# Levinson's Theorem and the Nodes of Zero-Energy Wave Functions for Potentials with Repulsive Coulomb Tails

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Levinson's theorem relation phase shifts and bound states, developed for a short-range potential $V_{\rm sh}$, is extended to scattering by $V_{\rm sh}+V_{\rm C}$, where $V_{\rm C}$ is a repulsive Coulomb potential. The subtleties associated with $L=0$, $E=0$ bound states for $V_{\rm sh}$ alone are not present for $V_{\rm sh}+V_{\rm C}$. Information is also obtained on the relation between the nodal structure of the zero-incident-energy wave function and the number of bound states; some extensions to scattering by a compound target are possible.

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Levinson's theorem, which provides the only generally valid relation between phase shifts and bound states, is one of the classic results of scattering theory. Recall that for scattering by a short-range potential $V_{\rm sh}(r)$, where $r^2V_{\rm sh}(r)\sim 0$ for $r\sim 0$ and $r^3V_{\rm sh}(r)\sim 0$ as $r\sim\infty$, the theorem states that $\delta_L(0)-\delta_L(\infty)=N_L\pi$, where $\delta_L(k)$ is the phase shift for the partial wave of angular momentum $L$ for wave number $k$ and $N_L$ is the number of bound states (all of which have normalizable wave functions) of the given $L$. [We ignore for the moment the possibility of zero-energy (i.e., $E=0$) bound states.] We provide here a sketch of the extension of that fundamental theorem to include the very important case of potentials of the form $V_{\rm sh}(r)+V_{\rm C}(r)$, where $V_{\rm C}(r)=Z_1Z_2e^2/r$ is a repulsive Coulomb potential; our extension applies to the differences of the phases with and without $V_{\rm sh}$.

The usual proof of the theorem for $V_{\rm sh}$ alone is based on the analytic properties of the scattering amplitude in momentum space and our extension is given in that form. We very recently presented a new proof of the theorem for $V_{\rm sh}$.[1] The proof, which proceeds in coordinate space and is based on a minimum principle for the scattering length $A_L$, provides new insights *and* a new result, information on the nodal structure of the $E=0$ wave function $u_L(r)$ for scattering by $V_{\rm sh}$. This nodal-structure result is also extended here to include potentials of the form $V_{\rm sh}+V_{\rm C}$. We remark that a knowledge of the nodal structure of $u_L(r)$, the $E=0$ limit of the scattering wave function $w_L(k,r)$, provides a very useful check on numerical calculations of this function. Furthermore, when combined with a nodal definition of $\delta_L(k)$—a definition in terms of the nodal points of the free wave function and $w_L(k,r)$—a knowledge of the nodal structure enables one to give an absolute definition of $\delta_L(0)$ and thereby of $\delta_L(k)$. Most significantly, such nodal-structure analyses can be extended to a class of multiparticle single-channel scattering problems where they may be applied, in a useful way, independently of the validity of Levinson's theorem. One frequently introduces models of the multiparticle scattering problem based on the existence of an effective potential seen by each particle; analysis of the nodal structure of the model wave function provides explicit information which can be of considerable physical interest.[2]

Levinson's theorem is clearly invalid for scattering by $V_{\rm C}(r)$ or by a hard-core potential $V_{\rm hc}(r)$. Thus, $V_{\rm C}$ can support no bound states and its phase shift, conventionally denoted by $\sigma_L(k)$, has the values $\sigma_L(0)=\infty$ and $\sigma_L(\infty)=0$. Similarly, $V_{\rm hc}$ can support no bound states and its phase shift is 0 at $k=0$ and $-\infty$ at $k=\infty$. But consider scattering by $V_{\rm hc}+V_{\rm sh}$. It is then known[3] that the phase shift defined as the *difference* between the phase shifts associated with $V_{\rm hc}+V_{\rm sh}$ and with $V_{\rm hc}$ alone *does* satisfy Levinson's theorem. The corresponding result is transparently valid for the sum of two short-range potentials; one need merely apply Levinson's theorem to the sum of the two potentials and to one of them, and take the difference. These results suggest that the difference $\delta_L(k)=\Delta_L(k)-\sigma_L(k)$ between the phase shifts associated with $V_{\rm C}+V_{\rm sh}$ and with $V_{\rm C}$ alone might satisfy Levison's theorem, and we will show that this is indeed the case. [Parenthetically, we note that $\delta_L(\infty)=0$ for $V_{\rm sh}$, so that Levinson's theorem for $V_{\rm sh}$ can be written as $\delta_L(0)=N_L\pi$. When possible, the elimination of any reference to $\delta_L(\infty)$ can be a great advantage, as, for example, in an attempt to extend any results to scattering by a compound system.]

