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Levinson's theorem for non-local interactions

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Abstract. Levinson's theorem for a Schrödinger equation with both local and non-local symmetric potentials is studied in terms of the Sturm-Liouville theorem. A new convention for the phase shifts is applied instead of the usual one. It is proved that the usual Levinson theorem holds for the case with both local potential and non-local symmetric cutoff potential, which is not necessarily separable. The problems related to the positive-energy bound states and the physically redundant solutions are also discussed in this paper.

1. Introduction

Levinson's theorem (Levinson 1949) is one of the fundamental theorems in scattering theory, and has been confirmed by several authors (Jauch 1957, Ni 1979) in terms of a few different methods, and generalised to a variety of potentials and relativistic cases (Newton 1960, 1977a, b, Martin 1958, Wright 1965, Ma and Ni 1985). In comparison with previous proofs, the proof of Levinson's theorem by the Sturm-Liouville theorem, suggested by Yang, is more simple, intuitive and more easily generalised (Ma 1985a, b, c, 1986, Liang and Ma 1986, Chang and Ma 1987, Dai 1987). Some obstacles and ambiguities which may occur in the previous methods disappear in the new proof. In §§ 2 and 3 of this paper, we prove in terms of the Sturm-Liouville theorem that Levinson's theorem holds for the Schrödinger equation with both local and non-local symmetric potentials which are not necessarily separable. Some problems related to the positive-energy bound states and the physically redundant solutions will be discussed in §§ 4 and 5.

2. Sturm–Liouville theorem and the convention for the phase shifts

The radial Schrödinger equation with both local potential $V(r)$ and non-local symmetric potential $U(r, r')$ is ($\hbar = 1$, $2m = 1$)

$$\frac{d^2}{dr^2}u(r) + \left(E - V(r) - \frac{l(l+1)}{r^2}\right)u(r) = \int U(r, r')u(r')\,dr' \tag{1}$$

where $u(r)/r$ is the radial function, l denotes the angular momentum and E denotes the energy. The operator $U(r, r')$ is assumed to be real and symmetric:

$$U(r, r') = U(r', r). \tag{2}$$

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The mesonic theory of nuclear forces suggests that the interaction between two nucleons is local at great distances but becomes non-local if the two nucleons come close together. In order to simplify the demonstrations, we assume, following Martin (1958), that both interactions are well behaved in the finite region, i.e. non-singular out of the origin and not too singular at the origin (cf Chadan 1958), and they are vanishing at distances larger than a:

$$\left.\begin{aligned} |V(r)| &\sim r^{\alpha} \\ |U(r,r')| &\sim r^{\beta} \end{aligned}\right\} \qquad \alpha, \beta \geqslant -1 \text{ at } r \sim 0$$
$$\left.\begin{aligned} V(r) &= 0 \\ U(r,r') &= 0 \end{aligned}\right\} \qquad \text{at } r \geqslant a. \tag{3}$$

We call them cutoff potentials. The tail of the local potential in infinity will not change the essence of the proof and was discussed before (Ma 1985a, c). With this assumption, the integral range on the right-hand side of (1) is, in fact, from 0 to a, and the equation in the region $[a, \infty)$ simply becomes the one for the free particles:

$$\frac{d^2}{dr^2}u(r) + \left(E - \frac{l(l+1)}{r^2}\right)u(r) = 0. \tag{1'}$$

Firstly, we show the Sturm-Liouville theorem for equation (1). Denote u_1 as a solution of (1) with the energy E_1. Multiplying the equations for u and u_1 by u_1 and u, respectively, and subtracting one equation from the other, we obtain

$$\frac{d}{dr}(uu_1' - u'u_1) + (E_1 - E)uu_1$$
$$= u(r)\int U(r,r')u_1(r')\,dr' - u_1(r)\int U(r,r')u(r')\,dr'.$$

