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TOPICAL REVIEW

The Levinson theorem

Zhong-Qi Ma

Institute of High Energy Physics, Beijing 100049, People's Republic of China

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Abstract
The Levinson theorem is a fundamental theorem in quantum scattering theory, which shows the relation between the number of bound states and the phase shift at zero momentum for the Schrödinger equation. The Levinson theorem was established and developed mainly with the Jost function, with the Green function and with the Sturm–Liouville theorem. In this review, we compare three methods of proof, study the conditions of the potential for the Levinson theorem and generalize it to the Dirac equation. The method with the Sturm–Liouville theorem is explained in some detail. References to development and application of the Levinson theorem are introduced.

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1. Introduction

The Levinson theorem is a fundamental theorem in quantum scattering theory, which shows the relation between the number of bound states and the phase shift at zero momentum. Levinson first established and proved this theorem in 1949 [47] for the Schrödinger equation with a spherically symmetric potential $V(r)$. In a book on quantum scattering theory [72], Newton rigorously re-proved the Levinson theorem for the Schrödinger equation and studied the case with a half bound state. The spherically symmetric potential $V(r)$ in the Schrödinger equation is assumed to satisfy the asymptotic condition

$$\int_0^\infty \mathrm{d}r\, r|V(r)| < \infty. \tag{1.1}$$

This condition is necessary for the nice behaviours of the wavefunction at the origin and at infinity. In the analytic continuation of the Jost function to the complex plane of the momentum k, the additional demand for the potential $V(r)$ is required (see p 337 of [72]):

$$\int_0^\infty \mathrm{d}r\, r^2|V(r)| < \infty. \tag{1.2}$$

Under those conditions the phase shift $\delta_\ell(k)$ at zero momentum with the angular momentum ℓ is related to the number of bound states n_ℓ with the same angular momentum:

$$\delta_\ell(0) - \delta_\ell(\infty) = \begin{cases} (n_\ell + 1/2)\pi, & \text{a half bound state occurs,} \\ n_\ell \pi, & \text{the remaining cases.} \end{cases} \tag{1.3}$$

This is the Levinson theorem for the Schrödinger equation, where a half bound state may occur when $\ell = 0$. A zero-momentum state is called a half bound state if its wavefunction is finite but does not decay at infinity fast enough to be square integrable. As is well known, there is degeneracy of states for the magnetic quantum number due to the spherical symmetry. Usually, this degeneracy is not expressed explicitly in the statement of the Levinson theorem.

It is understood that the Levinson theorem (1.3) will not hold if the restriction (1.1) for the potential $V(r)$ is violated. However, the additional demand (1.2) for the potential $V(r)$ was required in the analytic continuity of the Jost function, and it is too strong for the Levinson theorem.

The phase shift $\delta_\ell(k)$ appears in a trigonometric function so that it is determined up to a multiple of π. In the Levinson theorem (1.3), the phase shift $\delta_\ell(0)$ at zero momentum is determined with respect to the phase shift $\delta_\ell(\infty)$ at infinity momentum, where the phase shift is assumed to be continuous with respect to the momentum k. In the usual case when the potential has a nice behaviour, the phase shift $\delta_\ell(\infty)$ is vanishing, but it may not in some special cases, where the appearance of the term $\delta_\ell(\infty)$ in the Levinson theorem will cause trouble [65, 96]. See the detail in section 5.

Most papers [3, 70, 85, 99] have been devoted to the proof of the Levinson theorem and its generalization based on the Jost function. In the proof, the Jost function is made the analytic continuation to the upper complex plane of k. The study of the analytic property and the multiplicities of zeros of the Jost function on the complex plane is quite complicated. It obstructs the generalization of the Levinson theorem to the relativistic cases [3, 44, 45, 85, 99].

Jauch [41] proved the Levinson theorem with the orthogonality and completeness relations for the eigenfunctions of the Hamiltonian, where the restriction (2) for the potential was released [96]. He applied the operator formulism of the scattering theory to the proof, which was similar to the method of the Green function [76]. The total number of the eigenstates of the Hamiltonian is proved to be invariant as the potential changes. In other words, the bound state is transformed from the scattering state or vice versa as the potential changes. This is an important idea for simplifying the proof of the Levinson theorem. Jauch [41] claimed that, if without any inelastic scattering, his conclusion is in principle suitable for the relativistic case. However, he did not give the explicit relativistic form of the Levinson theorem.

Ni [76] used the retarded Green function to explicitly prove the Levinson theorem for the Schrödinger equation and to generalize it for the Dirac equation and for the Klein–Gordon equation. Unfortunately, there were some mistakes in his proof for the relativistic cases. The correct statement of the Levinson theorem for the Dirac equation with a spherically symmetric potential was first proved with the retarded Green function [53]. The method of the Green function was also applied to generalization of the Levinson theorem for the relativistic cases in one or two spatial dimensions [11, 50–52]. In the proof with the Green function, the difference of total numbers of the eigenstates of the Hamiltonian with and without the potential is calculated. But it is a difference of two infinite quantities. In the proof, two limit processes are interchanged without a strict proof. The term of $\delta_\ell(\infty)$ still appears in the obtained Levinson theorem for the Schrödinger equation.

In a talk on monopole theory [103, 104], Professor C N Yang presented a new form of the Sturm–Liouville theorem for the coupled partial differential equations of first order. The proof of the Levinson theorem with the new form of the Sturm–Liouville theorem for the Schrödinger equation [54] is more simple, intuitive and easy for generalization than the previous methods. The term of $\delta_\ell(\infty)$ is removed in the obtained Levinson theorem. The additional demand (1.2) on the potential $V(r)$ is released. It becomes evident that as the potential changes, the phase shift at zero momentum jumps by π when a scattering state transforms into a bound state and vice versa. The modified form of the Levinson theorem when the potential $V(r)$ has a tail r^{-2} at infinity is easy to obtain [54] and holds for two counterexamples raised by Newton [72]. With the Sturm–Liouville theorem, the Levinson theorem is generalized to the Dirac equation [55, 56, 58], to the Klein–Gordon equation [48], as well as to the non-local interaction [59]. Recently, the Levinson theorem was established for the cases with the arbitrary spatial dimensions [11, 24–27, 29, 35, 50, 51, 93], including one spatial dimension [4–7, 16, 18, 20, 28, 30, 34, 42, 52, 61, 62].

Another approach to the Levinson theorem with the Sturm–Liouville theorem was presented by Iwinski–Rosenberg–Sprouch [36], where the nodal structure of zero-energy wavefunctions was related to the number of bound states through the Sturm–Liouville theorem and then to the zero-energy phase shift. They extended the method to scattering in a potential with repulsive Coulomb tail [37], to the multiparticle single-channel scattering [38, 88] and to the electron–atom scattering [89].

The Levinson theorem was also established for a charged particle moving in the field of the Aharonov–Bohm magnetic flux with a short-range potential [49], for a fermion-monopole system [68, 102] and for time-periodic potential [7, 67]. The Levinson-type theorems were derived for the systems with non-central potentials [70, 78], for the KdV system [64], for the integral equation of the vertex function [17], for three-body systems [101] and for the eigenfrequency models of fluctuating fields at a sphaleron [2]. This theorem and the technique used in its proof were developed and applied in relation to the problems of fractional charge [9, 32, 57], regularized index [10] and anomalies in quantum field theories [12, 77], as well as in the method of bosonization [13, 100]. The technique was widely used in the inverse scattering method [18, 71, 73, 74], in the study of low momentum scattering [21, 22] and in the multichannel scattering with non-local and confining potentials [98]. The applications of this theorem to the two-dimensional electron gas [83, 84], to spontaneous fermion production [15], to cosmology [43, 90], to the second virial coefficient [33] and to the exact solutions of the Dirac equation with surface delta interactions [23] were investigated. The threshold behaviour of the Jost function for the atom polarization potential was evaluated up to the order k^4 [63]. The semiclassical version of the Levinson theorem was derived and applied to the sine-Gordon theory [39].

The plan of this review is as follows. We sketch the main idea of the proof of the Levinson theorem based on the Jost function in section 2 and on the Green function in section 3. In section 4, we first introduce the Sturm comparison theorem and then we show a new form of the Sturm–Liouville theorem where a phase angle is monotonic with respect to the energy. This monotonic property of a phase angle is the main spirit in the proof of the Levinson theorem with the Sturm–Liouville theorem. In terms of this method, the Levinson theorem is proved for the Schrödinger equation in section 4 and for the Dirac equation in section 6. Some special cases for the Schrödinger equation are discussed in section 5. Finally, a conclusion is given in section 7.

2. The Levinson theorem and the Jost function

Newton gave an elegant review [72] of the Levinson theorem based on the Jost function. In this section, we will sketch the main idea of this proof.

2.1. Solutions of the Schrödinger equation

The three-dimensional Schrödinger equation with a spherically symmetric potential $V(r)$ is

$$-\frac{\hbar^2}{2M}\,\nabla^2\,\psi(\boldsymbol{r},E,\lambda) = [E-\lambda V(r)]\,\psi(\boldsymbol{r},E,\lambda). \tag{2.1}$$

A real parameter λ is introduced for convenience and eventually λ is set to be 1. The radial function $R_\ell(r,k,\lambda)$ with the angular momentum ℓ satisfies the radial equation

$$\begin{aligned}&\psi(\boldsymbol{r},E,\lambda) = r^{-1}R_\ell(r,k,\lambda)Y_m^\ell(\hat{\boldsymbol{r}}),\\ &R_\ell''(r,k,\lambda)+[k^2-\lambda U(r)-\ell(\ell+1)r^{-2}]R_\ell(r,k,\lambda)=0,\\ &k=\sqrt{2ME}/\hbar, \qquad U(r)=2MV(r)/\hbar^2,\end{aligned} \tag{2.2}$$

where the prime denotes the derivative with respect to r. Provided that

$$\int_0^\infty \mathrm{d}r\, r|U(r)| < \infty, \tag{2.3}$$

$R_\ell(r,k,\lambda)$ is an entire function of λ for each fixed k and r, and an entire function of k for each fixed λ and r (see p 334 in [72]). Equation (2.3) demands the potential $U(r)$ be less singular than r^{-2} near the origin and to vanish at infinity faster than r^{-2}.

Equation (2.2) becomes the Bessel equation for $z(r)=r^{-1/2}R_\ell(r,k,\lambda)$ when the potential can be neglected:

$$z''+r^{-1}z'+[k^2-(\ell+1/2)^2r^{-2}]z=0. \tag{2.4}$$

Thus, the regular solution $R_\ell(r,k,\lambda)$ has the asymptotic behaviour at the origin like $\sqrt{r}J_{\ell+1/2}$. In this section, following Newton [72], we choose the normalization factor such that the regular solution $R_\ell(r,k,\lambda)$ satisfies the boundary condition at the origin:

$$\lim_{r\to 0} r^{-\ell-1}R_\ell(r,k,\lambda)=1. \tag{2.5}$$

Since the dependence on k in equation (2.2) is only via k^2, and the boundary condition of $R_\ell(r,k,\lambda)$ is independent of k, $R_\ell(r,k,\lambda)$ is an everywhere regular function of k^2, and an even function of k,

$$R_\ell(r,-k,\lambda)=R_\ell(r,k,\lambda). \tag{2.6}$$

In the analytic continuation to the complex value of k, one has

$$R_\ell^*(r,k^*,\lambda)=R_\ell(r,k,\lambda). \tag{2.7}$$

There are two linearly independent solutions for a linear differential equation of second order. Another solution of equation (2.2) is irregular with the behaviour $r^{-\ell}$ near the origin.

Two solutions $R_{\ell\pm}(r,k,\lambda)$ of equation (2.2) are defined from the boundary condition at infinity:

$$\begin{aligned}&\lim_{r\to\infty} \mathrm{e}^{\mp \mathrm{i}kr}R_{\ell\pm}(r,k,\lambda)=1,\\ &R_{\ell+}(r,k,\lambda)=R_{\ell-}(r,-k,\lambda)=R_{\ell-}(r,k^*,\lambda)^*.\end{aligned} \tag{2.8}$$

Generally speaking, $R_{\ell\pm}(r,k,\lambda)$ both are irregular at the origin. The regular solution $R_\ell(r,k,\lambda)$ is a combination of $R_{\ell\pm}(r,k,\lambda)$:

$$R_\ell(r,k,\lambda)=a_+(k,\lambda)R_{\ell+}(r,k,\lambda)+a_-(k,\lambda)R_{\ell-}(r,k,\lambda). \tag{2.9}$$

For a free particle, $\lambda=0$, one has

$$R_\ell(r,k,0)=\frac{(2\ell+1)!!}{k^{\ell+1}}\sqrt{\frac{\pi kr}{2}}J_{\ell+1/2}(kr)\xrightarrow{r\to\infty}\frac{(2\ell+1)!!}{k^{\ell+1}}\sin(kr-\ell\pi/2). \tag{2.10}$$

For a given λ, due to the restriction (2.3), $R_\ell(r, k, \lambda)$ with $E > 0$ is an oscillatory solution and describes a scattering state. The phase shift $\delta_\ell(k, \lambda)$ is introduced to describe the asymptotic behaviour of the scattering state at infinity:

$$R_\ell(r, k, \lambda) \propto \sin[kr - \ell\pi/2 + \delta_\ell(k, \lambda)], \qquad r \to \infty. \tag{2.11}$$

Comparing equation (2.11) with equation (2.9) one has

$$\frac{a_+(k, \lambda)}{a_-(k, \lambda)} = -\mathrm{e}^{\mathrm{i}[-\ell\pi + 2\delta_\ell(k,\lambda)]}. \tag{2.12}$$

The phase shift $\delta_\ell(k, \lambda)$ is determined from equation (2.11) up to a multiple of π. In comparison with equation (2.10), equation (2.11) implies a convention for the phase shift:

$$\delta_\ell(k, 0) = 0. \tag{2.13}$$

The phase shift is determined uniquely if $\delta_\ell(k, \lambda)$ with $k > 0$ is assumed to be a continuous function of λ.

When $E \leqslant 0$, a regular solution of equation (2.2) in the whole space does not always exist. If $a_-(\mathrm{i}\omega, \lambda) = 0$ in equation (2.9), there is a regular solution $R_\ell(r, \mathrm{i}\omega, \lambda)$ of equation (2.2), which describes a bound state at the energy $E = -\hbar^2\omega^2/(2M)$. In fact, $R_{\ell+}(0, \mathrm{i}\omega, \lambda) = 0$ in this case. Equivalently, the condition for the existence of a bound state can also be expressed as $a_+(-\mathrm{i}\omega, \lambda) = 0$ and $R_{\ell-}(0, -\mathrm{i}\omega, \lambda) = 0$.

As pointed out by Newton (p 337 of [72]), for the continuity of the derivative of $R_{\ell\pm}(r, k, \lambda)$ to include the point $k = 0$, the additional demand for the potential $U(r)$ is required:

$$\int_0^\infty \mathrm{d}r\, r^2|U(r)| < \infty. \tag{2.14}$$

If equations (2.3) and (2.14) hold, $R_{\ell+}(r, k, \lambda)$ for each r is an analytic function of k regular for Im $k > 0$ and a continuous function with a continuous k derivative in the region Im $k \geqslant 0$. The restriction (2.14) demands the potential $U(r)$ to vanish at infinity faster than r^{-3}. In fact, this restriction (2.14) is not necessary for the Levinson theorem [96], but is required in the proof for the Levinson theorem with the Jost function.