Following the standard procedure[3] we define the Jost function $\mathscr{F}_L(k)$ for $V_{\rm sh}+V_{\rm C}$ as the Wronskian $W(f_L,\phi_L)$, where $f_L(k,r)$ is the Jost solution, behaving as $\exp(ikr-\eta\ln 2kr)$ for $r\sim\infty$; here $\eta=(ka)^{-1}$ and $a=\hbar^2/mZ_1Z_2e^2$, with $m$ the reduced mass. The regular analytic solution $\phi_L(k,r)$ is defined by the boundary condition $\phi_L(k,r)\sim r^{L+1}$, $r\sim 0$. The analyticity of $\mathscr{F}_L(k)$ in the upper-half $k$ plane can be proven by straightforward generalization of the standard proof applicable for $V_{\rm sh}$, with the restrictions on the behavior of $V_{\rm sh}$ at $r\sim 0$ and at $r\sim\infty$ unchanged. [That proof required the development of relatively simple bounds on the free wave functions $j_L(kr)$ and $n_L(kr)$, for $k$ complex. Those bounds, *and* bounds on the standard Coulombic functions $F_L$ and $G_L$, follow easily from a knowledge of the forms of the functions at $r \sim 0$ and $r \sim \infty$.] Though division by the rather simple $V=0$ Jost function is often not explicitly remarked on, it is important to recognize that in the standard derivation of Levinson's theorem for $V_{\rm sh}$ one deals with the ratio of two Jost functions, one associated with $V=V_{\rm sh}$ and the other $V=0$. A $k^{-1}$ singularity present in each Jost function at $k=0$ then disappears from the ratio. Similarly, the results indicated above for the sum of two short-range potentials relative to one and for $V_{\rm hc}+V_{\rm sh}$ vs $V_{\rm hc}$ can be based on a ratio of Jost functions. The essential point is that for real positive $k$ the argument of the Jost function for a given $v$ is the negative of the phase shift for that $V$, so that the argument of the ratio of Jost functions is the *difference* $\delta_L(k)$, often the physically interesting entity. The above considerations suggest that in the case of present interest one should introduce the ratio $R_L(k)=\mathscr{F}_L(k)/\mathscr{F}_L^{(\rm C)}(k)$, where $\mathscr{F}_L^{(\rm C)}(k)$ is the Jost function for $V_{\rm C}$ alone. An explicit expression for $\mathscr{F}_L^{(\rm C)}(k)$ is known.[3] Here we need only note that this function is analytic and has no zeros in the upper-half $k$ plane, and has an essential singularity at $k=0$, and for positive real $k$ has the phase $-\sigma_L(k) = -\arg\Gamma(L+1+i\eta)$. With $\Delta_L(k)$ defined as the phase shift associated with $V_{\rm sh}+V_{\rm C}$, the argument of $R_L(k)$ is $-[\Delta_L(k)-\sigma_L(k)] \equiv -\delta_L(k)$, the phase shift that we wish to study.

