Levinson's Theorem

Levinson's theorem, published in 1949, relates some properties of bound states and of scattering states for a potential $V(r)$ that satisfy simple conditions at $r = o$ and at $r \sim \infty$. The theorem fascinated theorists and stimulated the publication of many papers that extended the theory to include spin, tensor forces, non-local potentials, and relativistic effects, for example. There not has been much research in the area in recent years, largely because the theorem has been of limited use – there re some cases where it can be helpful. On the other hand the theorem has retained its intellectual appeal and is often discussed in textbooks and cited in research papers.

We begin with a rough statement of the theorem. Consider zero-energy scattering by a potential, and ignore subtleties associated with zero-energy bound states. (The subtleties arise for zero angular momentum – $\ell = 0$ - only. There are normalizable zero-energy bound states for $\ell > 0$ but not for $\ell = 0$.) Let $d_\ell(E)$ be the phase shift for a particle incident at an energy E with an angular momentum $\ell\hbar$. $d_\ell(E)$ is given an absolute meaning, that is, with no ambiguity with regard to multiples of π, by setting $d_\ell(E = \infty) = 0$. The theorem states that $d_\ell(0) = N_\ell p$, where N_ℓ is the number of bound states with angular momentum $\ell\hbar$.

We extended the theorem to include scattering by a repulsive Coulomb potential [139].

The relevant phase shift for this case is the phase shift relative to the Coulomb phase shift.

Now it's clear that the important extension would be to scattering by a compound system. One immediate difficulty is that whereas single channel scattering is characterized by a phase shift $d_\ell(E)$, scattering as $E \sim \infty$ is a multi-channel process. Another difficulty is that $d_1(E)$ for $E \sim 0$ is defined by $A_\ell = -\lim_{k \to o} \tan d_\ell(h) \big| k$, but A_ℓ undergoes infinite jumps as one introduces better and better tried wavefunctions; the jumps occur when a bound state appears.

Years ago, Swan provided the essence of an extension to electron-atom scattering in a very suggestive paper in which he attempted to take into account the Pauli exclusion principle. (He also, much less successfully, discussed nucleon-nucleus scattering.) Assume that the atom can support N_ℓ composite bound states, ions consisting of the atom and an electron, the latter with angular momentum $\ell\hbar$. Assume further that, in the shell model, the atom contains $N_{Pauli\,\ell}$ closed shells with angular momentum $\ell\hbar$. Swan's basic idea was that $d_\ell(0)$ consists of a sum of two terms, one for composite bound states, as for potential scattering, and one for states excluded by the Pauli principle. The basic idea is fine, but the proofs involved many-body analyticity theorems that have not been proven. The statements he makes for $\ell > 0$ are not generally correct. It was one purpose to provide a rigorous extension of Levinson's theorem to scattering by a compound system.

Before discussing any formal proofs, we consider a simple model that provides some physical insight. We assume an independent-particle model for a neutral target atom, with zero

spin-orbit coupling, and with an effective one-body potential $V_{eff}(r)$. We assume further that the incident electron is subject to the same potential. $d_\ell(0)$ is taken to be the number of modes of the radial function $R_{o\ell}(r)$ of the incident e^-, the subscript o denoting that the incident energy is zero. To simplify the discussion we discuss three concrete cases of e^- scattering. In the first case the target is the Ne atom in its closed shell $(ls)^2(2s)^2(2p)^6\ {}^1S_o$ ground state; there are no composite bound states, that is, no bound states $(Nere^-)$. For $\ell > 1$, the effective one-body potential $V(r)$ cannot support any bound states and by the original (one-body) Levinson theorem $d_\ell(0) = 0$ for $\ell > 1$. For $\ell > l$, $V(r)$ can support one bound state, a $2p$ state, and thus $d_1(0) = p$. For $\ell = 0$ $V(r)$ can support two bound states, $1s$ and $2s$, and $d_0(0) = 2p$.

variational bound on the scattering length A if no composite bound state exists, just as in the usual application of the theorem it provides a variational bound on the energy if only one bound state exists. If we treat the zero energy state as if it were a bound state, we can apply Sturm-Liouville theory to the Schroedinger equation for angular momentum $\ell\hbar$ and a potential $V(r)$. One then obtains the same results as obtained just above using the Levinson theorem for potential scattering.)