2.2. The Jost function

The Wronskian of any two solutions of equation (2.2) is defined as

$$W\left[R_\ell^{(1)}(r, k_1, \lambda_1), R_\ell^{(2)}(r, k_2, \lambda_2)\right] = R_\ell^{(1)}(r, k_1, \lambda_1)\frac{\mathrm{d}}{\mathrm{d}r}R_\ell^{(2)}(r, k_2, \lambda_2) - R_\ell^{(2)}(r, k_2, \lambda_2)\frac{\mathrm{d}}{\mathrm{d}r}R_\ell^{(1)}(r, k_1, \lambda_1). \tag{2.15}$$

By making use of the radial equation (2), one obtains

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}r}W\left[R_\ell^{(1)}(r, k_1, \lambda), R_\ell^{(2)}(r, k_2, \lambda)\right] &= R_\ell^{(1)}(r, k_1, \lambda)\frac{\mathrm{d}^2}{\mathrm{d}r^2}R_\ell^{(2)}(r, k_2, \lambda) - R_\ell^{(2)}(r, k_2, \lambda)\frac{\mathrm{d}^2}{\mathrm{d}r^2}R_\ell^{(1)}(r, k_1, \lambda)\\ &= \left(k_1^2 - k_2^2\right) R_\ell^{(1)}(r, k_1, \lambda)R_\ell^{(2)}(r, k_2, \lambda).\end{aligned} \tag{2.16}$$

Similarly, one has

$$\frac{\mathrm{d}}{\mathrm{d}r}W\left[R_\ell^{(1)}(r, k, \lambda_1), R_\ell^{(2)}(r, k, \lambda_2)\right] = -(\lambda_1 - \lambda_2)U(r)R_\ell^{(1)}(r, k, \lambda_1)R_\ell^{(2)}(r, k, \lambda_2). \tag{2.17}$$

When $k_1 = k_2 = k$ and $\lambda_1 = \lambda_2 = \lambda$,

$$\frac{d}{dr} W\big(R_\ell^{(1)}, R_\ell^{(2)}, k, \lambda\big) = 0,$$
$$W\big(R_\ell^{(1)}, R_\ell^{(2)}, k, \lambda\big) \equiv W\big[R_\ell^{(1)}(r, k, \lambda), R_\ell^{(2)}(r, k, \lambda)\big]. \tag{2.18}$$

The Wronskian $W\big(R_\ell^{(1)}, R_\ell^{(2)}, k, \lambda\big)$ is a constant with respect to r and can be evaluated in any r. For example, the Wronskian $W(R_{\ell+}, R_{\ell-}, k, \lambda)$ can be evaluated in the limit as $r \to \infty$:

$$W(R_{\ell+}, R_{\ell-}, k, \lambda) = -2ik. \tag{2.19}$$

Hence, the combinative coefficients $a_\pm(k, \lambda)$ of $R_\ell(r, k, \lambda)$ in equation (2.9) can be expressed by the Wronskians:

$$a_\pm(k, \lambda) = \pm \frac{W(R_{\ell\mp}, R_\ell, k, \lambda)}{2ik}. \tag{2.20}$$

The Jost function $\mathcal{J}_\ell(k, \lambda)$ and its auxiliary function $\mathcal{J}_{\ell-}(k, \lambda)$ are defined as

$$\mathcal{J}_\ell(k, \lambda) = \frac{k^\ell e^{-i\pi\ell/2}}{(2\ell+1)!!} W(R_{\ell+}, R_\ell, k, \lambda), \tag{2.21}$$

$$\mathcal{J}_{\ell-}(k, \lambda) = \frac{k^\ell e^{i\pi\ell/2}}{(2\ell+1)!!} W(R_{\ell-}, R_\ell, k, \lambda). \tag{2.22}$$

For real λ and complex k one has

$$\mathcal{J}_{\ell-}(-k, \lambda) = \mathcal{J}_\ell(k, \lambda), \qquad \mathcal{J}_{\ell-}(k, \lambda) = \mathcal{J}_\ell^*(k^*, \lambda). \tag{2.23}$$

Substituting the definitions of the Jost functions into equations (2.12) and (2.20), one obtains

$$\frac{\mathcal{J}_{\ell-}(k, \lambda)}{\mathcal{J}_\ell(k, \lambda)} = e^{i\pi\ell} \frac{W(R_{\ell-}, R_\ell, k, \lambda)}{W(R_{\ell+}, R_\ell, k, \lambda)} = e^{2i\delta_\ell(k,\lambda)}. \tag{2.24}$$

Due to the boundary conditions (2.5) and (2.8), equation (2.21) becomes

$$\mathcal{J}_\ell(k, \lambda) = \frac{k^\ell e^{-i\pi\ell/2}}{(2\ell-1)!!} \lim_{r\to 0} r^\ell R_{\ell+}(r, k, \lambda). \tag{2.25}$$

$\mathcal{J}_\ell(k, \lambda) = 0$ means that $R_{\ell+}(r, k, \lambda)$ is a regular solution of equation (2.2) such that it is proportional to $R_\ell(r, k, \lambda)$.

When $|k| \to \infty$ with $\mathrm{Im}\, k > 0$, the potential $\lambda U(r)$ in equation (2.2) can be neglected, and due to equation (2.10)

$$R_\ell(r, k, \lambda) \sim (2\ell+1)!!k^{-\ell-1} \sin(kr - \pi\ell/2). \tag{2.26}$$

In evaluating $W(R_{\ell+}, R_\ell, k, \lambda)$ of equation (2.21) at a large r, $\sin(kr - \pi\ell/2)$ in $R_\ell(r, k, \lambda)$ can be replaced with $i\, e^{-ikr+i\pi\ell/2}/2$ due to $\mathrm{Im}\, k > 0$,

$$\lim_{|k|\to\infty} \mathcal{J}_\ell(k, \lambda) = 1, \qquad \mathrm{Im}\, k > 0. \tag{2.27}$$

2.3. The Levinson theorem

In this subsection, we set $\lambda = 1$ and omit the argument λ in all functions. Under the restrictions (2.3) and (2.14), the Jost function $\mathcal{J}_\ell(k)$ is analytic and contains finite number of zeros in the upper half of complex plane of k so that

$$\frac{1}{2\pi i} \oint_C d \ln \mathcal{J}_\ell(k) = n, \tag{2.28}$$

where the contour C is a path along the real axis from $-\infty$ to $+\infty$, avoiding the origin by a small upper semicircle of radius ϵ and closed by a large semicircle of radius K in the upper half plane. n is the residue number. We are going to analyse the positions and the multiplicities of zeros of the Jost function in the upper half of the k plane.

First, we prove that the zeros of $\mathcal{J}_\ell(k)$ in the upper half of the k plane must be located on the imaginary axis. In fact, if $\mathcal{J}_\ell(k) = 0$, from equation (2.25) there is a regular complex solution $R_\ell(r, k)$ of equation (2.2):

$$R_\ell(r, k) = a_+(k) R_{\ell+}(r, k) \neq 0, \qquad k = k_0 + \mathrm{i}\omega, \quad \omega \geqslant 0. \tag{2.29}$$

$R_\ell(r, k)$ is vanishing at the origin and its logarithmic derivative at infinity is $\mathrm{i}k = \mathrm{i}k_0 - \omega$. The Wronskian $W[R_\ell(r, k)^*, R_\ell(r, k)]$ satisfies equation (2.16):

$$\frac{\mathrm{d}}{\mathrm{d}r} W[R_\ell(r, k)^*, R_\ell(r, k)] = (k^{2*} - k^2)|R_\ell(r, k)|^2.$$

Integrating it from 0 to r_0, where $r_0 \sim \infty$, one has

$$2\mathrm{i}k_0 |R_\ell(r_0, k)|^2 = -4\mathrm{i}k_0\omega \int_0^{r_0} \mathrm{d}r |R_\ell(r, k)|^2. \tag{2.30}$$

The coefficients of $(\mathrm{i}k_0)$ on both sides of equation (2.30) have different signs, so that $k_0 = 0$.

Second, we prove that the zeros of $\mathcal{J}_\ell(k)$ on the positive imaginary axis are simple. If yes, n is the number of the bound states of equation (2.2) except for the possible bound state at $k = 0$. Now, the solution $R_\ell(r, k_1)$ with $k_1 = \mathrm{i}\omega$ in equation (2.29) is real. Calculate $\dot{\mathcal{J}}_\ell(k_1)$, where the dot denotes the derivative with respect to k_1. Due to $\mathcal{J}_\ell(k_1) = 0$, one obtains from equation (2.21)

$$\dot{\mathcal{J}}_\ell(k_1) = \frac{k_1^\ell \, \mathrm{e}^{-\mathrm{i}\ell\pi/2}}{(2\ell+1)!!} \{W[\dot{R}_{\ell+}(r, k_1), R_\ell(r, k_1)] + W[R_{\ell+}(r, k_1), \dot{R}_\ell(r, k_1)]\}.$$

From equations (2.16) and (2.29)

$$\begin{aligned}
W[\dot{R}_{\ell+}(r, k_1), R_\ell(r, k_1)] &= \lim_{k\to k_1} \frac{\partial}{\partial k_1} W[R_{\ell+}(r, k_1), R_\ell(r, k)] \\
&= \lim_{k\to k_1} \frac{\partial}{\partial k_1} \left\{ \left[k_1^2 - k^2\right] \int_0^r \mathrm{d}r' R_{\ell+}(r', k_1) R_\ell(r', k) \right\} \\
&= 2k_1 a_+(k_1)^{-1} \int_0^r \mathrm{d}r' R_\ell(r', k_1)^2, \\
W[R_{\ell+}(r, k_1), \dot{R}_\ell(r, k_1)] &= \lim_{k\to k_1} \frac{\partial}{\partial k_1} W[R_{\ell+}(r, k), R_\ell(r, k_1)] \\
&= \lim_{k\to k_1} \frac{\partial}{\partial k_1} \left\{ \left[k_1^2 - k^2\right] \int_r^\infty \mathrm{d}r' R_{\ell+}(r', k) R_\ell(r', k_1) \right\} \\
&= 2k_1 a_+(k_1)^{-1} \int_r^\infty \mathrm{d}r' R_\ell(r', k_1)^2.
\end{aligned}$$

Thus,

$$\dot{\mathcal{J}}_\ell(k_1) = \frac{2k_1^{\ell+1} \, \mathrm{e}^{-\mathrm{i}\ell\pi/2}}{a_+(k_1)(2\ell+1)!!} \int_0^\infty \mathrm{d}r' R_\ell(r', k_1)^2 \neq 0. \tag{2.31}$$

It shows that the zero $k_1 = \mathrm{i}\omega$ of $\mathcal{J}_\ell(k)$ is simple.

Third, if $k = 0$ is a zero of $\mathcal{J}_\ell(k)$, careful calculation shows [69] that the multiplicity of this zero is 2 for $\ell \geqslant 1$ and 1 for $\ell = 0$. Note that the asymptotic behaviour of the regular solution $R_\ell(r, k)$ of equation (2.2) with $k = 0$, if it exists, is $r^{-\ell}$ at infinity, which means that $R_\ell(r, 0)$ is square integrable for $\ell \geqslant 1$ and finite but not square integrable for $\ell = 0$. The zero-momentum solution with $\ell = 0$ does not describe a bound state.

Now, evaluate the integral along the contour C. Due to equation (2.27), the integral along the large semicircle ($|k| \to \infty$) is vanishing. Then, as discussed above, if $\mathcal{J}_\ell(0) = 0$, $\mathcal{J}_\ell(k)$ when $k \sim 0$ is proportional to k^2 for $\ell \geqslant 1$ and to k for $\ell = 0$, so that the integral along the small semicircle is

$$\int_\epsilon \mathrm{d}\ln \mathcal{J}_\ell(k) = \begin{cases} 0 & \text{when} \quad \mathcal{J}_\ell(0) \neq 0, \\ -2\pi \mathrm{i} & \text{when} \quad \mathcal{J}_\ell(0) = 0 \quad \text{with} \quad \ell \geqslant 1, \\ -\pi \mathrm{i} & \text{when} \quad \mathcal{J}_\ell(0) = 0 \quad \text{with} \quad \ell = 0. \end{cases} \tag{2.32}$$

Moving this term to the right-hand side of equation (2.28), n is replaced with $n_\ell + 1/2$ when $\ell = 0$ and $\mathcal{J}_0(0) = 0$, and with n_ℓ for the remaining cases, where n_ℓ is the number of bound states of equation (2.2) with the angular momentum ℓ. At last, from equations (2.23) and (2.24) one obtains that on the real axis of the k plane, $\mathcal{J}_\ell(k) = \mathcal{J}_{\ell-}(k)^* = \mathcal{J}_\ell(-k)^* = |\mathcal{J}_\ell(k)|\,\mathrm{e}^{-\mathrm{i}\delta_\ell(k)}$. Namely, $|\mathcal{J}_\ell(-k)| = |\mathcal{J}_\ell(k)|$ and $\delta_\ell(-k) = -\delta_\ell(k)$. Thus, the integral along the real axis is

$$\lim_{K\to\infty}\lim_{\epsilon\to 0}\left\{\int_{-K}^{-\epsilon} \mathrm{d}\ln\mathcal{J}_\ell(k) + \int_\epsilon^K \mathrm{d}\ln\mathcal{J}_\ell(k)\right\} = 2\mathrm{i}\,[\delta_\ell(0) - \delta_\ell(\infty)]\,. \tag{2.33}$$

When $\ell = 0$ and $\mathcal{J}_0(0) = 0$, the wavefunction $R_0(r, 0)$ is finite but not square integrable. In this case, the state is not a bound state, but called a half bound state. A half bound state occurs only when $\ell = 0$ and $\mathcal{J}_0(0) = 0$. Altogether, the Levinson theorem for the three-dimensional Schrödinger equation with a spherically symmetric potential is proved:

$$\delta_\ell(0) - \delta_\ell(\infty) = \begin{cases} (n_\ell + 1/2)\pi, & \text{a half bound state occurs,} \\ n_\ell \pi, & \text{the remaining cases.} \end{cases} \tag{2.34}$$

The Levinson theorem (2.34) contains a difference of two phase shifts, namely the phase shift $\delta_\ell(0)$ is determined with respect to the phase shift $\delta_\ell(\infty)$ at infinite momentum. In some literature, the phase shift $\delta_\ell(\infty, 1)$ at infinite momentum was 'defined to be zero' (e.g. p 357 in [72]). However, $\delta_\ell(\infty, 1)$ may not be zero in some special cases as discussed in sections 4 and 5.

2.4. *Brief summary*

The proof of the Levinson theorem with the Jost function is based on the property of the Jost function in the analytic continuation to the complex plane of k. In order to study the analytic property of the Jost function, a stronger restriction (2.14), which is not necessary for the Levinson theorem, has to be imposed on the potential. The positions and the multiplicities of zeros of the Jost function in the upper half of the complex plane of k are quite difficult to study. This difficulty is an obstacle for the generalization of the Levinson theorem. The phase shift $\delta_\ell(0)$ in the Levinson theorem (2.34) is given with respect to the phase shift $\delta_\ell(\infty)$ at infinite energy, which is vanishing conditionally. In some special cases where $\delta_\ell(\infty)$ is not vanishing, the form (2.34) of the Levinson theorem will not hold.

3. The Levinson theorem and the Green function

In this section, we will sketch the proof of the Levinson theorem for the Schrödinger equation with the Green function [76]. The main idea is the same as, but more intuitive than, that with the operator formulism of the scattering theory raised by Jauch [41].

3.1. Orthonormal eigenfunctions

The radial equation (2.2) of the Schrödinger equation with a spherically symmetric potential $V(r)$ is rewritten in a Hamiltonian form:

$$\begin{aligned} &H_\ell(r,\lambda)R_\ell(r,E,\lambda) = ER_\ell(r,E,\lambda), \\ &H_\ell(r,\lambda) = H_\ell(r,0) + \lambda V(r) = -\frac{\hbar^2}{2M}\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\ell(\ell+1)}{r^2}\right] + \lambda V(r). \end{aligned} \tag{3.1}$$

In this section, the variable k in the radial function is replaced with the variable E for convenience. The real regular solution $R_\ell(r,E,\lambda)$ in equation (3.1) is orthonormal:

$$\int_0^\infty \mathrm{d}r\, R_\ell(r,E,\lambda)R_\ell(r,E',\lambda) = \begin{cases} \delta(E-E'), & \text{when} \quad E>0, \\ \delta_{EE'}, & \text{when} \quad E\leqslant 0. \end{cases} \tag{3.2}$$

There is a continuum for scattering states when $E>0$, and a discrete spectrum for bound states when $E\leqslant 0$. Denote by n_ℓ the number of bound states of the system. The complete condition for $R_\ell(r,E,\lambda)$ is

$$\sum_E R_\ell(r,E,\lambda)R_\ell(r',E,\lambda) = \delta(r-r'), \tag{3.3}$$

where $\sum_E$ is a symbolic sign which means an integral for the continuum and a sum over the discrete spectrum:

$$\sum_E R_\ell(r,E,\lambda)R_\ell(r',E) = \int_0^\infty \mathrm{d}E\, R_\ell(r,E,\lambda)R_\ell(r',E,\lambda) + \sum_{\nu=1}^{n_\ell} R_\ell(r,E_\nu,\lambda)R_\ell(r',E_\nu,\lambda). \tag{3.4}$$

For a free particle, $\lambda=0$, $H_\ell(r,0)$ only has a continuum. The explicit form of $R_\ell(r,E,0)$ for a scattering state with $E=\hbar^2k^2/(2M)>0$ is

$$\begin{aligned} &R_\ell(r,E,0) = \sqrt{Mr}\,J_{\ell+1/2}(kr)/\hbar, \\ &\int_0^\infty \mathrm{d}r\, R_\ell(r,E,0)R_\ell(r,E',0) = \delta(E-E') = \frac{M}{\hbar^2 k}\delta(k-k'). \end{aligned} \tag{3.5}$$

The set of $R_\ell(r,E,0)$ is also complete

$$\sum_E R_\ell(r,E,0)R_\ell(r',E,0) = \int_0^\infty \mathrm{d}E\, R_\ell(r,E,0)R_\ell(r',E,0) = \delta(r-r'). \tag{3.6}$$

The asymptotic behaviours of $R_\ell(r,E,0)$ near the origin and at infinity are

$$R_\ell(r,E,0) = \begin{cases} \dfrac{(kr)^{\ell+1}}{\hbar(2\ell+1)!!}\sqrt{\dfrac{2M}{\pi k}}, & \text{when} \quad r\to 0, \\ \dfrac{1}{\hbar}\sqrt{\dfrac{2M}{\pi k}}\sin(kr-\ell\pi/2), & \text{when} \quad r\to\infty. \end{cases} \tag{3.7}$$