Integrating it over the variable r in the interval $[0, a]$ and noting the symmetric property (2) of $U(r, r')$, we get

$$(uu_1' - u'u_1)\Big|_0^a = -(E_1 - E)\int_0^a uu_1\,dr'.$$

We apply the physical boundary condition at the origin (see the appendix)

$$u(r) \sim 0 \qquad \text{at } r \sim 0 \tag{4}$$

so

$$u^2(a)\frac{d(u'/u)}{dE}\bigg|_{a-} = \lim_{E_1 \to E}\frac{uu_1' - u'u_1}{E_1 - E}\bigg|_0^a$$
$$= -\int_0^a u^2(r')\,dr'. \tag{5}$$

The logarithmic derivative u'/u of the radial function u at $a-$ decreases monotonically with respect to the energy. Similarly, we discuss the solutions in the region $[a, \infty)$ instead of the region $[0, a]$, and from the boundary condition

$$u(r) \sim 0 \qquad \text{when } E < 0,\ r \sim \infty \tag{4'}$$

so that u'/u is not continuous at a except for a bound state. Then we have

$$u^2(a)\frac{d(u'/u)}{dE}\bigg|_{a+} = \int_a^{\infty} u^2(r')\,dr' \qquad E < 0. \tag{5'}$$

Equations (5) and (5′) are the Sturm-Liouville theorem for the case with both local and non-local symmetric potentials. Notice that the non-local symmetric cutoff potential does not need to be separable for the validity of the Sturm-Liouville theorem.

Secondly, we make a convention for the phase shifts. The phase shift is determined by its tangent function up to an integral multiple of π. In the usual convention, the phase shift is defined by the relative value with respect to the phase shift at infinite energy; it is assumed that $\delta(0)-\delta(\infty)$ is finite and $\delta(E)$ is a continuous function of energy. In some cases there may be trouble with the usual convention. For example, Levinson's theorem for the case with the repulsive hard core for which $\delta(\infty)\sim-\infty$ used to be considered as being violated (Newton 1982). In the case with a positive-energy bound state, both numerator and denominator of $\tan\delta$ vanish and there is no reason to require the phase shift to be continuous at this energy (Kermode 1976).

As a matter of fact, according to Levinson's theorem, the number of bound states is only related to the behaviour of phase shifts near zero energy (or near $E=\pm M$ for the Dirac equation). The above problems come from the convention of phase shifts (Ma 1985c).

Now, we make a new convention to give an absolute definition to the phase shift:

$$\delta(E)=0 \qquad \text{for zero potentials.} \tag{6}$$

The phase shift $\delta(E)$ changes as the potential changes from zero to the given value. We do not require that the phase shift be continuous with respect to the potential. On the contrary, the phase shift $\delta(0)$ at zero energy jumps when a bound state is created or annihilated. The jumps are the essence of Levinson's theorem. However, the logarithmic derivative of the radial function $(u'/u)|_{a-}\equiv A(E)$ changes as the potential changes, and the phase shift is monotonic with respect to $A(E)$ (e.g. see (14)). Therefore, the phase shift $\delta(0)$ at zero energy changes determinately as the potential changes, no matter whether the phase shift at the infinite energy is finite or not, and whether the phase shift jumps or not at the energy where a positive-energy bound state occurs.

3. Levinson's theorem

Under this convention of the phase shift we can prove Levinson's theorem for the case with both local and non-local symmetric potentials in terms of the Sturm-Liouville theorem in a similar way to that for the case with only a local potential (Ma 1985a). We are going to sketch the proof here.

At first, we discuss the solutions with $E<0$. In the region $[a,\infty)$, there is only one solution of (1′) vanishing in infinity:

$$\begin{aligned} u(r) &= [\pi k_1 r/2]^{1/2}\exp[\mathrm{i}(\pi/2)(l+\tfrac{3}{2})]H^{(1)}_{l+1/2}(\mathrm{i}k_1 r) \\ &= [\pi k_1 r/2]^{1/2}K_{l+1/2}(k_1 r)\sim\begin{cases}\dfrac{(2l-1)!!}{(k_1 r)^l} & \text{at } k_1 r\sim 0\\ e^{-k_1 r} & \text{at } k_1 r\sim\infty\end{cases} \\ u(r)&\sim 0 \qquad \text{at } r\sim\infty. \end{aligned} \tag{7}$$