Our second example is scattering by Na in its $(1s)^2(2s)^2(2p)^6 3s\ \ {}^2S_{\frac{1}{2}}$ ground state, with an open $3s$ shell. We again have $d_\ell(0) = 0$ for $\ell > 1$. Since there is a 2p state, it follows that $d_1(0) = p$. For $\ell > 0$ we must distinguish between the spin-symmetric spatially-antisymmetric triplet states and the spin-antisymmetric spatially-symmetric singlet state. The $3s$ state can be occupied by the incident e^-; the spatial wave functions for $Na + e^-$ is then symmetric but the spin function is antisymmetric, so that the Pauli principle is satisfied. Only the $1s$ and $2s$ states are excluded, so the Pauli principle gives a contribution to the phase shift of $2p$. There is one composite bound state, so that the full phase shift is $3p$. For the triplet state the incident e^- cannot occupy the open $3s$ state, for the $Na + e^-$ wavefunction would be symmetric in space and spin. Thus, the $1s$, $2s$ and $3s$ states re excluded, and the Pauli phase shift is $3p$, as is the full phase shift since there are no composite bound states for the triplet state.

(Table I in the published article [170] has a major typo: Na appears twice. The correct entry is the one for which the full phase shift is $3p$ for both the singlet and triplet cases.)

For our third example the target is the open-shell $(is)^2(2s)^2(2p)\ \ {}^2P_J$ ground state of B - the value of J is irrelevant – and we consider an $\ell = 2$ incident e^-. As just one indication of the complexity of this example, note that if the total orbital angular momentum, target plus incident e^-, is unity, the emergent electron can have $\ell = 2$ or $\ell = 0$ and we are faced with a multichannel scattering situation.

The discussion thus far represents a definition of $d_\ell(0)$. We showed in our papers that the definition is a useful one. Thus, we provided a new approach to a proof of Levinson's

theorem for potential scattering, based on the model structure of the zero-energy scattering wavefunction [138]. We made some progress toward the extension of the theorem to scattering by a compound system in [140], but in an attempt to make the extension we were confronted with the difficulty, in addition to those noted above, that little is known of the model structure of bound state or scattering wavefunctions for many fermion systems. We now give a schematic description of how we bypassed this difficulty. We constructed a one-body function $F(r_1)$ by taking the inner product of the antisymmetrized bound state wavefunction $y(1,2,...,2)$ with the antisymmetrizied product $U(1,2,...,Z+1) = A\Phi(Z_0+1)\Psi$, where A is the antisymmetrization operator; Φ is the free one-particle zero-energy wavefunction [169]. For short-range potentials Φ would be $r^{\ell+1}$; for e^- - atom scattering, Φ takes into account, asymptotically, the long-range $1/r^4$ polarization potential. To obtain $F(r_1)$ for other than He or He, we took $y(1,2,...,Z)$ to be the Hartree-Fock wavefunctions given in analytic form by Clemente. The number of modes of $F(r_1)$ for the many atoms for which we checked – some with closed shells only and some with one open shell – agreed with the number obtained by adding the number of composite bound states and the number of states excluded by the Pauli principle [170].

A very interesting and desirable – and remarkable – feature of the definition of $F(r_1)$ is that the dynamics of the scattering process plays no role whatsoever; only the free one-body function Φ enters. (This may not be quite as remarkable as it first appears to be; presumably the dynamics is largely determined by the Pauli principle.) Furthermore the bound-state wavefunctions need not be exact; the check is on a discrete entity, an integer, not a continuous variable.

The arguments which led to our introduction of $F(r_1)$ included the introduction of a "length phase" h_ℓ [51]. Thus, an essential element of Levinson's theorem is that a single-channel scattering amplitude for a given value of ℓ is characterized by a phase shift $d_\ell(E)$ and that $d_\ell{}^{(E)}$ can be defined in an absolute fashion, though physically it is only $d_\ell \bmod p$ which is meaningful. We defined h_ℓ by writing $A_\ell = a_\ell \cot h_\ell$, where a_ℓ is arbitrary and the length phase h_ℓ varies continuously as we introduce more and more terms in our trial scattering function while A_ℓ undergoes infinite jumps when a bound state is introduced. The arugments also included theorems on variational bounds in scattering theory which Lenny Rosenberg and I developed over the years, going back to 1959.

Rosenberg, Phys. Rev. C 58, (1385) (1998), extended the theorem to the nuclear scattering processes $n-p$, $n-d$, and $p-d$. He took tensor forces into account in the $n-p$ process, and therefore had to consider eigemphase shifts rather than phase shifts. For the $n-d$ and $p-d$ processes, tensor forces were ignored; in the $p-d$ case Coulomb forces had to be accounted for.