Although the solution $R_\ell(r,E,\lambda)$ with a given λ is hard to solve explicitly, some of its asymptotic behaviours are known. If the potential $V(r)$ satisfies the restriction (2.3), $R_\ell(r,E,\lambda)$ is proportional to $r^{\ell+1}$ near the origin. Since the integral in the orthogonality (3.2) is equal to a Dirac delta function for a scattering state, the main contribution to the integral in equation (3.2) comes from the part of the wavefunction at large r, so that the asymptotic behaviour of $R_\ell(r, E, \lambda)$ at infinity can be written as the following combination of a Bessel function and a Neumann function:

$$R_\ell(r, E, \lambda) \propto r^{\ell+1} \to 0, \qquad \text{when} \quad r \to 0,$$

$$\begin{aligned} R_\ell(r, E, \lambda) &= \frac{\sqrt{Mr}}{\hbar}[\cos\delta_\ell(k,\lambda) J_{\ell+1/2}(kr)/\hbar - \sin\delta_\ell(k,\lambda) N_{\ell+1/2}(kr)] \\ &\to \frac{1}{\hbar}\sqrt{\frac{2M}{\pi k}} \sin[kr - \ell\pi/2 + \delta_\ell(k,\lambda)], \qquad \text{when} \quad r \to \infty. \end{aligned} \tag{3.8}$$

The asymptotic behaviours of $R_\ell(r, E, \lambda)$ for a bound state with $E = E_\nu < 0$ are

$$R_\ell(r, E_\nu, \lambda) \propto \begin{cases} r^{\ell+1} \sim 0, & \text{when} \quad r \to 0, \\ \mathrm{e}^{-\sqrt{-2ME_\nu}r/\hbar} \sim 0, & \text{when} \quad r \to \infty. \end{cases} \tag{3.9}$$

3.2. The retarded Green function

The retarded Green function $G(r, r', E, \lambda)$ is defined as

$$[E - H_\ell(r, \lambda) + \mathrm{i}\eta]\, G(r, r', E, \lambda) = \delta(r - r'). \tag{3.10}$$

From equation (3.3) one has

$$G(r, r', E, \lambda) = \sum_{E'} \frac{R_\ell(r, E', \lambda) R_\ell(r', E', \lambda)}{E - E' + \mathrm{i}\eta}. \tag{3.11}$$

The retarded Green function $G(r, r', E, 0)$ for a free particle is

$$[E - H_\ell(r, 0) + \mathrm{i}\eta] G(r, r', E, 0) = \delta(r - r'), \tag{3.12}$$

$$G(r, r', E, 0) = \sum_{E'} \frac{R_\ell(r, E', 0) R_\ell(r', E', 0)}{E - E' + \mathrm{i}\eta}. \tag{3.13}$$

The Dyson equation can be shown by multiplying it with $E - H_\ell(r, 0) + \mathrm{i}\eta$:

$$G(r, r'', E, \lambda) = G(r, r'', E, 0) + \int_0^\infty \mathrm{d}r' G(r, r', E, 0) \lambda V(r') G(r', r'', E, \lambda). \tag{3.14}$$

Taking $r'' = r$ and integrating equation (3.14) with respect to r, one has

$$\begin{aligned} \int_0^\infty \mathrm{d}r \{G(r, r, E, \lambda) - G(r, r, E, 0)\} &= \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' G(r, r', E, 0) \lambda V(r') G(r', r, E, \lambda) \\ &= \sum_{E'} \sum_{E''} \left[\int_0^\infty \mathrm{d}r\, R_\ell(r, E'', \lambda) R_\ell(r, E', 0) \right] \\ &\quad \times \frac{\left[\int_0^\infty \mathrm{d}r' R_\ell(r', E', 0) \lambda V(r') R_\ell(r', E'', \lambda)\right]}{(E - E' + \mathrm{i}\eta)(E - E'' + \mathrm{i}\eta')}. \end{aligned} \tag{3.15}$$

Due to $\lambda V(r) = H_\ell(r, \lambda) - H_\ell(r, 0)$,

$$\int_0^\infty \mathrm{d}r' R_\ell(r', E', 0) \lambda V(r') R_\ell(r', E'', \lambda) = (E'' - E') \int_0^\infty \mathrm{d}r' R_\ell(r', E', 0) R_\ell(r', E'', \lambda). \tag{3.16}$$

In the meaning of integral one has (see [40], for example)

$$\frac{1}{E - E' + \mathrm{i}\eta} = P \frac{1}{E - E'} - \mathrm{i}\pi\delta(E - E'), \tag{3.17}$$

where P denotes to take the principal value. Thus, the imaginary part of the following fraction is

$$\begin{aligned}
\mathrm{Im}\frac{E''-E'}{(E-E'+\mathrm{i}\eta)(E-E''+\mathrm{i}\eta')} \\
&= -\pi(E''-E')\left\{P\frac{1}{E-E''}\delta(E-E')+P\frac{1}{E-E'}\delta(E-E'')\right\} \\
&= \pi[\delta(E-E')-\delta(E-E'')]. \qquad (3.18)
\end{aligned}$$

Substituting equations (3.16) and (3.18) into equation (3.15) and integrating it with respect to E from $-\infty$ to ∞, one finds that the contributions from two delta functions are exactly the same and cancel each other:

$$\begin{aligned}
\mathrm{Im}\int_{-\infty}^{\infty}\mathrm{d}E\int_0^{\infty}\mathrm{d}r\,\{G(r,r,E,\lambda)-G(r,r,E,0)\} \\
&= \pi\int_{-\infty}^{\infty}\mathrm{d}E\sum_{E'}\sum_{E''}\left[\int_0^{\infty}\mathrm{d}r\,R_\ell(r,E'',\lambda)R_\ell(r,E',0)\right] \\
&\quad\times\left[\int_0^{\infty}\mathrm{d}r'R_\ell(r',E',0)R_\ell(r',E'',\lambda)\right][\delta(E-E')-\delta(E-E'')]=0. \qquad (3.19)
\end{aligned}$$

From the complete conditions (3.3) and (3.6), equation (3.19) can be rewritten as

$$\begin{aligned}
\mathrm{Im}\int_{-\infty}^{\infty}\mathrm{d}E\int_0^{\infty}\mathrm{d}r\{G(r,r,E,\lambda)-G(r,r,E,0)\} \\
&= \pi\int_{-\infty}^{\infty}\mathrm{d}E\sum_{E'}\delta(E-E')\int_0^{\infty}\mathrm{d}r\,R_\ell(r,E',0)R_\ell(r,E',0) \\
&\quad-\pi\int_{-\infty}^{\infty}\mathrm{d}E\sum_{E''}\delta(E-E'')\int_0^{\infty}\mathrm{d}r\,R_\ell(r,E'',\lambda)R_\ell(r,E'',\lambda)=0. \qquad (3.20)
\end{aligned}$$

Namely, equation (3.19) contains a cancellation of two infinite quantities which are exactly the same. Its physical meaning is shown in equation (3.20) that the number of eigenstates of $H(r,\lambda)$ is the same as that of $H(r,0)$.

Furthermore, if the integral of E in equation (3.19) runs from $-\infty$ to 0, the term with $\delta(E-E')$ vanishes because there is no bound state for a free particle. Thus, setting $\lambda=1$, one has

$$\begin{aligned}
\mathrm{Im}\int_{-\infty}^{0}\mathrm{d}E\int_0^{\infty}\mathrm{d}r\{G(r,r,E,1)-G(r,r,E,0)\} \\
&= -\pi\int_{-\infty}^{0}\mathrm{d}E\,\delta(E-E'')\sum_{E''}\left[\int_0^{\infty}\mathrm{d}r\,R_\ell(r,E'',1)R_\ell(r,E'',1)\right] \\
&= -n_\ell\pi. \qquad (3.21)
\end{aligned}$$

Due to equation (3.19) one has

$$\begin{aligned}
n_\ell &= \pi^{-1}\,\mathrm{Im}\int_0^{\infty}\mathrm{d}E\int_0^{\infty}\mathrm{d}r\{G(r,r,E,1)-G(r,r,E,0)\} \\
&= \int_0^{\infty}\mathrm{d}E\int_0^{\infty}\mathrm{d}r\,\{R_\ell(r,E,0)R_\ell(r,E,0)-R_\ell(r,E,1)R_\ell(r,E,1)\}. \qquad (3.22)
\end{aligned}$$

It shows that when λ changes from 0 to 1, some scattering states may transform into bound states or vice versa, but the total number of the eigenstates remains invariant. The Levinson theorem will be proved from equation (3.22). In the proof of equation (3.22), two infinite quantities cancel each other (see equation (3.19)). This problem also occurs in the operator formulism [41]. This cancellation seems to be strict because two infinite quantities are exactly the same.

3.3. The Levinson theorem

Integrating equation (2.16) with respect to r from the origin to infinity, one has

$$\frac{1}{k^2 - k'^2} \lim_{r\to\infty} W\left[R_\ell(r, E, \lambda), R_\ell(r, E', \lambda)\right] = \int_0^\infty \mathrm{d}r' R_\ell(r', E, \lambda) R_\ell(r', E', \lambda). \tag{3.23}$$

From the boundary condition (3.8) the Wronskian becomes

$$\begin{aligned}
&\lim_{r\to\infty} W[R_\ell(r, E, \lambda), R_\ell(r, E', \lambda)] \\
&\quad = \lim_{r\to\infty} \frac{2M}{\hbar^2\pi\sqrt{kk'}}\{k' \sin[kr - \ell\pi/2 + \delta_\ell(k, \lambda)] \cos[k'r - \ell\pi/2 + \delta_\ell(k', \lambda)] \\
&\qquad - k \sin[k'r - \ell\pi/2 + \delta_\ell(k', \lambda)] \cos[kr - \ell\pi/2 + \delta_\ell(k, \lambda)]\} \\
&\quad = \lim_{r\to\infty} \frac{M}{\hbar^2\pi\sqrt{kk'}}\{(k' - k) \sin[(k + k')r - \ell\pi + \delta_\ell(k, \lambda) + \delta_\ell(k', \lambda)] \\
&\qquad + (k' + k) \sin[(k - k')r + \delta_\ell(k, \lambda) - \delta_\ell(k', \lambda)]\} \\
&\quad = \lim_{r\to\infty} \frac{M(k^2 - k'^2)}{\hbar^2\pi\sqrt{kk'}} \left\{(-1)^{\ell+1} \cos[\delta_\ell(k, \lambda) + \delta_\ell(k', \lambda)] \frac{\sin[(k + k')r]}{k + k'}\right. \\
&\qquad + \cos[\delta_\ell(k, \lambda) - \delta_\ell(k', \lambda)] \frac{\sin[(k - k')r]}{k - k'} \\
&\qquad + (-1)^{\ell+1} \cos[(k + k')r] \frac{\sin[\delta_\ell(k, \lambda) + \delta_\ell(k', \lambda)]}{k + k'} \\
&\qquad \left. + \cos[(k - k')r] \frac{\sin[\delta_\ell(k, \lambda) - \delta_\ell(k', \lambda)]}{k - k'}\right\}.
\end{aligned} \tag{3.24}$$

Due to rapid oscillation, $\cos[(k + k')r] \to 0$ as $r \to \infty$ and

$$\lim_{r\to\infty} \frac{\sin xr}{\pi x} = \delta(x). \tag{3.25}$$

Substituting equation (3.24) into equation (3.23), one obtains

$$\begin{aligned}
&\lim_{E'\to E} \int_0^\infty \mathrm{d}r\, R_\ell(r, E, \lambda) R'_\ell(r, E', \lambda) \\
&\quad = \frac{M}{\hbar^2 k}\left\{(-1)^{\ell+1} \cos[2\delta_\ell(k, \lambda)]\delta(2k) + \lim_{E'\to E} \delta(k - k') + \frac{1}{\pi}\frac{\mathrm{d}\delta_\ell(k, \lambda)}{\mathrm{d}k}\right\},
\end{aligned} \tag{3.26}$$

where

$$\lim_{E'\to E} \frac{\sin[\delta_\ell(k, \lambda) - \delta_\ell(k', \lambda)]}{(k - k')} = \frac{\mathrm{d}\delta_\ell(k, \lambda)}{\mathrm{d}k}. \tag{3.27}$$

For a free particle, the phase shift is zero such that

$$\lim_{E'\to E} \int_0^\infty \mathrm{d}r\, R_\ell(r, E, 0) R'_\ell(r, E', 0) = \frac{M}{\hbar^2 k}\left\{(-1)^{\ell+1}\delta(2k) + \lim_{E'\to E} \delta(k - k')\right\}. \tag{3.28}$$

Substituting equations (3.26) and (3.28) into equation (3.22) and noting

$$\int_0^\infty \mathrm{d}E \frac{M}{\hbar^2 k}\delta(2k) = \frac{1}{2}\int_0^\infty \mathrm{d}E\, \delta(E) = \frac{1}{4}, \tag{3.29}$$

one obtains the Levinson theorem

$$n_\ell = \frac{1}{\pi}\left[\delta_\ell(0) - \delta_\ell(\infty)\right] - \frac{1}{2}(-1)^\ell \sin^2[\delta_\ell(0)], \tag{3.30}$$

where $\delta_\ell(k) \equiv \delta_\ell(k, 1)$. The Levinson theorem (3.30) coincides with the form (2.34) because $\sin^2[\delta_\ell(0)]$ is one for the half bound state of S-wave and zero for the remaining cases.

3.4. Brief summary

The proof of the Levinson theorem with the Green function is much simpler than that with the Jost function. The restriction (2.14) for the potential is released in this proof. This method of proof is generalized to the Dirac equation [53, 76], to the Klein–Gordon equation [76] and to the equations with different dimensions [50–52]. On the other hand, some problems appear in the proof, such as the difference of two infinite quantities and the interchange of two limits of $E' \to E$ and $r \to \infty$. The phase shift $\delta_\ell(0)$ in the Levinson theorem (3.30) is also given with respect to the phase shift $\delta_\ell(\infty)$ of infinite energy, which is vanishing conditionally.

4. The Levinson theorem and the Sturm–Liouville theorem

The Sturm–Liouville theorem [95, 103] is a fundamental theorem in the theory of differential equations. It studies the eigenvalue problems in the differential equations of second order, and was generalized to those of higher order, to the coupled ones of second order and to the partial differential equations [1, 19, 87, 97]. This theorem has a broad application in physics because the Schrödinger equation is a Sturm-type equation. In this section, the Levinson theorem will be proved with the Sturm–Liouville theorem.

4.1. The Sturm comparison theorem

The Sturm comparison theorem. If $y(x)$ and $Y(x)$ satisfy

$$\begin{aligned} &y'' + f(x)y = 0, \qquad && Y'' + F(x)Y = 0,\\ &y(a) = Y(a) = 0, && y'(a+) = Y'(a+) > 0, \end{aligned} \tag{4.1}$$

where f and F are continuous functions with $f(x) < F(x)$ in the region $[a, b]$, and c is the first zero of Y to the right of a in $[a, b]$, then (a) $y(x) > Y(x)$ in (a, c); (b) there is at least one zero of Y between two neighbouring zeros of y in $[a, b]$; (c) the kth zero of y in $[a, b]$ is located at the right of the kth zero of Y.

Proof. Taking the Wronskian of equation (4.1), one has from equation (2.16)

$$[y'Y - yY']_{x_1}^{x_2} = \int_{x_1}^{x_2} [F(t) - f(t)]y(t)Y(t)\,\mathrm{d}t. \tag{4.2}$$

Letting $x_1 = a$, one obtains

$$\lim_{x\to a} \frac{y}{Y} = 1, \qquad \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{y}{Y}\right) > 0, \qquad \text{when} \quad a < x < c,$$

(a) is proved. If d_1 and $d_2 > d_1$ are two neighbouring zeros of y in $[a, b]$, y does not change its sign in (d_1, d_2), and both $y'(d_1)$ and $-y'(d_2)$ have the same sign as that of y in (d_1, d_2). Hence, Y has to change its sign in (d_1, d_2) because from equation (4.2)

$$y'(d_2)Y(d_2) - y'(d_1)Y(d_1) = \int_{d_1}^{d_2} [F(t) - f(t)]\, y(t)Y(t)\,\mathrm{d}t.$$

This conclusion holds when $d_1 = a$, namely, the first zero of y in (a, b) is located at the right of c. Thus, (b) is proved and (c) is obvious. □

The Sturm comparison theorem studies the positions of zeros of $y(x)$ as $f(x)$ changes. It has broad application both in mathematics and in physics. For example [46], with it one is able to prove that the kth zero $\theta_k^{(n)}$ of the Legendre function $P_n(\cos\theta)$ in $[0, \pi]$ satisfies $\theta_k^{(n)} > \theta_k^{(n+1)}$ $(k \leqslant n)$ and $\theta_{k+1}^{(n)} - \theta_k^{(n)} > \theta_{k+1}^{(n+1)} - \theta_k^{(n+1)}$ $(k < n/2)$. For the kth zero $x_{\nu k}$ of the Bessel function $J_\nu(x)$ one has $x_{\nu k} > x_{\mu k}$ if $\nu > \mu \geqslant 0$ and $x_{\nu k}/\nu \geqslant x_{\mu k}/\mu$ if $\nu > \mu > 0$.

4.2. Monotonic property of a phase angle

For the three-dimensional Schrödinger equation (2.1) with a spherically symmetric potential, its radial equation is a Sturm-type equation,

$$\begin{aligned} &R_\ell''(r, E, \lambda) + F(r, E, \lambda) R_\ell(r, E, \lambda) = 0, \\ &F(r, E, \lambda) = \left\{ \frac{2M}{\hbar^2} [E - \lambda V(r)] - \frac{\ell(\ell+1)}{r^2} \right\}. \end{aligned} \tag{4.3}$$

The zero of the wavefunction $R_\ell(r, E, \lambda)$ is usually called the node of $R_\ell(r, E, \lambda)$ in physics. A regular solution contains a node at the origin. Due to the Sturm comparison theorem, the remaining nodes in the solution move towards the origin as the energy E increases. A new bound state occurs when a new node appears at infinity as E $(E \leqslant 0)$ increases. Namely, the number of nodes contained in the radial functions of bound states increases one by one as the energy E increases, and the radial function of the ground state contains no node except for two nodes at the origin and at infinity.