In the region $[0, a]$, there is also only one solution of (1) vanishing at the origin. When $V(r) = U(r, r') = 0$, we have the solution in the region $[0, a]$

$$u(r) = (2\pi k_1 r)^{1/2} \exp\left(-i\frac{\pi}{2}(l+\tfrac{1}{2})\right) J_{l+1/2}(ik_1 r)$$

$$= (2\pi k_1 r)^{1/2} I_{l+1/2}(k_1 r) \sim \begin{cases} \dfrac{2(k_1 r)^{l+1}}{(2l+1)!!} & \text{at } k_1 r \sim 0 \\ e^{k_1 r} & \text{at } k_1 r \sim \infty \end{cases} \tag{8a}$$

$$u(r) \sim 0 \qquad \text{at } r \sim 0$$

where $k_1 = [-E]^{1/2}$ and $K_{l+1/2}(x)$ and $I_{l+1/2}(x)$ are the modified Bessel functions (Bateman 1953). Then we obtain the logarithmic derivatives near $r \sim a$

$$A(E) \equiv \left.\frac{u'}{u}\right|_{a-} = \frac{1}{2a} + \frac{k_1 I'_{l+1/2}(k_1 a)}{I_{l+1/2}(k_1 a)}$$

$$\sim \begin{cases} (l+1)/a & \text{when } E \leqslant 0 \\ k_1 \sim \infty & \text{when } E \sim -\infty \end{cases} \tag{9a}$$

and

$$B(E) \equiv \left.\frac{u'}{u}\right|_{a+} = \frac{1}{2a} + \frac{k_1 K'_{l+1/2}(k_1 a)}{K_{l+1/2}(k_1 a)}$$

$$\sim \begin{cases} -l/a & \text{when } E \leqslant 0 \\ -k_1 \sim -\infty & \text{when } E \sim -\infty. \end{cases} \tag{9b}$$

$A(E)$ decreases monotonically and $B(E)$ increases monotonically as energy E increases from negative infinity to zero. These monotonical properties hold for non-vanishing potentials V and U because of the Sturm-Liouville theorem. When V and U change from zero to the given values, $B(E)$ does not change but $A(E)$ changes. Because of the monotonical property, if there is an overlapping region between the variable areas of $A(E)$ and $B(E)$, there must be a bound state at some negative energy E. From (9a) and (9b) there is no overlapping region, so no bound state for the case with $V = U = 0$. For the finite potentials, $A(\infty)$ does not change and the variable area of $A(E)$ only depends on the boundary value $A(0)$ as the potentials change. Note that as the potential changes $u(a)|_{E=0}$ may change to cross zero and $A(0)$ may cross infinity, which is not a singularity of the solution. There may be several overlapping regions between the variable areas because $A(0)$ may change to cross infinity several times. Owing to the Sturm-Liouville theorem, there is only one energy E in each overlapping region with which the matching condition is satisfied:

$$\left.\frac{u'}{u}\right|_{a-} = \left.\frac{u'}{u}\right|_{a+} \tag{10}$$

namely, there is a bound state. The number n_l of bound states is equal to the number of the overlapping regions between the variable areas of $A(E)$ and $B(E)$. We denote by n_+ the number of times $A(0)$ decreases to cross the value $-l/a$, and by n_- the number of times $A(0)$ increases to cross that value as potentials $V(r)$ and $U(r, r')$ change from zero to the given values. Then we have

$$n_l = n_+ - n_-. \tag{11}$$

Secondly, we discuss the solutions with $E > 0$. There is only one solution vanishing at the origin for the potential $V(r)$ and $U(r, r')$ and the logarithmic derivative $A(E)$

of the solution at $a-$ can be calculated in principle. $A(E)$ changes as the potentials change. In the region $[a, \infty)$ the general solution to (1′) is

$$\begin{aligned} u(r) &= (kr)[\cos\delta(E) j_l(kr) - \sin\delta(E) n_l(kr)] \\ &\overset{r\sim\infty}{\sim} \sin(kr - l\pi/2 + \delta) \\ k &= [E]^{1/2} \end{aligned} \tag{12}$$

