0 \qquad (8)$$

$$\frac{1}{\varepsilon}\,[H_\varepsilon - E_0 - \varepsilon E_1]\psi_\varepsilon \xrightarrow[\varepsilon\to 0]{s} 0.$$

The common way to interpret equation (8) is to say that $E_0 + \varepsilon E_1$ represents to first order the real part of a pole of the Green's function of H_ε on the (unphysical) second sheet [11]. This pole, if it lies near the real axis, would cause a resonance with long life time which may be physically indistinguishable from a bound state. Thus, ψ_ε is something like an "almost stationary" state.

Mathematically, the existence of a first order pseudoeigenvalue for H_ε is equivalent to the phenomenon of first order spectral concentration [7]: One says that the spectrum of H_ε is asymptotically concentrated to first order in the interval $I_\varepsilon = (E_0 + \varepsilon E_1 - o(\varepsilon), E_0 + \varepsilon E_1 + o(\varepsilon))$ if and only if for all $\phi \in L^2((0,\infty);dr)$

$$P_\varepsilon(I_\varepsilon)\phi \xrightarrow[\varepsilon\to 0]{s} \psi_0(\psi_0,\phi) \tag{9}$$

($P_\varepsilon(I)$ denotes the spectral measure of H_ε associated with the interval I, $(\ ,\ )$ is the scalar product). Roughly speaking, this means that in an expansion of ϕ with respect to the eigenfunctions of H_ε the energies in a small neighbourhood I_ε of $E_0 + \varepsilon E_1$ are the most important ones.

For generalizations of this concept to spectral concentration of order $p > 0$ and to isolated eigenvalues of finite multiplicity re refer to the literature [7-12].

In our case E_0 is a negative eigenvalue of $h_\ell + V$, and E_1 is given by first order perturbation theory, i.e.

$$E_1 = (\psi_0, k_{\ell,\kappa}\,\psi_0). \tag{10}$$

Can one prove that $E_0 + E_1/c^2$ is a first order pseudoeigenvalue for the family of operators $h_{\ell,\kappa}(c)$? The basic assumption one has to verify is that ψ_0 lies in the domain of $k_{\ell,\kappa}$ [7-10]. For $\gamma = 0$, i.e. for short-range interactions $V_s(r)$ this is indeed the case for all $\ell \geq 0$. But for $\gamma \neq 0$ this condition is not fulfilled for $\ell = 1$ which can be seen from the fact that the corresponding eigenfunction ψ_0 is not in the domain of $\gamma(\gamma+1)/r^3$ (ψ_0 behaves like r^γ at the origin and therefore ψ_0/r^3 is not

square integrable). This indeed prevents the application of the abstract theory outlined above for $\ell = 1$ in spite of $(\psi_0, k_{\ell,\kappa}\,\psi_0)$ being still finite when considered as a quadratic form. Existing theorems [12] then only predict spectral concentration to lower order than one [5].

We summarize these results on first order pseudoeigenvalues in the following

Theorem: Let $V(r) = \gamma/r + V_s(r)$, $\ell \geq 2$ if $\gamma \neq 0$ or $\ell \geq 0$ if $\gamma = 0$. If E_0 is an eigenvalue of $h_\ell + V$ with corresponding eigenfunction ψ_0, and $E_1 = (\psi_0, k_{\ell,\kappa}\,\psi_0)$, then $E_0 + E_1/c^2$ is a first order pseudoeigenvalue of $h_{\ell,\kappa}(c)$, i.e. the spectrum of $h_{\ell,\kappa}(c)$ is asymptotically concentrated to first order in the interval $(E_0 + E_1/c^2 - o(1/c^2), E_0 + E_1/c^2 + o(1/c^2))$ as $c \to \infty$.

We finally note that in the case of short-range interactions, i.e. if $\gamma = 0$, the above theorem generalizes to systems including nonspherically symmetric interactions $V_s(\vec{x})$ and magnetic vector potentials $\vec{A}(\vec{x})$ decreasing at infinity [4].

Acknowledgement

One of us (B.T.) thanks Prof. W. Thirring for his kind hospitality at the University of Vienna.

References

[1] L.L. Foldy, S.A. Wouthuysen, Phys. Rev. 78 (1950) 29.

[2] A. Messiah, Quantum Mechanics, Vol. 2 (North Holland, Amsterdam, 1970), and
J.D. Bjørken, S.D. Drell, Relativistic Quantum Mechanics (McGraw-Hill, New York, 1964).

[3] T.P. Das, Relativistic Quantum Mechanics of Electrons (Harper & Row, New York, 1973) and the references cited therein.

[4] F. Gesztesy, H. Grosse, B. Thaller, First order relativistic corrections and spectral concentration, to appear.

[5] F. Gesztesy, H. Grosse, B. Thaller, in preparation.

[6] S. Albeverio, F. Gesztesy, R. Høegh-Krohn, L. Streit, Charged particles with short range interactions, preprint 1982.

[7] R.C. Riddell, Pac. J. Math. 23 (1967) 377.

[8] C.C. Conley, P.A. Rejto, in: Perturbation theory and its applications in quantum mechanics, ed. C.H. Wilcox (Wiley, New York, 1966).

[9] K. Veselic, Glasnik Math. Ser. III., 4 (1969) 213 and 231.

[10] T. Kato, Perturbation Theory of Linear Operators (Springer, Berlin, Heidelberg, New York, 1980),
M. Reed, B. Simon, Methods of Modern Mathematical Physics, Vol. 4 (Academic Press, New York, San Francisco, London, 1978)
W. Thirring, A Course in Mathematical Physics, Vol. 3 (Springer, New York, Wien, 1979).

[11] J.B. Mc.Leod in: Perturbation theory and its applications in quantum mechanics, ed. C.H. Wilcox (Wiley, New York, 1966),
J.S. Howland, Trans. Am. Math. Soc. 162 (1971) 141.

[12] W.M. Greenlee, J. Func. Anal. 5 (1970) 66.