Another form of the Sturm comparison theorem is called the Sturm–Liouville theorem. Professor C N Yang said in a talk on magnetic monopole theory [103]: 'For the Sturm–Liouville problem, the fundamental trick is the definition of a phase angle which is monotonic with respect to the energy'. The phase angle is the logarithmic derivative of the wavefunction for the Schrödinger equation:

$$\phi_\ell(r, E, \lambda) = R_\ell(r, E, \lambda)^{-1} \frac{\mathrm{d}}{\mathrm{d}r} R_\ell(r, E, \lambda). \tag{4.4}$$

From equation (2.16), the Wronskian of the radial equation (4.3) satisfies

$$\begin{aligned} &\left[R_\ell(r, E, \lambda) \frac{\mathrm{d}}{\mathrm{d}r} R_\ell(r, E', \lambda) - R_\ell(r, E', \lambda) \frac{\mathrm{d}}{\mathrm{d}r} R_\ell(r, E, \lambda) \right]_{r_1}^{r_2} \\ &\quad = \frac{2M}{\hbar^2} [E - E'] \int_{r_1}^{r_2} R_\ell(r', E, \lambda) R_\ell(r', E', \lambda)\, \mathrm{d}r'. \end{aligned} \tag{4.5}$$

Letting $r_1 = 0$ and $r_2 = r_0$ in equation (4.5), due to $R_\ell(0, E, \lambda) = R_\ell(0, E', \lambda) = 0$ one obtains

$$\begin{aligned} &R_\ell(r_0, E, \lambda)^2 \frac{\partial}{\partial E} \phi_\ell(r_0-, E, \lambda) \\ &\quad = \lim_{E' \to E} \left. \frac{R_\ell(r, E, \lambda) \frac{\mathrm{d}}{\mathrm{d}r} R_\ell(r, E', \lambda) - R_\ell(r, E', \lambda) \frac{\mathrm{d}}{\mathrm{d}r} R_\ell(r, E, \lambda)}{E' - E} \right|_{r_0-} \\ &\quad = -\frac{2M}{\hbar^2} \int_0^{r_0} R_\ell(r', E, \lambda')^2 \mathrm{d}r' < 0. \end{aligned} \tag{4.6}$$

The logarithmic derivative $\phi_\ell(r_0-, E, \lambda)$ at a given point r_0- decreases monotonically as the energy increases.

Similarly, if the solution $R_\ell(r, E, \lambda)$ with $E < 0$ tends to zero as r goes to infinity,

$$\begin{aligned} R_\ell(r_0, E, \lambda)^2 \frac{\partial}{\partial E}\phi_\ell(r_0+, E, \lambda) &= \lim_{E'\to E} \left. \frac{R_\ell(r, E, \lambda)\frac{\mathrm{d}}{\mathrm{d}r}R_\ell(r, E', \lambda) - R_\ell(r, E', \lambda)\frac{\mathrm{d}}{\mathrm{d}r}R_\ell(r, E, \lambda)}{E' - E}\right|_{r_0+} \\ &= \frac{2M}{\hbar^2}\int_{r_0}^{\infty} R_\ell(r', E, \lambda)^2\,\mathrm{d}r' > 0. \end{aligned} \tag{4.7}$$

The logarithmic derivative $\phi_\ell(r_0+, E, \lambda)$ at a given point r_0+ with $E < 0$ increases monotonically as the energy increases.

For two solutions with the same energy E but different λ, equation (4.5) becomes

$$\begin{aligned} &\left[R_\ell(r, E, \lambda)\frac{\mathrm{d}}{\mathrm{d}r}R_\ell(r, E, \lambda') - R_\ell(r, E, \lambda')\frac{\mathrm{d}}{\mathrm{d}r}R_\ell(r, E, \lambda)\right]_{r_1}^{r_2} \\ &\quad = \frac{2M}{\hbar^2}[\lambda' - \lambda]\int_{r_1}^{r_2} V(r')R_\ell(r', E, \lambda)R_\ell(r', E, \lambda')\,\mathrm{d}r'. \end{aligned} \tag{4.8}$$

Letting $r_1 = 0$ and $r_2 = r_0$ in equation (4.8), one has

$$\begin{aligned} R_\ell(r_0, E, \lambda)^2 \frac{\partial}{\partial \lambda}\phi_\ell(r_0-, E, \lambda) &= \lim_{\lambda'\to\lambda} \left. \frac{R_\ell(r, E, \lambda)\frac{\mathrm{d}}{\mathrm{d}r}R_\ell(r, E, \lambda') - R_\ell(r, E, \lambda')\frac{\mathrm{d}}{\mathrm{d}r}R_\ell(r, E, \lambda)}{\lambda' - \lambda}\right|_{r_0-} \\ &= \frac{2M}{\hbar^2}\int_0^{r_0} V(r')R_\ell(r', E, \lambda)^2\,\mathrm{d}r'. \end{aligned} \tag{4.9}$$

The logarithmic derivative $\phi_\ell(r_0-, E, \lambda)$ at a given point r_0- is monotonic with respect to λ if the potential $V(r)$ does not change its sign in the region $(0, r_0)$.

For a scattering state, the asymptotic behaviour of $R_\ell(r, E, \lambda)$ at infinity is given in equation (3.8). Substituting it into equation (4.9) where r_0 tends to infinity, one obtains

$$\begin{aligned} \lim_{r\to\infty}\lim_{\lambda'\to\lambda} & \frac{R_\ell(r, E, \lambda)\frac{\mathrm{d}}{\mathrm{d}r}R_\ell(r, E, \lambda') - R_\ell(r, E, \lambda')\frac{\mathrm{d}}{\mathrm{d}r}R_\ell(r, E, \lambda)}{\lambda' - \lambda} \\ &= -\frac{2M}{\hbar^2\pi}\lim_{\lambda'\to\lambda}\frac{\sin[\delta_\ell(k, \lambda') - \delta_\ell(k, \lambda)]}{\lambda' - \lambda} \\ &= \frac{2M}{\hbar^2}\int_0^{\infty} V(r')R_\ell(r', E, \lambda)^2\,\mathrm{d}r'. \\ \frac{\partial\delta_\ell(k, \lambda)}{\partial\lambda} &= -\pi\int_0^{\infty} V(r)R_\ell(r, E, \lambda)^2\,\mathrm{d}r. \end{aligned} \tag{4.10}$$

The phase shift $\delta_\ell(k, \lambda)$ is monotonic with respect to λ if the potential $V(r)$ does not change its sign in the whole space. If the potential $V(r)$ in equation (4.3) is neglectable as E goes to infinity, $R_\ell(r, E, \lambda)$ tends to $R_\ell(r, E, 0)$. Thus,

$$\begin{aligned} \lim_{E\to\infty}\frac{\partial\delta_\ell(k, \lambda)}{\partial\lambda} &\sim -\frac{\pi M}{\hbar^2}\lim_{E\to\infty}\int_0^{\epsilon} V(r) r J_{\ell+1/2}(kr)^2\,\mathrm{d}r \\ &\quad - \lim_{E\to\infty}\frac{2M}{\hbar^2 k}\int_{\epsilon}^{\infty}\sin^2(kr - \ell\pi/2)V(r)\,\mathrm{d}r, \end{aligned} \tag{4.11}$$

where ϵ is a small real number. Equation (4.11) means that it is conditional to set $\delta_\ell(\infty, \lambda) = 0$.

4.3. The bounded potential

We are going to prove the Levinson theorem with the Sturm–Liouville theorem through two steps. First, we assume that the interaction area of the potential $V(r)$ is finite. There is a distance r_0 far away from the interaction area such that out of r_0 the interaction can be neglected. Namely, in addition to the restriction (2.3), the potential $V(r)$ is assumed to be a bounded one:

$$V(r) = 0, \qquad \text{when} \quad r > r_0. \tag{4.12}$$

Second, we will discuss the case where the potential has a tail at infinity, and study under what condition the potential can be neglected in the region (r_0, ∞).

Solve the radial equation (4.3) separately in two regions, $[0, r_0)$ and (r_0, ∞), under the conditions (2.3) and (4.12), and then match the logarithmic derivatives of two solutions at r_0:

$$\phi_\ell(r_0-, E, \lambda) = \phi_\ell(r_0+, E, \lambda). \tag{4.13}$$

In the region $[0, r_0)$, the regular solution $R_\ell(r, E, \lambda)$ of equation (4.3) with $R_\ell(0, E, \lambda) = 0$ can be calculated in principle, although hardly. Then, its logarithmic derivative $\phi_\ell(r_0-, E, \lambda)$ at r_0- can be obtained as a function of E and λ. On the other hand, the solution of equation (4.3) in the region (r_0, ∞) is easy to solve due to $V(r) = 0$. When $E > 0$, there are two independent solutions of equation (4.3) in the region (r_0, ∞), and one can always find their linear combination such that its logarithmic derivative $\phi_\ell(r_0+, E, \lambda)$ matches $\phi_\ell(r_0-, E, \lambda)$. Namely, a scattering state exists for any $E > 0$. When $E \leqslant 0$, there is only one physically admissible solution of equation (4.3) in the region (r_0, ∞). If its logarithmic derivative $\phi_\ell(r_0+, E, \lambda)$ matches $\phi_\ell(r_0-, E, \lambda)$ at one energy E, a bound state appears at that energy. The monotonic property of $\phi_\ell(r_0-, E, \lambda)$ and $\phi_\ell(r_0+, E, \lambda)$ with respect to the energy will greatly help to determine how many bound states occur for the system.

4.4. The phase shift of zero momentum

For a scattering state with $E > 0$, the general solution of equation (4.3) in the region (r_0, ∞), where $V(r) = 0$, can be written as

$$\begin{aligned} R_\ell(r, E, \lambda) &= \frac{\sqrt{Mr}}{\hbar}[\cos\delta_\ell(k, \lambda) J_{\ell+1/2}(kr) - \sin\delta_\ell(k, \lambda) N_{\ell+1/2}(kr)] \\ &\to \frac{1}{\hbar}\sqrt{\frac{2M}{\pi k}}\sin[kr - \ell\pi/2 + \delta_\ell(k, \lambda)], \qquad \text{when} \quad kr \to \infty. \end{aligned} \tag{4.14}$$

In fact, the solution (4.14) holds approximately when $V(r)$ is not bounded but satisfies the restriction (2.3) (see equation (3.8)). Through the matching condition (4.13) at r_0 one is able to determine $\tan\delta_\ell(k, \lambda)$, where the normalization factor in $R_\ell(r, E, \lambda)$ plays no role. In fact,

$$\begin{aligned} \phi_\ell(r_0+, E, \lambda) &= R_\ell(r, E, \lambda)^{-1} \left.\frac{\mathrm{d}R_\ell(r, E, \lambda)}{\mathrm{d}r}\right|_{r=r_0+} \\ &= \frac{1}{2r_0} + \frac{\cos\delta_\ell(k, \lambda) kJ'_{\ell+1/2}(kr_0) - \sin\delta_\ell(k, \lambda) kN'_{\ell+1/2}(kr_0)}{\cos\delta_\ell(k, \lambda) J_{\ell+1/2}(kr_0) - \sin\delta_\ell(k, \lambda) N_{\ell+1/2}(kr_0)}, \end{aligned} \tag{4.15}$$

where the prime on the Bessel function (or the Neumann function and later the Hankel function) denotes its derivative with respect to the argument (kr). Substituting equation (4.15) into the matching condition (4.13), one has

$$\tan\delta_\ell(k, \lambda) = \frac{[\phi_\ell(r_0-, E, \lambda) - 1/(2r_0)]\, J_{\ell+1/2}(kr_0) - kJ'_{\ell+1/2}(kr_0)}{[\phi_\ell(r_0-, E, \lambda) - 1/(2r_0)]\, N_{\ell+1/2}(kr_0) - kN'_{\ell+1/2}(kr_0)}. \tag{4.16}$$

Thus, through the matching condition (4.13) the phase shift, as well as the solution (4.14), depends on λ. The phase shift $\delta_\ell(k,\lambda)$ is calculated from equation (4.16) up to a multiple of π. It can be determined uniquely by the convention (2.13) that $\delta_\ell(k,\lambda)$ with $k>0$ is a continuous function of λ and vanishing when $\lambda=0$.

The logarithmic derivative $\phi_\ell(r_0-,E,\lambda)$ changes as λ increases from 0 to 1, so does the phase shift $\delta_\ell(k,\lambda)$. For a given $k=(2ME)^{1/2}/\hbar$, one obtains from equation (4.16)

$$\left.\frac{\partial\delta_\ell(k,\lambda)}{\partial\phi_\ell(r_0-,E,\lambda)}\right|_k = -2(\pi r_0)^{-1}\cos^2[\delta_\ell(k,\lambda)] \times\{[\phi_\ell(r_0-,E,\lambda)-1/(2r_0)]N_{\ell+1/2}(kr_0)-kN'_{\ell+1/2}(kr_0)\}^{-2}\leqslant 0, \tag{4.17}$$

where the identity $J_\nu(z)N'_\nu(z)-J'_\nu(z)N_\nu(z)=2/(\pi z)$ is used. Namely, for a given k the phase shift $\delta_\ell(k,\lambda)$ increases monotonically as the logarithmic derivative $\phi_\ell(r_0-,E,\lambda)$ decreases. In fact, this conclusion coincides with the Sturm–Liouville theorem (see equations (4.9) and (4.10)).

The phase shift $\delta_\ell(0,\lambda)$ of zero momentum is defined to be the limit of $\delta_\ell(k,\lambda)$ as k tends to zero:

$$\delta_\ell(0,\lambda)=\lim_{k\to 0}\delta_\ell(k,\lambda). \tag{4.18}$$

In order to calculate $\delta_\ell(0,\lambda)$, one takes the series expansion of equation (4.16) with respect to kr_0,

$$\tan\delta_\ell(k,\lambda)=\frac{-\pi(kr_0)^{2\ell+1}}{2^{2\ell+1}\Gamma(\ell+3/2)\Gamma(\ell+1/2)}\frac{\phi_\ell(r_0-,0,\lambda)-(\ell+1)/r_0}{\phi_\ell(r_0-,0,\lambda)-c^2k^2-[-\ell/r_0+k^2r_0/(2\ell-1)]}, \tag{4.19}$$

where $c^2>0$ due to the Sturm–Liouville theorem (4.6). In equation (4.19), only the leading terms in the numerator are reserved, but the next leading terms in the denominator are also kept down because they are sensitive for the later calculation. When $\ell=0$, equation (4.19) reduces to

$$\tan\delta_0(k,\lambda)=-kr_0\frac{\phi_0(r_0-,0,\lambda)-1/r_0}{\phi_0(r_0-,0,\lambda)-c^2k^2+k^2r_0}. \tag{4.20}$$

The following conclusions can be made from equations (4.17)–(4.20).

(a) Due to a factor $(kr_0)^{2\ell+1}$ in equation (4.19), for a sufficiently small kr_0, $|\tan\delta_\ell(k,\lambda)|$ is very small, and $\delta_\ell(k,\lambda)=n_\ell(k,\lambda)\pi+\alpha_\ell(k,\lambda)$, where $n_\ell(k,\lambda)$ is an integer and $\alpha_\ell(k,\lambda)$ is a small acute angle, positive or negative. As k goes to zero, $n_\ell(k,\lambda)$ remains invariant and $\alpha_\ell(k,\lambda)$ tends to zero. Namely, $\delta_\ell(0,\lambda)$ is always equal to a multiple of π, and it changes discontinuously as λ increases. There is an exception with $\ell=0$ and $\phi_0(r_0-,0,\lambda)=0$, where $\tan\delta_0(k,\lambda)\sim(kr_0)^{-1}$ and $n_0(k,\lambda)$ is a half of odd integer.

(b) As λ increases from 0 to 1, $\phi_\ell(r_0-,0,\lambda)$ changes continuously except for the jump between $\pm\infty$ when $R_\ell(r_0-,0,\lambda)$ changes across zero. If $\phi_\ell(r_0-,0,\lambda)$ changes across the value $(\ell+1)/r_0$, the numerator of $\tan\delta_\ell(k,\lambda)$ changes its sign, where $\alpha_\ell(k,\lambda)$ changes sign but $n_\ell(k,\lambda)$ remains invariant. If $\phi_\ell(r_0-,0,\lambda)$ changes across the value $-\ell/r_0$, the denominator of $\tan\delta_\ell(k,\lambda)$ changes its sign and $\tan\delta_\ell(k,\lambda)$ jumps between $\pm\infty$ such that $n_\ell(k,\lambda)$ changes by one. For the critical case where $\phi_\ell(r_0-,0,1)=-\ell/r_0$, $\tan\delta_\ell(k,1)$ with small kr_0 is negative when $\ell\geqslant 1$ and is very large (proportional to $(kr_0)^{-1}$) when $\ell=0$.