where j_l and n_l are the spherical Bessel and Neumann functions. From the matching condition (10) the phase shift $\delta(E)$ can be determined:

$$\begin{aligned} \tan\delta(E) &= \frac{j_l(ka)}{n_l(ka)} \frac{A(E) - kj_l'(ka)/j_l(ka) - 1/a}{A(E) - kn_l'(ka)/n_l(ka) - 1/a} \\ &\overset{k\sim 0}{\sim} -\frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!} \frac{A(0) - (l+1)/a}{A(0) - (-l/a)}. \end{aligned} \tag{13}$$

If $V = U = 0$, the solution in the region $[0, a]$ is $(kr)j_l(kr)$ and the numerator of $\tan\delta(E)$ vanishes, so it is possible to make the convention (6) for the phase shift. For the non-vanishing potentials, the factor $(ka)^{2l+1}$ ensures $\delta(0) = n\pi$. There is an exception for the case with a half-bound state which will be discussed below. Now, $\delta(0)$ will be $2m\pi$ if $\tan\delta(E)$ for a positive energy E small enough falls in the first or fourth quadrant, or $(2m+1)\pi$ if it falls in the second or third quadrant. $\delta(0)$ changes by π only if $\tan\delta(E)$ changes to cross infinity. On the other hand, from (13) we obtain

$$\left.\frac{\partial\delta}{\partial A}\right|_E = -\frac{\cos^2\delta}{ka^2[(A-1/a)n_l(ka) - kn_l'(ka)]^2} \leqslant 0. \tag{14}$$

Therefore, the phase shift $\delta(0)$ at zero energy increases by π each time when $A(0)$ decreases to cross the value $(-l/a)$ and $\delta(0)$ decreases by π each time when $A(0)$ increases to cross that value, i.e.

$$\delta(0) = (n_+ - n_-)\pi = n_l\pi. \tag{15}$$

Finally, we discuss the critical case where $A(0)$ is equal to $(-l/a)$ for the given potentials $V(r)$ and $U(r, r')$. There is a bound state with $E = 0$ for this case with $l > 0$ and the solution in the region $[a, \infty)$ is as follows:

$$\begin{aligned} &u(r) = r^{-l} \\ &(u'/u)|_{a+} = -l/a. \end{aligned} \tag{16}$$

For the S wave it is not a bound state and is usually called a half-bound state. For definiteness, we assume that $A(0)$ decreases to reach the value $(-l/a)$ as the potentials change to reach the given values. We are going to see whether the phase shift $\delta(0)$ increases an additional π to match the zero-energy bound state with $l > 0$; namely, we should show in this case

$$A(E) - \frac{kn_l'(ka)}{n_l(ka)} - \frac{1}{a} \sim -|c|^2k^2 \qquad \text{when } ka \ll 1. \tag{17}$$

From the Sturm-Liouville theorem (5) we have

$$A(E) \sim -l/a - |c_1|^2k^2 \tag{18a}$$

and it is easy to check that

$$-kn_l'(ka)/n_l(ka) \sim (l+1)/a - |c_2|^2k^2 \tag{18b}$$

so we have (17). In fact, equation (18*b*) can also be proved in terms of the Sturm-Liouville theorem similarly to (5′). In the region $[a, \infty)$ the solution with $E = 0$ is given in (16) and the solution with $E_1 \geqslant 0$ is taken as follows:

$$u(r) = ckrn_l(kr) \overset{k\sim 0}{\sim} r^{-l} \qquad l > 0. \tag{19}$$

As E_1 goes to zero we obtain for any $r > a$

$$u^2(a)\frac{\mathrm{d}(u'/u)}{\mathrm{d}E}\bigg|_{a+} - u^2(r)\frac{\mathrm{d}(u'/u)}{\mathrm{d}E}\bigg|_{r} = \int_a^r u^2(r')\,\mathrm{d}r'.$$

For $l > 0$ the second term on the left-hand side vanishes as r goes to infinity, so we obtain (18*b*).