We now subject $R_L(k)$ to the standard analysis, that is, we integrate its logarithmic derivative over a contour in the complex $k$ plane. This contour consists of the real axis, but passes over the origin, and an infinite semicircle in the upper-half plane. Along with the fundamental analyticity property, and the identification of the phase of $R_L(k)$ as $-\delta_L(k)$, the theorem makes use of the following additional properties, familiar from a study of the analogous short-range case: (i) $R_L^*(k)=R_L(-k)$, $k$ real. (ii) The zeros of $R_L(k)$ in the upper-half plane lie on the imaginary axis, are simple, and correspond to bound states in $V_{\rm sh}+V_{\rm C}$. (iii) $R_L(k)\sim 1$ for $k\sim\infty$ in the upper-half plane and remains finite as $k$ approaches the real axis from above. If there is an $E=0$ bound state the rate at which $R_L(k)$ vanishes for $k\sim 0$ must be determined and here the presence of $V_{\rm C}$ plays a particularly interesting role. Thus, in analogy to Newton's treatment[4] of $V_{\rm sh}$, one readily shows, starting from $R_L(k)=W(f_L,\phi_L)\mathscr{F}_L^{(\rm C)}(k)$ and $R_L(0)=0$, that, as $k\sim 0$,

$$dR_L(k)/dk \sim b_L k \int \phi_L^2(0,r)\,dr, \tag{1}$$

where $b_L$ is a nonvanishing constant. Since $\phi_L(0,r)$, the $E=0$ bound-state wave function, has the asymptotic form $r^{1/4}\exp[-(8r/a)^{1/2}]$, the integral (over the range 0 to $\infty$) is finite, and of course nonvanishing, for all $L$. It follows that $R_L(k)\sim\beta_L k^2$ for $k\sim 0$, with $\beta_L\neq 0$. In this regard the $V_{\rm sh}+V_{\rm C}$ problem is simpler than the $V_{\rm sh}$ problem. In the latter case, $E=0$ bound-state wave functions behave as $r^{-L}$ for $r\sim\infty$ and are therefore normalizable only for $L>0$. Therefore, the analog of Eq. (1) fails to determine the behavior of the $L=0$ Jost function for $k\sim 0$. Further analysis[4] shows, in fact, that it behaves as $k$, not $k^2$, so that the contribution to the contour integral from the neighborhood of $k=0$ differs for $L=0$ and $L>0$. Thus, the precise form of the theorem for $V_{\rm sh}$ is $\delta_L(0)=(N_L+\frac{1}{2}\zeta_L)\pi$, where $N_L$ is the number of bound states, including $E=0$ bound states if and only if they are normalizable, where $\zeta_L=0$ for $L>0$, and where $\zeta_0=0$ if there is no $E=0$, $L=0$ bound state and $\zeta_0=1$ if there is. (An $L=0$, $E=0$ state is only "half bound."[3]) For $V_{\rm sh}+V_{\rm C}$, on the other hand, we have simply $\delta_L(0)=N_L\pi$.

We turn now to a discussion of the nodal structure of $u_L(r)$ for $V_{\rm sh}+V_{\rm C}$. The nodal structure of the eigenfunction of a discrete state, the bound-state wave function in the present context, is a subject on which there is a large body of literature going back to the work of Sturm and Liouville (SL). The SL studies are based on a minimum principle for the eigenvalue which characterizes the $n$th state, its energy $E_n$. Correspondingly, the information gained on the nodal structure of $u_L(r)$ for $V_{\rm sh}$ was based on a minimum principle[5] for the parameter which characterizes $u_L(r)$, namely, $A_L$. Now one may readily extend the minimum principle to the $A_L$ associated with $V_{\rm C}+V_{\rm sh}$. Under the assumption, for simplicity, that $V_{\rm sh}$ vanishes exponentially for $r\sim\infty$, $u_L(r)$ behaves asymptotically as a linear combination of Coulombic (rather than free) and (decreasing) irregular solutions and $A_L$ is the relative amplitude of these solutions. The trial $E=0$ scattering function has a similar asymptotic form. Use of the minimum principle in the manner described earlier[1] leads to the conclusion that $u_L(r)$ has $n_L$ nodes, where $n_L$ is the number of negative-energy bound states in the potential $V_{\rm sh}+V_{\rm C}$. To convert this result to a statement concerning $\delta_L(0)$, we adopt the nodal definition of $\Delta_L(k)$ and make use of the known threshold behavior of $\delta_L(k)$. The latter is obtained from the effective-range expansion