(c) Due to equation (4.17) $\delta_\ell(k,\lambda)$ increases (decreases) as $\phi_\ell(r_0-,0,\lambda)$ decreases (increases). For a sufficiently small but fixed kr_0 and $\ell\geqslant 1$, as λ increases from 0 to 1, each time $\phi_\ell(r_0-,0,\lambda)$ decreases to reach or across the value $-\ell/r_0$, $\tan\delta_\ell(k,\lambda)$

increases from a positive value to a negative value through a jump from positive infinity to negative infinity, and $n_\ell(k,\lambda)$ increases by one. Conversely, each time $\phi_\ell(r_0-, 0, \lambda)$ increases across the value $-\ell/r_0$, $\tan\delta_\ell(k,\lambda)$ decreases from a negative value to a positive value through a jump from negative infinity to positive infinity, and $n_\ell(k,\lambda)$ decreases by one. Note that when $\phi_\ell(r_0-, 0, \lambda)$ increases to reach the value $-\ell/r_0$, $\tan\delta_\ell(k,\lambda)$ decreases but remains negative, and $n_\ell(k,\lambda)$ does not decrease.

The situation is a little bit different for $\ell = 0$. For a sufficiently small but fixed kr_0 and $\ell = 0$, each time $\phi_0(r_0-, 0, \lambda)$ increases to reach the value 0, $\tan\delta_0(k,\lambda)$ decreases from a negative value to infinity and $n_0(k,\lambda)$ decreases by 1/2, and each time $\phi_0(r_0-, 0, \lambda)$ increases from 0, $\tan\delta_0(k,\lambda)$ decreases from infinity to a positive value and $n_0(k,\lambda)$ also decreases by 1/2. Conversely, each time $\phi_0(r_0-, 0, \lambda)$ decreases to reach the value 0, or decreases from 0, $n_0(k,\lambda)$ increases by 1/2.

In summary, as λ increases continuously, $\delta_\ell(0,\lambda)$ changes by jumps. As λ increases, $\delta_\ell(0,\lambda)$ jumps by π if $\phi_\ell(r_0-, 0, \lambda)$ decreases across the value $-\ell/r_0$ and jumps by $-\pi$ if $\phi_\ell(r_0-, 0, \lambda)$ increases across the value $-\ell/r_0$. Denote $n_\ell(0, 1)$ by n_ℓ for simplicity. If $\phi_\ell(r_0-, 0, 1) \neq -\ell/r_0$, $\delta_\ell(0) = n_\ell\pi$ where n_ℓ is equal to the times $\phi_\ell(r_0-, 0, \lambda)$ decreases across the value $-\ell/r_0$ as λ increases from 0 to 1, minus the times $\phi_\ell(r_0-, 0, \lambda)$ increases across that value. If $\phi_\ell(r_0-, 0, 1) = -\ell/r_0$, as λ increases to reach 1, n_ℓ with $\ell \geqslant 1$ increases an additional one if $\phi_\ell(r_0-, 0, \lambda)$ decreases to reach $-\ell/r_0$, but does not decrease if $\phi_\ell(r_0-, 0, \lambda)$ increases to reach $-\ell/r_0$, and n_0 with $\ell = 0$ increases (or decreases) an additional 1/2 if $\phi_0(r_0-, 0, \lambda)$ decreases (or increases) to reach 0.

4.5. Number of bound states

Discuss the solutions of equation (4.3) with $E \leqslant 0$ in two regions $[0, r_0)$ and (r_0, ∞). There is only one regular solution of equation (4.3) in both regions, respectively. For a given energy $E < 0$, if the logarithmic derivatives of two regular solutions in two regions satisfy the matching condition (4.13) at r_0, there is a bound state with that energy E. Otherwise, no physical admissible solution in the whole space $[0, \infty)$. We will neglect the normalization factor in the solution because it does not matter with the matching condition (4.13). The case with $E = 0$ needs specification.

In the region (r_0, ∞), where $V(r) = 0$, the real regular solution of equation (4.3) does not depend on λ,

$$R_\ell(r, E) = \mathrm{e}^{\mathrm{i}(\ell+3/2)\pi/2}\sqrt{\pi k_1 r/2}\,H^{(1)}_{\ell+1/2}(\mathrm{i}k_1 r) = \begin{cases} [(2\ell-1)!!](k_1 r)^{-\ell}, & \text{when} \quad k_1 r \to 0, \\ \mathrm{e}^{-k_1 r}, & \text{when} \quad k_1 r \to \infty, \end{cases} \tag{4.21}$$

where $k_1 = \sqrt{-2ME}/\hbar$ and $H^{(1)}_\nu(z)$ is the Hankel function of the first kind. The logarithmic derivative $\phi_\ell(r_0+, E)$ of $R_\ell(r, E)$ at r_0+ is

$$\phi_\ell(r_0+, E) = R_\ell(r, E)^{-1}\left.\frac{\mathrm{d}R_\ell(r, E)}{\mathrm{d}r}\right|_{r=r_0+} = \begin{cases} -\ell/r_0, & \text{when} \quad E \to 0, \\ -k_1 \to -\infty, & \text{when} \quad E \to -\infty. \end{cases} \tag{4.22}$$

When $E = 0$, the finite solution of equation (4.3) in the region (r_0, ∞) is

$$R_\ell(r, 0) = r^{-\ell}, \qquad \phi_\ell(r_0+, 0) = -\ell/r_0. \tag{4.23}$$

The solution (4.23) is square integrable when $\ell \geqslant 1$ and is equal to a finite constant when $\ell = 0$. If $\phi_\ell(r_0-, 0, 1)$ is equal to $-\ell/r_0$, a bound state with $E = 0$ occurs for $\ell \geqslant 1$, but only a half bound state with $E = 0$ occurs for $\ell = 0$.

Equation (4.3) is difficult to solve analytically in the region $[0, r_0)$ except for $\lambda = 0$. When $\lambda = 0$ the real regular solution $R_\ell(r, E, \lambda)$ of equation (4.3) is

$$\begin{aligned} R_\ell(r, E, 0) &= \mathrm{e}^{-\mathrm{i}(\ell+1/2)\pi/2}\sqrt{2\pi k_1 r}\, J_{\ell+1/2}(\mathrm{i}k_1 r) \\ &= \begin{cases} 2(k_1 r)^{\ell+1}/(2\ell+1)!!, & \text{when} \quad k_1 r \to 0, \\ \mathrm{e}^{k_1 r}, & \text{when} \quad k_1 r \to \infty. \end{cases} \end{aligned} \tag{4.24}$$

The logarithmic derivative $\phi_\ell(r, E, 0)$ of $R_\ell(r, E, 0)$ at r_0- is

$$\begin{aligned} \phi_\ell(r_0-, E, 0) &= R_\ell(r, E, 0)^{-1} \left.\frac{\mathrm{d}R_\ell(r, E, 0)}{\mathrm{d}r}\right|_{r=r_0-} \\ &= \begin{cases} (\ell+1)/r_0, & \text{when} \quad E \to 0, \\ k_1 \to +\infty, & \text{when} \quad E \to -\infty. \end{cases} \end{aligned} \tag{4.25}$$

It can be seen from equations (4.22) and (4.25) that as E increases from negative infinity to 0, $\phi_\ell(r_0+, E)$ increases monotonically from negative infinity to $-\ell/r_0$ and $\phi_\ell(r_0-, E, 0)$ decreases monotonically from positive infinity to $(\ell+1)/r_0$. There is no overlap between two variant ranges of two logarithmic derivatives when $\lambda = 0$, such that there is no bound state for a free particle.

As λ increases from 0 to 1, $\phi_\ell(r_0+, E)$ remains invariant, but $\phi_\ell(r_0-, E, \lambda)$ changes. Due to the Sturm–Liouville theorem (4.6), one only needs to pay attention to variance of $\phi_\ell(r_0-, 0, \lambda)$ at $E = 0$. For the repulsive potential, $V(r) > 0$, from equation (4.9) $\phi_\ell(r_0-, 0, \lambda)$ increases as λ increases, so that no overlap occurs and no bound state appears for the repulsive potential. $\phi_\ell(r_0-, 0, \lambda)$ cannot increase to be larger than $\phi_\ell(r_0-, -\infty, \lambda)$ owing to the Sturm–Liouville theorem (4.6). For the attractive potential, $V(r) < 0$, $\phi_\ell(r_0-, 0, \lambda)$ decreases as λ increases. If $\phi_\ell(r_0-, 0, \lambda)$ decreases across the value $-\ell/r_0$, one overlap occurs between two variant ranges of two logarithmic derivatives at two sides of r_0. Due to the Sturm–Liouville theorem, there is one and only one energy with which the matching condition (4.13) is satisfied and one bound state appears. As λ increases again, $\phi_\ell(r_0-, 0, \lambda)$ may decrease to negative infinity, jumps to positive infinity, and decrease again. If $\phi_\ell(r_0-, 0, \lambda)$ decreases second time across the value $-\ell/r_0$, a new overlap occurs between two variant ranges of two logarithmic derivatives, such that another bound state appears.

Generally speaking, as λ increases from 0 to 1, a new bound state appears if $\phi_\ell(r_0-, 0, \lambda)$ decreases across the value $-\ell/r_0$, and a bound state disappears if $\phi_\ell(r_0-, 0, \lambda)$ increases across the value $-\ell/r_0$. For the critical case where $\phi_\ell(r_0-, 0, 1) = -\ell/r_0$ with $\ell \geqslant 1$, as λ increases to reach 1, a new bound state appears if $\phi_\ell(r_0-, 0, \lambda)$ decreases to reach $-\ell/r_0$, but no bound state disappears if $\phi_\ell(r_0-, 0, \lambda)$ increases to reach $-\ell/r_0$. For the critical case where $\ell = 0$ and $\phi_0(r_0-, 0, 1) = 0$, as λ increases to reach 1, no new bound state, but a half bound state, appears if $\phi_0(r_0-, 0, \lambda)$ decreases to reach the value 0, and a bound state becomes a half bound state if $\phi_0(r_0-, 0, \lambda)$ increases to reach 0.

Together with the conclusion in the preceding subsection, the Levinson theorem comes. As λ increases from 0 to 1, each time $\phi_\ell(r_0-, 0, \lambda)$ decreases across the value $-\ell/r_0$, the phase shift $\delta_\ell(0, \lambda)$ jumps by π and a bound state appears, and each time $\phi_\ell(r_0-, 0, \lambda)$ increases across $-\ell/r_0$, $\delta_\ell(0, \lambda)$ jumps by $-\pi$ and a bound state disappears. For the critical case where $\phi_\ell(r_0-, 0, 1) = -\ell/r_0$ with $\ell \geqslant 1$, as λ increases to reach 1, the phase shift $\delta_\ell(0, \lambda)$ jumps by an additional π and a new bound state appears at $E = 0$ if $\phi_\ell(r_0-, 0, \lambda)$ decreases to reach $-\ell/r_0$, but $\delta_\ell(0, \lambda)$ does not jump and no bound state disappears if $\phi_\ell(r_0-, 0, \lambda)$ increases to reach $-\ell/r_0$. For the critical case where $\ell = 0$ and $\phi_0(r_0-, 0, 1) = 0$, as λ increases to reach 1, the phase shift $\delta_0(0, \lambda)$ jumps by $\pi/2$ and no new bound state with $E = 0$ (only a half bound state) appears if $\phi_0(r_0-, 0, \lambda)$ decreases to reach the value 0. Similarly, $\delta_0(0, \lambda)$ jumps by $-\pi/2$ and a bound state becomes a half bound state if $\phi_0(r_0-, 0, \lambda)$ increases to reach 0. Therefore, the Levinson theorem is written as

$$\delta_\ell(0) = \begin{cases} (n_\ell + 1/2)\,\pi, & \text{a half bound state occurs,} \\ n_\ell \pi, & \text{the remaining cases,} \end{cases} \tag{4.26}$$

where $\delta_\ell(0) = \delta_\ell(0, 1)$ and n_ℓ, respectively, are the phase shift of zero momentum and the number of bound states with the angular momentum ℓ and $\lambda = 1$. The half bound state only occurs when $\ell = 0$ and $\phi_0(r_0-, 0, 1) = 0$. We would like to emphasize the difference of equation (4.26) from equations (2.34) and (3.30) that the phase shift $\delta_\ell(0)$ here is determined not with respect to the phase shift $\delta_\ell(\infty)$ of infinite momentum.

4.6. Potential with a tail

Now, we turn to the case where the potential has a tail at $r > r_0$ [54]:

$$V(r) \sim br^{-m}, \qquad \text{when} \quad r > r_0. \tag{4.27}$$

Let r_0 be so large that only the leading term of $V(r)$ is concerned in the region (r_0, ∞). Divide the potential into two parts for convenience:

$$V_1 = \begin{cases} V(r) & \text{when} \quad r < r_0, \\ 0 & \text{when} \quad r > r_0, \end{cases} \qquad V_2 = \begin{cases} 0 & \text{when} \quad r < r_0, \\ V(r) \sim br^{-m} & \text{when} \quad r > r_0, \end{cases} \tag{4.28}$$

and $\lambda V(r)$ in equation (4.3) is replaced with $\lambda V_1(r) + \tau V_2(r)$. τ first increases from 0 to 1, and then λ increases from 0 to 1.

In the region (r_0, ∞), equation (4.3) becomes

$$\frac{d^2 R_\ell(r, E, \lambda, \tau)}{dr^2} + \left\{ \frac{2M}{\hbar^2} \left[E - \frac{\tau b}{r^m} \right] - \frac{\ell(\ell+1)}{r^2} \right\} R_\ell(r, E, \lambda, \tau) = 0. \tag{4.29}$$

Although equation (4.29) does not depend on λ, the solution $R_\ell(r, E, \lambda, \tau)$ with $E > 0$ depends on λ through the matching condition, but the solution $R_\ell(r, E, \tau)$ with $E \leqslant 0$ does not depend on λ. If $m = 1$, the tail of potential is like the Coulomb potential, where, as is well known, there is an infinite number of bound state and the phase shift changes logarithmically. If $m \geqslant 3$, the potential term is too small to affect the phase shift (see the end of this subsection). For $m = 2$, let

$$a_\tau\,(a_\tau + 1) = \frac{2M}{\hbar^2}\tau b + \ell(\ell+1), \qquad a_1 = a. \tag{4.30}$$

If $2Mb/\hbar^2 + \ell(\ell+1) < -1/4$, this potential causes an infinite number of bound states, which is not interesting to us. The case with $2Mb/\hbar^2 + \ell(\ell+1) = -1/4$ is complicated where the next leading term in equation (4.27) becomes important. For the case with $2Mb/\hbar^2 + \ell(\ell+1) > -1/4$ ($a_\tau > -1/2$), the solutions (4.14) and (4.21) in the region (r_0, ∞) become

$$\begin{aligned} R_\ell(r, E, \lambda, \tau)|_{E>0} &= \frac{\sqrt{Mr}}{\hbar}[\cos\eta_\ell(k, \lambda, \tau) J_{a_\tau+1/2}(kr) - \sin\eta_\ell(k, \lambda, \tau) N_{a_\tau+1/2}(kr)] \\ &\to \frac{1}{\hbar}\sqrt{\frac{2M}{\pi k}} \sin[kr - a_\tau\pi/2 + \eta_\ell(k, \lambda, \tau)], \qquad \text{when} \quad kr \to \infty, \end{aligned} \tag{4.31}$$

$$R_\ell(r, E, \tau)|_{E<0} = \mathrm{e}^{\mathrm{i}(a_\tau+3/2)\pi/2}\sqrt{\pi k_1 r/2}H^{(1)}_{a_\tau+1/2}(\mathrm{i}k_1 r)$$
$$= \begin{cases} [2^{a_\tau}\Gamma(a_\tau + 1/2)]\pi^{-1/2}(k_1 r)^{-a_\tau}, & \text{when} \quad k_1 r \to 0, \\ \mathrm{e}^{-k_1 r}, & \text{when} \quad k_1 r \to \infty, \end{cases} \tag{4.32}$$

where $k = \sqrt{2ME}/\hbar$ and $k_1 = \sqrt{-2ME}/\hbar$. Comparing equation (4.31) with equation (4.14) one finds that the phase shift is

$$\delta_\ell(k, \lambda, \tau) = \eta_\ell(k, \lambda, \tau) + (\ell - a_\tau)\pi/2. \tag{4.33}$$

For a free particle, $\lambda = \tau = 0$. Thus, the convention (2.13) for the phase shift becomes

$$\delta_\ell(k, 0, 0) = 0. \tag{4.34}$$

From equation (4.32), the logarithmic derivative $\phi_\ell(r_0+, E, \tau)$ with $E \leqslant 0$ and $\tau = 1$ is

$$\phi_\ell(r_0+, E, 1) = \begin{cases} -a/r_0, & \text{when} \quad E \to 0, \\ -k_1 \sim -\infty, & \text{when} \quad E \to -\infty. \end{cases} \tag{4.35}$$

The solution $R_\ell(r, E, \lambda)$ of equation (4.3) in the region $[0, r_0)$ and its logarithmic derivative $\phi_\ell(r_0-, E, \lambda)$ at r_0- do not depend on τ. From the matching condition (4.13) one obtains

$$\tan \eta_\ell(k, 0, \tau) = \frac{[\phi_\ell(r_0-, E, 0) - 1/(2r_0)]\, J_{a_\tau+1/2}(kr_0) - kJ'_{a_\tau+1/2}(kr_0)}{[\phi_\ell(r_0-, E, 0) - 1/(2r_0)]\, N_{a_\tau+1/2}(kr_0) - kN'_{a_\tau+1/2}(kr_0)}, \tag{4.36}$$

$$\tan \eta_\ell(k, \lambda, 1) = \frac{[\phi_\ell(r_0-, E, \lambda) - 1/(2r_0)]\, J_{a+1/2}(kr_0) - kJ'_{a+1/2}(kr_0)}{[\phi_\ell(r_0-, E, \lambda) - 1/(2r_0)]\, N_{a+1/2}(kr_0) - kN'_{a+1/2}(kr_0)}. \tag{4.37}$$

For a sufficiently small kr_0, the series expansion of equation (4.36) with the leading terms is

$$\tan \eta_\ell(k, 0, \tau) = \frac{-\pi (kr_0)^{2a_\tau+1}}{2^{2\ell+1}\Gamma(a_\tau + 3/2)\Gamma(a_\tau + 1/2)} \frac{\phi_\ell(r_0-, 0, 0) - (a_\tau + 1)/r_0}{\phi_\ell(r_0-, 0, 0) + a_\tau/r_0}. \tag{4.38}$$

Since $\phi_\ell(r_0-, 0, 0) = (\ell+1)/r_0$, the denominator in equation (4.38) is never equal to zero, so that $\eta_\ell(k, 0, 1)$ is very small for a sufficiently small kr_0. On the other hand, when kr_0 is large, the matching condition (4.13) requests $-a\pi/2 + \eta_\ell(k, 0, 1) = -\ell\pi/2$, so that $\delta_\ell(k, 0, 1) = 0$.