Note that (18*b*) holds only for $l > 0$. For the S wave the numerator of $\tan\delta(E)$ in (13) is proportional to k, and the denominator to k^2, that is, $\tan\delta(E)$ is proportional to k^{-1} and $\delta(0)$ increases an additional $\pi/2$ as $A(0)$ decreases to reach the value zero. This $\pi/2$ should be subtracted in (15) because there is no zero-energy bound state for the critical case in the S wave, so we obtain Levinson's theorem

$$\eta_l = (1/\pi)\delta(0) - \tfrac{1}{2}\sin^2\delta(0) \tag{20}$$

where n_l is the number of non-positive-energy bound states and $\delta(E)$ is the phase shift at energy E in our convention. Levinson's theorem holds without any modification for the case with both local and non-local cutoff symmetric potentials.

4. Positive-energy bound states

In the case with only a local interaction, the wavefunction and its first derivative would never vanish at the same point except for the origin, so there is no positive-energy bound state. However, in the case with a non-local interaction, Martin (1958) showed that while the potentials satisfy some condition, the solution with an asymptotic form is not unique, i.e. there exists the positive-energy bound state with a vanishing asymptotic form. If a small perturbative potential, non-local or local, is added, the positive-energy bound state will disappear and the phase shift at this energy increases rapidly by almost π. It can be seen explicitly in all the examples given by Martin (1958) and Kermode (1976).

It was pointed out by Kermode (1976) that the inverse tangent function is not single-valued and it is physically more satisfying to include a jump by π to the phase shift at the energy E_0 where a positive-energy bound state occurs. Martin (1958) and Chadan (1958) defined the phase shift to be continuous even at E_0 so that an additional π will be included into $\delta(0) - \delta(\infty)$ for each positive-energy bound state. This is their reason to modify Levinson's theorem by a term $\sigma\pi$ where σ denotes the number of positive-energy bound states. But in the viewpoint of Kermode, no modification to Levinson's theorem is needed.

However, the phase shift at zero energy in our convention does not change, no matter which viewpoint is used, i.e. no matter whether the phase shift jumps or not at the energy with a positive-energy bound state. Therefore, Levinson's theorem (20) holds for the cases where positive-energy bound states may occur.

5. Redundant state

The resonating group model of the scattering of nuclei, or other composite systems, derives an effective two-body interaction in which a non-local potential appears. There are some physically redundant states which describe Pauli-forbidden states for the compound system, and the physical two-body states must be orthogonal to these redundant states (Tamagaki 1968). Saito (1968, 1969) and Okai *et al* (1972) proposed a simple non-local term which guarantees the required orthogonality, and verified that it is a good representation of the interaction. If there is just one redundant state represented by the real normalised wavefunction $U(r)$, then Saito's equation (Okai *et al* 1972, Englefield and Shoukry 1974) is ($\hbar = 2m = 1$):

$$\frac{d^2}{dr^2}\Psi + \left(E - V(r) - \frac{l(l+1)}{r^2}\right)\psi = U(r)\int_0^\infty U(s)\left(\frac{d^2}{ds^2} - V(s) - \frac{l(l+1)}{s^2}\right)\psi(s)\,ds \qquad \int_0^\infty U^2(s)\,ds = 1. \tag{21}$$

Multiplying by $U(r)$ and integrating over r, one gets

$$E\int_0^\infty U(r)\psi(r)\,dr = 0. \tag{22}$$

The solution of (10) satisfies the orthogonality constraint except for that of zero energy. Saito's non-local potential is separable, but not symmetric, so the Sturm–Liouville theorem is hard to prove in this case.

Englefield and Shoukry (1974) generalised Chadan's method to prove a modified Levinson theorem for this case:

$$n_l + 1 = (1/\pi)\delta(0) \tag{23}$$

whereas they did not pay attention to the critical case because it was irrelevent to the problem in which they were interested.