$$K_L(k^2)\sim -A_L^{-1}+\tfrac{1}{2}r_L k^2+\ldots,\quad k\sim 0.$$

We define $K_L(k^2)/k^{2L+1}\Pi(\eta)$ as $C^2(\eta)\cot\delta_L(k) + 2\eta[\mathrm{Re}\,\psi(i\eta)-\ln\eta]$, where $\psi(i\eta)$ is the digamma function and

$$\Pi(\eta)=\prod_{s=1}^{L}\left(1+\frac{\eta^2}{s^2}\right),\quad C^2(\eta)=\frac{2\pi\eta}{\exp(2\pi\eta)-1}.$$

If there is no $E=0$ bound state one finds that $\delta_L(0)=n_L\pi=N_L\pi$. If an $E=0$ bound state exists then $|A_L| = \infty$ and $\cot\delta_L(k)$ diverges in the $E=0$ limit, for all $L$, because of the exponential decay of the Coulomb penetration factor appearing in the effective-range function $K_L$. The leading term in the effective-range expansion is now proportional to $k^2$, and by careful investigation of this term one finds that $\delta_L(0) = (n_L+1)\pi = N_L\pi$, in agreement with our previously derived statement of Levinson's theorem for $V_{sh}+V_C$.

We note that the value of $\delta(0)(\text{mod}\pi)$ follows immediately from effective-range theory [more explicitly, from the fact that the effective-range function $K_L(k^2)$ is analytic in $k^2$ near $k^2=0$] both for $V_{sh}$ and for $V_{sh}+V_C$. Thus, for $A_L$ finite or infinite, we find for $V_{sh}+V_C$ for all $L$ and for $V_{sh}$ for $L>0$ that $\cot\delta_L(0)=\infty$ and therefore that $\delta_L(0)(\text{mod}\pi)=0$; for $V_{sh}$ and $L=0$, the argument is the same if $A_L$ is finite, but if $|A_L|=\infty$ one finds that $\cot\delta_L(0)=0$ and therefore that $\delta_0(0)(\text{mod}\pi)=\frac{1}{2}\pi$. For $V_{sh}$ plus an *attractive* Coulomb potential effective-range theory was used to show[6] that $\delta_L(0)(\text{mod}\pi)=\mu(\infty)\pi$, where $\mu(n)$ is the quantum defect, defined by writing the $n$th energy level as $E_n = -(\hbar^2/2m)/a^2[n-\mu(n)]^2$. Because of the appearance of infinitely many bound states the two approaches developed here for the derivation of the theorems of the Levinson type are not directly applicable to the $V_{sh}$ plus attractive Coulomb case. However, one can trace the change in the number of nodes introduced by the existence of $V_{sh}$ and relate that to the number of additional bound states due to this potential. This leads to the relation $\delta_L(0)=\mu(\infty)\pi$ as the analog of Levinson's theorem, with the value of the largest integer contained in $\mu(\infty)$ representing the number of additional bound states due to $V_{sh}$. The fact that $\delta_L(0)/\pi$ need not be an integer may be traced to the behavior of the Coulomb penetration factor in the zero-energy limit; it is exponentially vanishing in the repulsive Coulomb case but remains finite for $V_C$ attractive.

Turning now to scattering by a compound target, we note that SL theory for the nodal structure of a bound-state wave function is not limited to a particle in a potential, though the information obtainable on a many-body wave function is not always as complete as for a one-body wave function. We previously extended the many-body SL nodal theory to the nodal structure of the wave function for a particle incident with zero energy on a compound system when no Coulomb tail is present. The further extension when there is a repulsive tail is trivial, since a minimum principle for $A_L$ for that case is known. (When applied to proton or neutron scattering by *very* heavy nuclei the theorem might well be useless since there will be very many states of the projectile plus target system lying below the energy level of the target elsewhere.

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