$\eta_\ell(k, 0, 1)$ is the initial condition of $\eta_\ell(k, \lambda, 1)$ in equation (4.37). From equation (4.37) one has

$$\left.\frac{\partial \eta_\ell(k, \lambda, 1)}{\partial \phi_\ell(r_0-, E, \lambda)}\right|_k \leqslant 0. \tag{4.39}$$

The series expansion of equation (4.37) when $a > 1/2$ and $a = 0$ is

$$\tan \eta_\ell(k, \lambda, 1) = \frac{-\pi (kr_0)^{2a+1}}{2^{2a+1}\Gamma(a + 3/2)\Gamma(a + 1/2)} \times \frac{\phi_\ell(r_0-, 0, \lambda) - (a + 1)/r_0}{\phi_\ell(r_0-, 0, \lambda) - c_1^2 k^2 - [-a/r_0 + k^2 r_0/(2a - 1)]}. \tag{4.40}$$

Straightforward calculation shows when $a = 1/2$

$$\tan \eta_\ell(k, \lambda, 1) = \frac{-\pi (kr_0)^2\, [\phi_\ell(r_0-, 0, \lambda) - 3/(2r_0)]}{4\left[\phi_\ell(r_0-, 0, \lambda) - c_2^2 k^2 + 1/(2r_0) + k^2 r_0 \ln(kr_0)\right]}, \tag{4.41}$$

and where $-1/2 < a < 1/2$ but $a \neq 0$,

$$\tan\eta_\ell(k,\lambda,1) = \frac{-\pi(kr_0)^{2a+1}}{2^{2a+1}\Gamma\left(a+\frac{3}{2}\right)\Gamma\left(a+\frac{1}{2}\right)} \times \frac{\phi_\ell(r_0-,0,\lambda)-(a+1)/r_0}{\phi_\ell(r_0-,0,\lambda)-c_3^2k^2+a/r_0+k(kr_0/2)^{2a}\pi\cot\left(a+\frac{1}{2}\right)\pi\big/\left[\Gamma\left(a+\frac{1}{2}\right)\right]^2}. \tag{4.42}$$

In the critical case where $\phi_\ell(r_0-,0,1) = -a/r_0$, for a sufficiently small kr_0, $\tan\eta_\ell(k,1,1)$ is negative when $a \geqslant 1/2$ and is equal to $\tan(a+1/2)\pi$ when $-1/2 < a < 1/2$. On the other hand, when $\phi_\ell(r_0-,0,1) = -a/r_0$, the zero-energy solution of equation (4.29) in the region (r_0,∞) is $R_\ell(r,0,1,1) \sim r^{-a}$, which describes a bound state when $a > 1/2$ and not when $-1/2 < a \leqslant 1/2$.

In terms of the similar analysis to that in the preceding subsections, we obtain the modified Levinson theorem [54]:

$$\delta_\ell(0)/\pi = \begin{cases} n_\ell + (\ell+a+1)/2, & \text{the critical case with } -1/2 < a \leqslant 1/2, \\ n_\ell + (\ell-a)/2, & \text{the remaining cases,} \end{cases} \tag{4.43}$$

where $\delta_\ell(0) \equiv \delta_\ell(0,1,1)$ and the critical case means $\phi_\ell(r_0-,0,1) = -a/r_0$ with $-1/2 < a \leqslant 1/2$. In the critical case, the zero-energy solution of equation (4.29) in the region (r_0,∞) is $R_\ell(r,0,1,1) \sim r^{-a}$, which does not describe a bound state because it is not square integrable.

Finally, we will further discuss the restriction (2.3) which demands the potential $V(r)$ to vanish at infinity faster than r^{-2}. Let

$$\begin{aligned} &|V(r)| < |V(r_0)|(r_0/r)^2, \qquad \text{when} \quad r > r_0, \\ &a(a+1) = \frac{2M}{\hbar^2}V(r_0)r_0^2 + \ell(\ell+1). \end{aligned} \tag{4.44}$$

For an arbitrarily chosen small number ϵ, one can always find a large r_0 such that

$$|\ell - a| < \epsilon. \tag{4.45}$$

Thus, the effect of the tail of the potential at infinity to the phase shift is small enough to be neglected.

4.7. Brief summary

The proof of the Levinson theorem with the Sturm–Liouville theorem is simpler and more intuitive than the other methods. The restriction (2.14) on the potential is released in this proof. The phase shift $\delta_\ell(\infty)$ of infinite energy does not appear in the Levinson theorem (4.26). Due to its simplicity, the Levinson theorem with this proof was introduced in a textbook on quantum mechanics [31]. The modified Levinson theorem (4.43) is proved for the case where the potential has a tail of r^{-2} at infinity, which violates the restriction (2.3). The proof of the Levinson theorem with the Sturm–Liouville theorem is easy to generalize to the Dirac equation [55], to the Klein–Gordon equation [48] and to the equations with different dimensions [24, 25, 27–29, 35, 61].

5. Release of restriction on potential

The phase shift $\delta_\ell(k,\lambda)$ in the form (4.26) of the Levinson theorem is determined with respect to the phase shift $\delta_\ell(k,0)$ of a free particle, which is vanishing owing to the convention

(2.13). But in the forms (2.34) and (3.30) of the Levinson theorem, the phase shift $\delta_\ell(k, \lambda)$ is determined with respect to the phase shift $\delta_\ell(\infty, \lambda)$ at infinite energy. This difference plays an important role in some special examples discussed in this section.

5.1. An infinite square-well potential

The radial equation (2.2) with an infinite square-well potential

$$V(r) = \begin{cases} \infty & \text{when} \quad r \leqslant a, \\ 0 & \text{when} \quad r > a, \end{cases} \tag{5.1}$$

can be solved exactly. The scattering solution $R_\ell(r, E, \lambda)$ with $E > 0$ and $\lambda = 1$ is

$$\begin{aligned} R_\ell(r, E, 1) &= \frac{\sqrt{Mr}}{\hbar} J_{\ell+1/2}[k(r-a)] \\ &\rightarrow \frac{1}{\hbar}\sqrt{\frac{2M}{\pi k}} \sin(kr - \ell\pi/2 - ka) \qquad \text{when} \quad r \rightarrow \infty. \end{aligned} \tag{5.2}$$

The phase shift is $\delta_\ell(k, 1) = -ka$ [96]. The restriction (2.3) is violated for the infinite square-well potential, and the forms (2.34) and (3.30) of the Levinson theorem do not hold owing to $\delta_\ell(\infty, 1) = -\infty$. But the form (4.26) of the Levinson theorem still holds.

5.2. The non-local interaction

The radial equation (2.2) of the Schrödinger equation with a spherically symmetric non-local interaction is

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2} R_\ell(r, E, \lambda) + k^2 R_\ell(r, E, \lambda) = \frac{2M}{\hbar^2} \int_0^\infty V(r, r') R_\ell(r', E, \lambda)\, \mathrm{d}r'. \tag{5.3}$$

The potential $V(r, r')$ is assumed to be Hermitian, real and vanishing at a distance larger than r_0:

$$V(r, r') = V(r', r), \qquad V(r, r') = 0 \qquad \text{if} \quad r > r_0 \quad \text{or} \quad r' > r_0. \tag{5.4}$$

Martin [65] investigated the possibility of a degeneracy of the wavefunction for a positive energy and found that the Levinson theorem (2.34) has to be slightly modified as

$$\delta_\ell(0) - \delta_\ell(\infty) = \pi(n_\ell + n'_\ell), \tag{5.5}$$

where n_ℓ is the number of bound states and n'_ℓ is the number of eigenstates of positive energy with vanishing asymptotic form.

As a matter of fact, when an eigenstate of positive energy with vanishing asymptotic form occurs, the phase shift $\delta_\ell(\infty)$ decreases by π (see figures 1 and 2 in [65]) and the form (2.34) of the Levinson theorem is modified. On the other hand, the form (4.26) of the Levinson theorem still holds, because in its proof with the Sturm–Liouville theorem, including for the non-local interaction [26, 59], the property of scattering states only with small k is concerned.

5.3. Newton's two counterexamples

Newton (see pp 438–439 in [72]) gave two counterexamples where the potential has a tail r^{-2} at infinity such that the Levinson theorem (2.34) does not hold. However, the modified Levinson theorem (4.43) holds in those cases.

Example 1

$$U(r) = \frac{2a^2}{(1+ar)^2} \longrightarrow \frac{2}{r^2}, \qquad \text{as} \quad r \longrightarrow \infty. \tag{5.6}$$

The regular S-wavefunction is given by

$$R_0(r,E) = \frac{\sin(kr)}{k} - \frac{a^2}{k^3}\frac{kr\cos(kr)-\sin(kr)}{1+ar}$$
$$\rightarrow \frac{\sin(kr)}{k} - \frac{a\cos(kr)}{k^2} = C\sin[kr+\delta_0(k)], \qquad \text{as} \quad r\rightarrow\infty,$$

where $\tan\delta_0(k) = -a/k$ and $\sin\delta_0(k) < 0$. The phase shifts of S-wave are $\delta_0(0) = -\pi/2$ and $\delta_0(\infty) = 0$. There is no bound state for S-wave, $n_0 = 0$, such that the Levinson theorem (2.34) is violated. However, since the potential has a tail of $a(a+1)r^{-2}$ with $a = 1$ at infinity, the modified Levinson theorem (4.43) holds.

Example 2

$$U(r) = -6r\frac{2N^2 - r^3}{(N^2+r^3)^2} \longrightarrow \frac{6}{r^2}, \qquad \text{as} \quad r\longrightarrow\infty, \tag{5.7}$$

where N is a constant. The regular S-wavefunction is

$$\begin{aligned} R_0(r,E) &= \frac{\sin kr}{k} - \frac{3r}{k^3(N^2+r^3)}(\sin kr - kr\cos kr) \\ &\xrightarrow{k\to 0} \sqrt{1/3}N\cdot\sqrt{3}Nr(N^2+r^3)^{-1}. \end{aligned} \tag{5.8}$$

Removing the factor $\sqrt{1/3}N$, one obtains the normalized wavefunction of a zero-energy bound state of S-wave. Since $\delta_0(0) = 0$, the Levinson theorem (2.34) does not hold. However, in this example, $\ell = 0, a = 2, n_0 = 1$ and $\delta_0(0) = 0$, so that the modified Levinson theorem (4.43) holds.

5.4. Brief summary

The form (2.34) of the Levinson theorem proved with the Jost function and the form (3.30) proved with the Green function both contain a term $\delta_\ell(\infty)$, but the form (4.26) of the Levinson theorem proved with the Sturm–Liouville theorem does not contain that term. In the usual cases, $\delta_\ell(\infty)$ is vanishing and three forms are equivalent. However, some special examples are discussed in this section where $\delta_\ell(\infty)$ is not vanishing and only the form (4.26) of the Levinson theorem holds.

In two counterexamples raised by Newton [72] where the potential has a tail r^{-2} at large r and the restriction (2.3) is violated, the forms (2.34), (3.30) and (4.26) of the Levinson theorem all do not hold, but the modified form (4.43) of the Levinson theorem proved with the Sturm–Liouville theorem holds for those examples.

6. The Levinson theorem for the Dirac equation

In this section, we will prove the Levinson theorem for the Dirac equation in (3+1)-dimensions with the generalized Sturm–Liouville theorem. It is assumed that only the zeroth component A_0 of the gauge potential is non-vanishing, $eA_0 = \lambda V(r)$, where $V(r)$ is spherically symmetric and satisfies the condition (2.3).

6.1. The Dirac equation in (3+1)-dimensions

The Dirac equation in the natural units $\hbar = c = 1$ is [8]

$$\mathrm{i}\sum_{\mu=0}^{3}\gamma^\mu(\partial_\mu + \mathrm{i}eA_\mu)\Psi(\boldsymbol{r},t) = M\Psi(\boldsymbol{r},t), \tag{6.1}$$

where $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu}\mathbf{1}$ and the metric tensor $\eta^{\mu\nu}$ is $\delta_{\mu\nu}$ when $\mu = 0$ and $-\delta_{\mu\nu}$ when $\mu \neq 0$. γ^μ are usually taken to be

$$\gamma^a = -\gamma_a = \begin{pmatrix} 0 & \sigma_a \\ -\sigma_a & 0 \end{pmatrix}, \qquad \gamma^0 = \gamma_0 = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}, \tag{6.2}$$

where $a = 1, 2, 3$ and σ_a is the Pauli matrix. We discuss a special case where only the zero component of A_μ is non-vanishing:

$$eA_0 = \lambda V(r), \qquad A_a = 0, \qquad a = 1, 2, 3, \tag{6.3}$$

where $V(r)$ is spherically symmetric and satisfies the condition (2.3). λ is a real parameter and eventually is set to be one. The Hamiltonian $H(\boldsymbol{r})$ of the system is expressed as

$$\begin{aligned} &\mathrm{i}\partial_0\Psi(\boldsymbol{r}, t) = H(\boldsymbol{r})\Psi(\boldsymbol{r}, t), \\ &H(\boldsymbol{r}) = \sum_{a=1}^{3} \gamma^0\gamma^a p_a + \lambda V(r) + \gamma^0 M, \end{aligned} \tag{6.4}$$

where $p_a = -\mathrm{i}\partial_a$, $1 \leqslant a \leqslant 3$. Since the tail of potential at large r can be neglected, we will first discuss the bounded potential

$$V(r) = 0, \qquad \text{when} \quad r > r_0. \tag{6.5}$$

The orbital angular-momentum operators L_a, the spinor operators S_a and the total angular-momentum operators J_a are defined as follows:

$$\begin{aligned} &L_a = -L^a = \mathrm{i}\sum_{bc} \epsilon_{abc}\left(x_b\partial_c - x_c\partial_b\right), && L^2 = \sum_{a=1}^{3} L_a L_a, \\ &S_a = -S^a = \mathrm{i}\sum_{bc} \epsilon_{abc}\gamma_b\gamma_c/2, && S^2 = \sum_{a=1}^{3} S_a S_a, \\ &J_a = L_a + S_a, && J^2 = \sum_{a=1}^{3} J_a J_a. \end{aligned} \tag{6.6}$$

There is another conservative quantity κ, which is commutable with the Hamiltonian $H(\boldsymbol{r})$ and the total angular-momentum J^2 and J_3,

$$\kappa = \gamma^0\left\{2\sum_{a=1}^{3} L_a S_a + 1\right\} = \gamma^0\{J^2 - L^2 - S^2 + 1\}, \tag{6.7}$$

κ here is different by a sign from that given in p 53 of [8], but the same as that in p 483 of [91].