In mathematics, there is a zero-energy solution $\psi_0(r)$

$$\frac{d^2}{dr^2}\psi_0(r) - \left(V(r) + \frac{l(l+1)}{r^2}\right)\psi_0(r) = U(r) \qquad \psi_0(r) \sim 0 \quad \text{at } r \sim 0. \tag{24}$$

ψ_0 satisfies (21) with zero energy. The general solution is $\psi_0 + c\phi_0$ where ϕ_0 satisfies (24) with $U(r) = 0$. If $U(r)$ vanishes fast enough in infinity, one can always choose the appropriate parameter c so that the solution $\psi_0 + c\phi_0$ vanishes in infinity, that is, there is always a zero-energy bound state for (21). This is a so-called physically redundant state. The additional one on the left-hand side of (23) describes the redundant state. As far as a mathematical equation (21) is concerned, the redundant state is one of the bound states. The number of all the non-positive-energy bound states for Saito's equation in the mathematical meaning still satisfies Levinson's theorem.

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Appendix. The asymptotic behaviours of the solutions at the origin

There are two independent solutions ϕ_1 and ϕ_2 to the homogeneous equation with $E>0$:

$$\phi''(r)+\left(E-V(r)-\frac{l(l+1)}{r^2}\right)\phi(r)=0. \tag{A1}$$

ϕ_1 and ϕ_2 satisfy the following asymptotic behaviours:

$$\begin{aligned}\phi_1(r)&\sim\begin{cases}c_1 r^{l+1} & \text{at } r\sim 0\\ [k]^{-1/2}\sin(kr-\frac{1}{2}l\pi+\delta_v) & \text{at } r\sim\infty\end{cases}\\ \phi_2(r)&\sim\begin{cases}c_2 r^{-l} & \text{at } r\sim 0\\ [k]^{-1/2}\cos(kr-\frac{1}{2}l\pi+\delta_v) & \text{at } r\sim\infty.\end{cases}\end{aligned} \tag{A2}$$

The Wronskian of (A1) gives

$$(\phi_1'\phi_2-\phi_2'\phi_1)=\text{constant}=1. \tag{A3}$$

When $E<0$, there are also two independent solutions ϕ_1 and ϕ_2 to (A1) in the region $[0, a]$ with the asymptotic behaviours at the origin

$$\phi_1(r)\sim c_1 r^{l+1}\qquad \phi_2(r)\sim c_2 r^{-l}\qquad \text{at } r\sim 0. \tag{A4}$$

$\phi_1(r)$ and $\phi_2(r)$ also satisfy (A3). Now, the Green function of (1) is as follows:

$$G(r, r')=\phi_1(r_1)\phi_2(r_2) \tag{A5}$$

where $r_1=\min(r, r')$, $r_2=\max(r, r')$, and

$$G''+\left(E-V-\frac{l(l+1)}{r^2}\right)G=-\delta(r-r'). \tag{A6}$$

We make an ansatz

$$\left|\int_0^a U(r, r')u(r')\,dr'\right|<\infty \tag{A7}$$

so the physically admissible solution to (1) in the region $[0, a]$ can be expressed as

$$\begin{aligned}u(r)&=c\phi_1(r)-\int\int G(r, r')U(r', r'')u(r'')\,dr'\,dr''\\ &=c\phi_1(r)-\phi_1(r)\int_0^a dr''\,u(r'')\int_r^a dr'\,\phi_2(r')U(r', r'')\\ &\quad-\phi_2(r)\int_0^a dr''\,u(r'')\int_0^r dr'\,\phi_1(r')U(r', r'').\end{aligned}$$

Near the origin, $\phi_1(r) \sim r^{l+1}$, $\phi_2(r) \sim r^{-l}$

$$\phi_1(r) \int_0^a \mathrm{d}r'' \, u(r'') \int_r^a \mathrm{d}r' \, \phi_2(r') U(r', r'') \sim r^{l+1-l+\beta+1} = r^{\beta+2}$$

$$\phi_2(r) \int_0^a \mathrm{d}r'' \, u(r'') \int_0^r \mathrm{d}r' \, \phi_1(r') U(r', r'') \sim r^{-l+l+\beta+2} = r^{\beta+2}.$$

Because of (3), (4) and (A7) are satisfied.

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