Denote by $\psi_K(\boldsymbol{r}, E, \lambda, m)$ the common eigenfunction of $H(\boldsymbol{r})$, J^2, J_3 and κ with the eigenvalues E, $j(j+1)$, m and K, respectively, where K is a non-vanishing integer and $j = |K| - 1/2$. Let [8]

$$\begin{aligned} &\Psi(\boldsymbol{r}, t) = \mathrm{e}^{-\mathrm{i}Et}\psi_K(\boldsymbol{r}, E, \lambda, m), \\ &\psi_K(\boldsymbol{r}, E, \lambda, m) = r^{-1}\begin{pmatrix} F_K(r, E, \lambda)\mathcal{Y}_{K,m}(\hat{\boldsymbol{r}}) \\ iG_K(r, E, \lambda)\mathcal{Y}_{-K,m}(\hat{\boldsymbol{r}}) \end{pmatrix}, \end{aligned} \tag{6.8}$$

where the spherical spinor function $\mathcal{Y}_{K,m}(\hat{\boldsymbol{r}})$ is constructed from the unit spinor $\chi(\rho)$ and the spherical harmonic $Y^{\ell}_{m}(\hat{\boldsymbol{r}})$ through the Clebsch–Gordan coefficients:

$$\begin{aligned}\mathcal{Y}_{|K|,m}(\hat{\boldsymbol{r}}) &= \begin{pmatrix}\sqrt{\frac{j+m}{2j}}Y^{\ell}_{m-1/2}(\hat{\boldsymbol{r}})\\ \sqrt{\frac{j-m}{2j}}Y^{\ell}_{m+1/2}(\hat{\boldsymbol{r}})\end{pmatrix}, \qquad \ell = j-1/2,\\ \mathcal{Y}_{-|K|,m}(\hat{\boldsymbol{r}}) &= \begin{pmatrix}\sqrt{\frac{j-m+1}{2j+2}}Y^{\ell}_{m-1/2}(\hat{\boldsymbol{r}})\\ -\sqrt{\frac{j+m+1}{2j+2}}Y^{\ell}_{m+1/2}(\hat{\boldsymbol{r}})\end{pmatrix}, \qquad \ell = j+1/2,\end{aligned} \tag{6.9}$$

$$\begin{aligned}(\boldsymbol{L}\cdot\boldsymbol{\sigma}+1)\,\mathcal{Y}_{K,m}(\hat{\boldsymbol{r}}) &= K\mathcal{Y}_{K,m}(\hat{\boldsymbol{r}}), \qquad \boldsymbol{L}\cdot\boldsymbol{\sigma} = \sum_{a=1}^{3}L_a\sigma_a,\\ (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\,\mathcal{Y}_{K,m}(\hat{\boldsymbol{r}}) &= \mathcal{Y}_{-K,m}(\hat{\boldsymbol{r}}), \qquad \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}} = \sum_{a=1}^{3}\sigma_a x^a/r.\end{aligned} \tag{6.10}$$

By making use of the following formula

$$\begin{aligned}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})^2\left(\sum_{a=1}^{3}\sigma_a p_a\right)r^{-1}f(r)r\mathcal{Y}_{K,m}(\hat{\boldsymbol{r}}) &= (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\,(-\mathrm{i}\partial_r+\mathrm{i}r^{-1}\boldsymbol{\sigma}\cdot\boldsymbol{L})r^{-1}f(r)\mathcal{Y}_{K,m}(\hat{\boldsymbol{r}})\\ &= \frac{\mathrm{i}}{r}\left[-\frac{\mathrm{d}f(r)}{\mathrm{d}r}+\frac{Kf(r)}{r}\right](\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\,\mathcal{Y}_{K,m}(\hat{\boldsymbol{r}}),\end{aligned} \tag{6.11}$$

one obtains the radial equation by substituting equation (6.8) into the Dirac equation (6.4) [8], where the γ_μ matrices (6.2) are applied:

$$\begin{aligned}\frac{\mathrm{d}G_K(r,E,\lambda)}{\mathrm{d}r}+\frac{K}{r}G_K(r,E,\lambda) &= [E-\lambda V(r)-M]F_K(r,E,\lambda),\\ -\frac{\mathrm{d}F_K(r,E,\lambda)}{\mathrm{d}r}+\frac{K}{r}F_K(r,E,\lambda) &= [E-\lambda V(r)+M]G_K(r,E,\lambda).\end{aligned} \tag{6.12}$$

It is easy to see that the solution with a negative K can be obtained from that with a positive K by interchanging $F_K(r,E,\lambda) \leftrightarrow G_{-K}(r,-E,-\lambda)$. The negative λ can be understood as the change of the sign of the potential $V(r)$. Hereafter, we only discuss the solution with a positive K. The main results for the case with a negative K will be indicated in the text. In solving equation (6.12), two momentums k and k_1 are introduced for different energies:

$$\begin{aligned}k &= \sqrt{E^2-M^2}, \qquad \text{when} \quad |E| \geqslant M,\\ k_1 &= \sqrt{M^2-E^2}, \qquad \text{when} \quad |E| \leqslant M.\end{aligned} \tag{6.13}$$

For a free particle, $\lambda = 0$, there is no bound state ($|E| \leqslant M$) for equation (6.12), and the orthonormal radial functions of a scattering state with $|E| > M$ are

$$\begin{aligned}F_K(r,E,0) &= (E/|E|)\sqrt{|E+M|r/2}J_{K-1/2}(kr),\\ G_K(r,E,0) &= \sqrt{|E-M|r/2}J_{K+1/2}(kr).\end{aligned} \tag{6.14}$$

Their asymptotic behaviours are

$$F_K(r,E,0) = \begin{cases}\dfrac{E}{|E|}\dfrac{(kr)^K}{(2K-1)!!}\sqrt{\dfrac{|E+M|}{\pi k}} \to 0, & \text{when} \quad kr \to 0,\\ \dfrac{E}{|E|}\sqrt{\dfrac{|E+M|}{\pi k}}\cos\left(kr-\dfrac{K\pi}{2}\right), & \text{when} \quad kr \to \infty,\end{cases}$$

$$G_K(r, E, 0) = \begin{cases} \dfrac{(kr)^{K+1}}{(2K+1)!!}\sqrt{\dfrac{|E-M|}{\pi k}} \longrightarrow 0, & \text{when} \quad kr \to 0, \\ \sqrt{\dfrac{|E-M|}{\pi k}} \sin\left(kr - \dfrac{K\pi}{2}\right), & \text{when} \quad kr \to \infty. \end{cases} \tag{6.15}$$

For a given λ, equation (6.12) is solved in two regions $[0, r_0)$ and $(r_0\infty)$ separately, and then match two solutions through the matching condition at r_0:

$$\phi_K(r_0-, E, \lambda) = \phi_K(r_0+, E, \lambda), \qquad \phi_K(r_0, E, \lambda) = \frac{F_K(r_0, E, \lambda)}{G_K(r_0, E, \lambda)}. \tag{6.16}$$

As far as the matching condition is concerned, the normalization factors in the solutions are not important.

In the region $[0, r_0)$, there is only one regular solution to equation (6.12). The asymptotic forms of the regular solutions at the origin are

$$\begin{aligned} F_K(r, E, \lambda) &= c(E/|E|)(2K+1)r^K \stackrel{r\to 0}{\longrightarrow} 0, \\ G_K(r, E, \lambda) &= c(|E-M|)r^{K+1} \stackrel{r\to 0}{\longrightarrow} 0, \end{aligned} \qquad \text{when} \quad |E| > M, \tag{6.17}$$

$$\begin{aligned} F_K(r, E, \lambda) &= -c(2K+1)r^K \stackrel{r\to 0}{\longrightarrow} 0, \\ G_K(r, E, \lambda) &= c(M-E)r^{K+1} \stackrel{r\to 0}{\longrightarrow} 0, \end{aligned} \qquad \text{when} \quad |E| < M, \tag{6.18}$$

where c is the normalization factor. In the region (r_0, ∞), equation (6.12) can be solved analytically due to equation (6.5). There are two linearly independent solutions when $|E| > M$, which are combined to satisfy the matching condition (6.16). From the orthonormal condition

$$\int_0^\infty \mathrm{d}r[F_K(r, E', \lambda)F_K(r, E, \lambda) + G_K(r, E', \lambda)G_K(r, E, \lambda)] = \delta(E - E'), \tag{6.19}$$

the scattering solution is

$$\begin{aligned} F_K(r, E, \lambda) &= \frac{E}{|E|}\sqrt{\frac{|E+M|r}{2}}[\cos\delta_K(E, \lambda)J_{K-1/2}(kr) - \sin\delta_K(E, \lambda)N_{K-1/2}(kr)] \\ &\stackrel{kr\to\infty}{\longrightarrow} \frac{E}{|E|}\sqrt{\frac{|E+M|}{\pi k}} \cos\left[kr - \frac{K\pi}{2} + \delta_K(E, \lambda)\right], \\ G_K(r, E, \lambda) &= \sqrt{\frac{|E-M|r}{2}}[\cos\delta_K(E, \lambda)J_{K+1/2}(kr) - \sin\delta_K(E, \lambda)N_{K+1/2}(kr)] \\ &\stackrel{kr\to\infty}{\longrightarrow} \sqrt{\frac{|E-M|}{\pi k}} \sin\left[kr - \frac{K\pi}{2} + \delta_K(E, \lambda)\right]. \end{aligned} \tag{6.20}$$

The phase shift $\delta_K(E, \lambda)$, as well as the radial functions $F_K(r, E, \lambda)$ and $G_K(r, E, \lambda)$, depends on the parameter λ through the matching condition (6.16):

$$\tan\delta_K(E, \lambda) = \frac{\phi_K(r_0-, E, \lambda)kJ_{K+1/2}(kr_0) - (E/|E|)(|E+M|)J_{K-1/2}(kr_0)}{\phi_K(r_0-, E, \lambda)kN_{K+1/2}(kr_0) - (E/|E|)(|E+M|)N_{K-1/2}(kr_0)}. \tag{6.21}$$

Since the phase shift $\delta_K(E, \lambda)$ is calculated from its tangent function, it is determined up to a multiple of π. A convention for the phase shift is accepted to determine it uniquely that $\delta_K(E, \lambda)$ with $|E| > M$ is a continuous function of λ and vanishing at $\lambda = 0$:

$$\delta_K(E, 0) = 0. \tag{6.22}$$

In fact, the forms of the solutions (6.15) and (6.20) have implied this convention.

For a given k, one obtains from equation (6.21)

$$\left.\frac{\partial \delta_K(E,\lambda)}{\partial \phi_K(r_0-,E,\lambda)}\right|_k = -\frac{E}{|E|}\frac{2|E+M|}{\pi r_0}\cos^2[\delta_K(E,\lambda)] \times\{\phi_K(r_0-,E,\lambda)kN_{K+1/2}(kr_0)-(E/|E|)(|E+M|)N_{K-1/2}(kr_0)\}^{-2}, \qquad (6.23)$$

where the identity $J_\nu(z)N_{\nu-1}(z) - J_{\nu-1}(z)N_\nu(z) = 2/(\pi z)$ is used. Different from equation (4.17) in the Schrödinger case, equation (6.23) contains a factor $E/|E|$, namely, as the ratio $\phi_K(r_0-,E,\lambda)$ increases the phase angle $\delta_K(E,\lambda)$ decreases when $E > M$, but increases when $E < -M$.

There is only one regular solution for a given E with $|E| \leqslant M$ in the region (r_0,∞),

$$\begin{aligned} F_K(r,E) &= \mathrm{e}^{\mathrm{i}(K+1/2)\pi/2}\sqrt{(M+E)\pi k_1 r/2}H^{(1)}_{K-1/2}(\mathrm{i}k_1 r) \overset{k_1 r\to\infty}{\longrightarrow} \sqrt{M+E}\,\mathrm{e}^{-k_1 r},\\ G_K(r,E) &= \mathrm{e}^{\mathrm{i}(K+3/2)\pi/2}\sqrt{(M-E)\pi k_1 r/2}H^{(1)}_{K+1/2}(\mathrm{i}k_1 r) \overset{k_1 r\to\infty}{\longrightarrow} \sqrt{M-E}\,\mathrm{e}^{-k_1 r}. \end{aligned} \qquad (6.24)$$

6.2. The generalized Sturm–Liouville theorem

Usually, the Sturm–Liouville theorem refers to the eigenvalue problems in the differential equations of second order. The Dirac equation is a coupled differential equation of first order. The Sturm–Liouville theorem has to be developed to study the eigenvalue problems in the differential equations of first order. The new form of the Sturm–Liouville theorem, raised by Professor C N Yang, shows the monotonic property of a phase angle, and is suitable for the Dirac equation, where the phase angle is the ratio of two radial functions [66, 103, 104].

The radial equations (14) can be rewritten in the matrix form

$$\begin{aligned} \Phi = \Phi_K(r,E,\lambda) &= \begin{pmatrix} F_K(r,E,\lambda)\\ G_K(r,E,\lambda)\end{pmatrix},\\ \mathrm{i}\sigma_2\frac{\mathrm{d}\Phi}{\mathrm{d}r} + \frac{K}{r}\sigma_1\Phi &= [E-\lambda V(r)]\Phi - M\sigma_3\Phi. \end{aligned} \qquad (6.25)$$

The key for the monotonic property of the phase angle is that the matrix on the term with derivative in the radial equation is anti-symmetric and those on the remaining terms are symmetric. Letting $\Phi_E = \Phi_K(r,E',\lambda)$ and $\Phi_\lambda = \Phi_K(r,E,\lambda')$ for simplicity, one has from equation (6.25)

$$\frac{\mathrm{d}}{\mathrm{d}r}\left[\Phi_E^T i\sigma_2\Phi\right] = [E-E']\Phi_E^T\Phi, \qquad (6.26)$$

$$\frac{\mathrm{d}}{\mathrm{d}r}\left[\Phi_\lambda^T i\sigma_2\Phi\right] = [\lambda'-\lambda]\Phi_\lambda^T V(r)\Phi. \qquad (6.27)$$

From equation (6.26), one obtains the generalized form of the Sturm–Liouville theorem for the Dirac equation:

$$\begin{aligned} \{G_K(r_0,E,\lambda)\}^2\frac{\partial}{\partial E}\phi_K(r_0-,E,\lambda) &= \lim_{E'\to E}\left.\frac{\Phi_K(r,E',\lambda)^T i\sigma_2\Phi_K(r,E,\lambda)}{E'-E}\right|_{r_0-}\\ &= -\int_0^{r_0}\{F_K(r,E,\lambda)^2 + G_K(r,E,\lambda)^2\}\,\mathrm{d}r < 0. \end{aligned} \qquad (6.28)$$

The ratio $\phi_K(r_0-,E,\lambda)$ at a given point r_0- decreases monotonically as the energy increases. For the solution with $|E| < M$, $\Phi_K(r,E,\lambda)$ tends to zero as r goes to infinity (see equation (6.24)). Thus,

$$\{G_K(r_0,E,\lambda)\}^2\frac{\partial}{\partial E}\phi_K(r_0+,E,\lambda) = \int_{r_0}^{\infty}\{F_K(r,E,\lambda)^2 + G_K(r,E,\lambda)^2\}\,\mathrm{d}r > 0. \qquad (6.29)$$

The ratio $\phi_K(r_0+, E, \lambda)$ at a given point r_0+ with $|E| < M$ increases monotonically as the energy increases.

From equation (6.27), one has

$$\{G_K(r_0, E, \lambda)\}^2 \frac{\partial}{\partial\lambda}\phi_K(r_0-, E, \lambda) = \lim_{\lambda'\to\lambda} \left.\frac{\Phi_K(r, E, \lambda')^T i\sigma_2 \Phi_K(r, E, \lambda)}{\lambda' - \lambda}\right|_{r_0-}$$
$$= \int_0^{r_0} V(r)\{F_K(r, E, \lambda)^2 + G_K(r, E, \lambda)^2\}\,\mathrm{d}r. \tag{6.30}$$

The ratio $\phi_K(r_0-, E, \lambda)$ at a given point r_0- is monotonic with respect to λ if the potential $V(r)$ does not change its sign in the region $[0, r_0)$.

For a scattering state, the asymptotic behaviour of $\Phi_K(r, E, \lambda)$ at infinity is given in equation (6.20). Substituting it into equation (6.30) where r_0 tends to infinity, one obtains

$$\lim_{r\to\infty}\lim_{\lambda'\to\lambda} \frac{\Phi_K(r, E, \lambda')^T i\sigma_2 \Phi_K(r, E, \lambda)}{\lambda' - \lambda} = -\frac{1}{\pi}\frac{E}{|E|}\lim_{\lambda'\to\lambda}\frac{\sin[\delta_K(E, \lambda') - \delta_K(E, \lambda)]}{\lambda' - \lambda}$$
$$= \int_0^{\infty} V(r)\{F_K(r, E, \lambda)^2 + G_K(r, E, \lambda)^2\}\,\mathrm{d}r > 0.$$
$$\frac{\partial\delta_K(E, \lambda)}{\partial\lambda} = -\pi\frac{E}{|E|}\int_0^\infty V(r)\Phi_K(r, E, \lambda)^T\Phi_K(r, E, \lambda)\,\mathrm{d}r. \tag{6.31}$$

The behaviours of the phase shift $\delta_K(E, \lambda)$ depend upon the sign of the energy E, but the phase shifts both for positive and negative energy are monotonic with respect to λ if the potential $V(r)$ does not change its sign in the whole space.

If the potential $V(r)$ in equation (6.12) is neglectable as $|E|$ tends to infinity, $\Phi_K(r, E, \lambda)$ tends to $\Phi_K(r, E, 0)$. Thus, due to equation (6.14)

$$\lim_{E\to\infty}\frac{\partial\delta_K(E, \lambda)}{\partial\lambda} = -\pi\lim_{E\to\infty}\int_0^\infty V(r)\left\{\frac{(E+M)r}{2}(J_{K-1/2}(kr))^2 + \frac{(E-M)r}{2}(J_{K+1/2}(kr))^2\right\}\mathrm{d}r,$$
$$\lim_{E\to\infty}\frac{\partial\delta_K(-E, \lambda)}{\partial\lambda} = \pi\lim_{E\to\infty}\int_0^\infty V(r)\left\{\frac{(E-M)r}{2}(J_{K-1/2}(kr))^2 + \frac{(E+M)r}{2}(J_{K+1/2}(kr))^2\right\}\mathrm{d}r,$$

$$\lim_{E\to\infty}\frac{\partial}{\partial\lambda}\{\delta_K(E, \lambda) + \delta_K(-E, \lambda)\} = -M\pi\lim_{E\to\infty}\int_0^\epsilon rV(r)\{(J_{K-1/2}(kr))^2 - (J_{K+1/2}(kr))^2\}\,\mathrm{d}r$$
$$-\lim_{E\to\infty}\frac{2M}{k}\int_\epsilon^\infty V(r)\cos[2kr - K\pi]\mathrm{d}r = 0, \tag{6.32}$$

where ϵ is a small real number. Equation (6.32) means that it is conditional to set $\delta_K(\infty, \lambda) + \delta_K(-\infty, \lambda) = 0$ [3, 14].

6.3. The Levinson theorem for the Dirac equation in (3+1)-dimensions

We will pay more attention to the phase shift $\delta_K(\pm M, \lambda)$ of zero momentum, which is defined to be the limit of $\delta_K(E, \lambda)$ as k tends to zero:

$$\delta_K(\pm M, \lambda) = \lim_{E\to\pm M}\delta_K(E, \lambda). \tag{6.33}$$

For a sufficiently small kr_0, one takes the series expansion of equation (6.21) with respect to kr_0, where only the leading terms are reserved. But the next leading terms in the denominator are also kept down because they are sensitive to the later calculation:

$$\tan\delta_K(E,\lambda) = \frac{-\pi(kr_0)^{2K-1}}{2^{2K+1}\Gamma(K+3/2)\Gamma(K+1/2)} \times \frac{\phi_K(r_0-,M,\lambda)(kr_0)^2 - 2M(2K+1)r_0}{\phi_K(r_0-,M,\lambda) - c^2k^2 - \frac{2Mr_0}{2K-1}\left[1+\frac{(kr_0)^2}{(2K-1)(2K-3)}\right]}, \tag{6.34}$$

when $E > M$, and

$$\tan\delta_K(E,\lambda) = \frac{-\pi(kr_0)^{2K+1}}{2^{2K+1}\Gamma(K+3/2)\Gamma(K+1/2)} \times \frac{\phi_K(r_0-,-M,\lambda) + (2K+1)/(2Mr_0)}{\phi_K(r_0-,-M,\lambda) + c^2k^2 + k^2r_0/[2M(2K-1)]}, \tag{6.35}$$

when $E < -M$. The term c^2 occurs due to the generalized Sturm–Liouville theorem (6.28). Note that k^2 increases as E decreases when $E < -M$. When $K = 1$ and $E > M$, equation (6.34) reduces to

$$\tan\delta_1(E,\lambda) = -\frac{kr_0}{3}\frac{\phi_1(r_0-,M,\lambda)(kr_0)^2 - 6Mr_0}{\phi_1(r_0-,M,\lambda) - c^2k^2 - 2Mr_0[1-(kr_0)^2]}. \tag{6.36}$$

The analysis of equations (6.23) and (6.34)–(6.36) is similar to that in section 4.4. The different point is that now one has to consider the changes of both $\phi_K(r_0-,M,\lambda)$ and $\phi_K(r_0-,-M,\lambda)$. As λ increases continuously, $\delta_K(\pm M,\lambda)$ changes by jumps. As λ increases, $\delta_K(M,\lambda)$ jumps by π if $\phi_K(r_0-,M,\lambda)$ decreases across the value $2Mr_0/(2K-1)$ and jumps by $-\pi$ if $\phi_K(r_0-,M,\lambda)$ increases across the value $2Mr_0/(2K-1)$, and $\delta_K(-M,\lambda)$ jumps by $-\pi$ if $\phi_K(r_0-,-M,\lambda)$ decreases across zero and jumps by π if $\phi_K(r_0-,-M,\lambda)$ increases across zero.

If $\phi_K(r_0-,M,1) \neq 2Mr_0/(2K-1)$, $\delta_K(M,1) = n_K(M)\pi$ where $n_K(M)$ is equal to the times $\phi_K(r_0-,M,\lambda)$ decreases across the value $2Mr_0/(2K-1)$ as λ increases from 0 to 1, minus the times $\phi_K(r_0-,M,\lambda)$ increases across that value. If $\phi_K(r_0-,-M,1) \neq 0$, $\delta_K(-M,1) = n_K(-M)\pi$ where $n_K(-M)$ is equal to the times $\phi_K(r_0-,-M,\lambda)$ increases across zero as λ increases from 0 to 1, minus the times $\phi_K(r_0-,-M,\lambda)$ decreases across zero.

If $\phi_K(r_0-,M,1) = 2Mr_0/(2K-1)$, $\tan\delta_K(E,1)$ given in equation (6.34) is negative. As λ increases to reach 1, $\delta_K(M,1)$ with $K > 1$ increases an additional π if $\phi_K(r_0-,M,\lambda)$ decreases to reach $2Mr_0/(2K-1)$, but does not decrease if $\phi_K(r_0-,0,\lambda)$ increases to reach $2Mr_0/(2K-1)$. When $K = 1$, as λ increases to reach 1, $\delta_1(M,1)$ increases (or decreases) an additional $\pi/2$ if $\phi_1(r_0-,M,\lambda)$ decreases (or increases) to reach $2Mr_0$. If $\phi_K(r_0-,-M,1) = 0$, $\tan\delta_K(E,1)$ given in equation (6.35) is negative. As λ increases to reach 1, $\delta_K(-M,1)$ increases an additional π if $\phi_K(r_0-,-M,\lambda)$ increases to reach zero, but does not decrease if $\phi_K(r_0-,-M,\lambda)$ decreases to reach zero.

Now, we turn to discuss the number of bound states. In the region (r_0,∞), the solution (6.24) with $|E| < M$ gives

$$\phi_K(r_0+,E) = \begin{cases} \dfrac{2Mr_0}{2K-1}, & \text{when} \quad E \to M, \\[2ex] \dfrac{k_1^2 r_0}{2M(2K-1)} \sim 0, & \text{when} \quad E \to -M. \end{cases} \tag{6.37}$$

When $E = \pm M$, the finite solutions of equation (6.12) in the region (r_0,∞) are

$$F_K(r,M) = 2Mr^{-K+1}, \qquad G_K(r,M) = (2K-1)r^{-K}, \qquad \phi_K(r_0+,M) = \frac{2Mr_0}{2K-1}, \tag{6.38}$$

$$F_K(r,-M)=0,\quad G_K(r,-M)=r^{-K},\qquad \phi_K(r_0+,-M)=0. \tag{6.39}$$

If $\phi_K(r_0-,M,1) = 2Mr_0/(2K-1)$, the matching condition (6.16) is satisfied and the solution (6.38) describes a bound state at $E = M$ except for $K = 1$. When $K = 1$, the solution (6.38) describes a half bound state because it is finite but does not decay at infinity fast enough to be square integrable. If $\phi_K(r_0-,-M,1) = 0$, the solution (6.39) describes a bound state at $E = -M$.

In the region $[0, r_0)$, equation (6.12) is difficult to solve analytically except for $\lambda = 0$. When $\lambda = 0$, the real regular solution of equation (6.12) with $|E| \leqslant M$ is

$$\begin{aligned} F_K(r,E,0) &= \mathrm{e}^{-\mathrm{i}(K-1/2)\pi/2}\sqrt{2\pi(M+E)k_1r}\,J_{K-1/2}(\mathrm{i}k_1r),\\ G_K(r,E,0) &= \mathrm{e}^{-\mathrm{i}(K-3/2)\pi/2}\sqrt{2\pi(M-E)k_1r}\,J_{K+1/2}(\mathrm{i}k_1r).\end{aligned} \tag{6.40}$$

The asymptotic form at the origin coincides with equation (6.18). Their ratio $\phi_K(r,E,0)$ at r_0- is

$$\phi_K(r_0-,E,0)=\begin{cases}-\dfrac{2M(2K+1)}{k_1^2r_0}, & \text{when}\quad E\to M,\\[2ex] -\dfrac{2K+1}{2Mr_0}, & \text{when}\quad E\to -M.\end{cases} \tag{6.41}$$

It can be seen from equations (6.37) and (6.41) that as E increases from $-M$ to M, $\phi_K(r_0+,E)$ increases monotonically from zero to $2Mr_0/(2K-1)$ (see equation (6.29)) and $\phi_K(r_0-,E,0)$ decreases monotonically from $-(2K+1)/2Mr_0$ to negative infinity (see equation (6.28)). There is no overlap between two variant ranges of two ratios when $\lambda = 0$, such that there is no bound state for a free particle.

As λ increases from 0 to 1, $\phi_K(r_0+,E)$ remains invariant, but $\phi_K(r_0-,E,\lambda)$ changes. Due to the generalized Sturm–Liouville theorem (6.28), one only needs to pay attention to variances of $\phi_K(r_0-,\pm M,\lambda)$. If $\phi_K(r_0-,M,\lambda)$ decreases, through a jump from negative infinity to positive infinity, across the value $2Mr_0/(2K-1)$ as λ increases, one overlap appears between two variant ranges of the ratios at two sides of r_0. Due to the generalized Sturm–Liouville theorem, there is one and only one energy with which the matching condition (6.16) is satisfied and one bound state appears. As λ increases again, $\phi_K(r_0-,M,\lambda)$ may decrease, through another jump, second time across the value $2Mr_0/(2K-1)$, a new overlap occurs between two variant ranges of two ratios, such that another bound state appears. Different to the case of Schrödinger equation, $\phi_K(r_0-,-M,\lambda)$ also changes as λ increases. If $\phi_K(r_0-,-M,\lambda)$ decreases, through a jump, across zero as λ increases, one overlap between two variant ranges of the ratios at two sides of r_0 disappears and a bound state becomes a scattering state with a negative energy and vice versa.

Together with the conclusion for the phase shifts, each time $\phi_K(r_0-,M,\lambda)$ decreases across the value $2Mr_0/(2K-1)$ as λ increases, a scattering state with a positive energy becomes a bound state and the phase shift $\delta_K(M,\lambda)$ jumps by π. Conversely, each time $\phi_K(r_0-,M,\lambda)$ increases across the value $2Mr_0/(2K-1)$ as λ increases, a bound state becomes a scattering state with a positive energy and the phase shift $\delta_K(M,\lambda)$ jumps by $-\pi$. For the critical case where $\phi_K(r_0-,M,1) = 2Mr_0/(2K-1)$ with $K > 1$, if $\phi_K(r_0-,M,\lambda)$ decreases to reach $2Mr_0/(2K-1)$ as λ increases to reach 1, a new bound state appears at $E = M$ and the phase shift $\delta_K(M,\lambda)$ jumps by an additional π. Conversely, if $\phi_K(r_0-,M,\lambda)$ increases to reach $2Mr_0/(2K-1)$, no bound state disappears and $\delta_K(M,\lambda)$ does not jump. For the critical case where $\phi_1(r_0-,M,1) = 2Mr_0$ with $K = 1$, if $\phi_1(r_0-,M,\lambda)$ decreases to reach the value $2Mr_0$ as λ increases to reach 1, no new bound state (only a half bound state with

$E = M$) appears and the phase shift $\delta_1(M, \lambda)$ jumps by $\pi/2$. Conversely, if $\phi_1(r_0-, M, \lambda)$ increases to reach $2Mr_0$, a bound state becomes a half bound state and the phase shift $\delta_1(M, \lambda)$ jumps by $-\pi/2$.

Similarly, each time $\phi_K(r_0-, -M, \lambda)$ decreases (or increases) across zero, a bound state disappears (or appears) and the phase shift $\delta_K(-M, \lambda)$ jumps by $-\pi$ (or π). For the critical case where $\phi_K(r_0-, -M, 1) = 0$, if $\phi_K(r_0-, M, \lambda)$ increases to reach 0 as λ increases to reach 1, a new bound state appears at $E = -M$ and the phase shift $\delta_K(M, \lambda)$ jumps by π. Conversely, if $\phi_K(r_0-, -M, \lambda)$ decreases to reach 0, no bound state disappears and $\delta_K(M, \lambda)$ does not jump.

Through an interchanging $F_K(r, E, \lambda) \leftrightarrow G_{-K}(r, -E, -\lambda)$, the conclusion for a negative K can be made. Therefore, the Levinson theorem for the Dirac equation with a spherically symmetric potential is written as

$$[\delta_K(M) + \delta_K(-M)]/\pi = \begin{cases} n_K + 1/2, & \text{a half bound state occurs,} \\ n_K, & \text{the remaining cases,} \end{cases} \tag{6.42}$$

where n_K is the number of bound states with the angular momentum K, and $\delta_K(\pm M) = \delta_K(\pm M, 1)$ is the phase shifts at the energy $E = \pm M$. A half bound state may occur only when $K = \pm 1$. When $K = 1$ a half bound state with $E = M$ occurs if $\phi_1(r_0-, M, 1) = 2Mr_0$, and when $K = -1$ a half bound state with $E = -M$ occurs if $\phi_{-1}(r_0-, -M, 1) = (2Mr_0)^{-1}$.

6.4. Potential with a tail

Now, we turn to the general case where the potential has a tail at infinity. Since the potential $V(r)$ satisfies the restriction (2.3), $V(r)$ vanish at infinity faster than r^{-2}. We will explain why the potential $V(r)$ can be neglected at large $r > r_0$.

Differentiate equation (6.12) in the region (r_0, ∞) with respect to r:

$$\begin{aligned} &\frac{\mathrm{d}^2 g_K(r,E)}{\mathrm{d}r^2} + \left[\frac{1}{r} + \frac{V'}{E - V - M}\right]\frac{\mathrm{d}g_K(r,E)}{\mathrm{d}r} \\ &\qquad + \left[k^2 - \frac{(K+1/2)^2}{r^2} - 2EV + V^2 + \frac{V'(2K+1)}{2r(E-V-M)}\right] g_K(r,E) = 0, \\ &\frac{\mathrm{d}^2 f_K(r,E)}{\mathrm{d}r^2} + \left[\frac{1}{r} + \frac{V'}{E - V + M}\right]\frac{\mathrm{d}f_K(r,E)}{\mathrm{d}r} \\ &\qquad + \left[k^2 - \frac{(K-1/2)^2}{r^2} - 2EV + V^2 - \frac{V'(2K-1)}{2r(E-V+M)}\right] f_K(r,E) = 0, \end{aligned} \tag{6.43}$$

where $F_K(r, E) = \sqrt{r} f_K(r, E)$ and $G_K(r, E) = \sqrt{r} g_K(r, E)$. Obviously, if only the leading terms with respect to r^{-1} are remained in equation (6.43), all the terms related to $V(r)$, which vanishes at infinity faster than r^{-2}, are neglected. Namely, solutions (6.20) and (6.24) satisfy equation (6.12) in the region (r_0, ∞) approximately if the condition (2.3) holds.

6.5. Brief summary

The character of the Levinson theorem for the Dirac equation is that the number of the bound states is related to the sum of two phase shifts at the energies $\pm M$. The generalized Sturm–Liouville theorem holds for the coupled differential equations of first order and plays an important role in the proof of the Levinson theorem for the Dirac equation. The so-called 'strong Levinson theorem' [16, 80–82] showed that the phase shifts at the energies $\pm M$ were separately constrained by the numbers of bound states transformed from the positive energy continuum and by the numbers of bound states transformed from the negative energy continuum. Another 'stronger form of Levinson's theorem' constrained the phase shifts at the energies $\pm M$ separately by the numbers of bound states having even and odd numbers of nodes [86]. But it is hard to distinguish those two bound states. Those relations are only the medial step in the proof of the Levinson theorem [60, 61, 75]. In my opinion, the stronger version of the Levinson theorem does not make new sense.

7. Conclusion

At its beginning stage, the Levinson theorem (2.34) for the spherically symmetric Schrödinger equation was proved with the method of the Jost function. In the request of the analytic continuation of the Jost function to the complex plane, the potential $V(r)$ was restricted by the conditions (2.3) and (2.14). The condition (2.14) is too strong for the Levinson theorem. The term of the phase shift $\delta_\ell(\infty)$ at infinite energy appears in the Levinson theorem (2.34), but it is vanishing in the condition (2.3). In some special cases, for example, in the infinite square well and in the case with a non-local interaction, $\delta_\ell(\infty)$ is not vanishing and the Levinson theorem (2.34) has to be modified. The proof method with the Jost function is quite difficult to generalize to the relativistic equation of motion.

Later, the Levinson theorem was proved with the operator formulism of the scattering theory or, equivalently, with the method of the Green function. The restriction (2.14) was released, but the term of $\delta_\ell(\infty)$ still exists in the Levinson theorem (3.30). The proof method can be generalized to the relativistic cases. In this proof some problems have to be studied more carefully, such as the difference of two infinite quantities and the interchange of two limits of $E' \to E$ and $r \to \infty$.

Professor C N Yang raised another form of the Sturm–Liouville theorem where a phase angle is monotonic with respect to the energy. The monotonic property of a phase angle is very effective in the proof of the Levinson theorem. This proof method with the Sturm–Liouville theorem is intuitive in physical meaning and easy for generalization. The restriction (2.14) was released, and the term of $\delta_\ell(\infty)$ disappears. The obtained Levinson theorem (4.26) holds for the infinite square well and for the non-local interaction. When the potential has a tail of r^{-2} at infinity, which violates the restriction (2.3), a modified Levinson theorem (4.43) is proved by the Sturm–Liouville theorem and holds for two counterexamples raised by Newton. In terms of this method, the Levinson theorem is easy to be generalized to the Dirac equation, to the Klein–Gordon equation [27, 48, 76, 79, 92, 94], to the arbitrary spatial dimensions and to the cases with variant potentials.

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