Nonrelativistic Levinson's theorem in *D* dimensions

Shi-Hai Dong*
Institute of High Energy Physics, Beijing 100039, People's Republic of China
and Instituto de Ciencias Nucleares, UNAM, Apartado Postal 70-543, Circuito Exterior, C. U., 04510 México, Distrito Federal, Mexico

Zhong-Qi Ma†
China Center for Advanced Science and Technology (World Laboratory), P. O. Box 8730, Beijing 100080, People's Republic of China
and Institute of High Energy Physics, Beijing 100039, People's Republic of China

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The Levinson theorem for the Schrödinger equation with a spherically symmetric potential in *D* dimensions is uniformly established by the Sturm-Liouville theorem. It is shown that the Levinson theorem for the cases without a half bound state does not depend on the spatial dimension *D*, namely, the phase-shift $\delta_l(0)$ of the scattering state with angular momentum *l* at zero momentum is equal to the total number n_l of bound states multiplied by π. When a half bound state occurs the Levinson theorem may be modified.

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I. INTRODUCTION

The Levinson theorem [1] as an important theorem in quantum scattering theory establishes the relation between the total number n_l of bound states with angular momentum *l* and the phase shift $\delta_l(0)$ of the scattering state at zero momentum for the Schrödinger equation with a spherically symmetric potential $V(r)$ with the boundary conditions [1,2]

$$\int_0^1 r|V(r)|dr<\infty,$$

$$\int_1^\infty r^2|V(r)|dr<\infty. \tag{1}$$

The first condition is necessary for the nice behavior of the wave functions at the origin and the second one is required by the analytic property of the Jost function. Newton (see pages 438–439 in [2]) pointed out two examples where the Levinson theorem is violated when the second condition is not satisfied.

Since 1949, the Levinson theorem has been proved by different methods and generalized to the different equations and potentials [2–22]. With the interest of higher-dimensional field theory recently, we have a try to carry out the Levinson theorem for the Schrödinger equation in *D* dimensions by the Sturm-Liouville theorem (SLT), which is the main purpose of this paper.

This paper is organized as follows. We discuss scattering states and bound states for the *D*-dimensional Schrödinger equation in Sec. II and III, respectively. SLT is studied in Sec. IV. The nonrelativistic Levinson theorem in *D* dimensions is established in Sec. V. The general case is discussed in Sec. VI.

*Electronic address: dongsh2@yahoo.com
†Electronic address: mazq@sun.ihep.ac.cn

II. SCATTERING STATES AND PHASE SHIFTS

Let us consider the *D*-dimensional Schrödinger equation

$$\left(-\frac{\hbar^2}{2\mu}\nabla_D^2+V(r)\right)\Psi(\mathbf{r})=E\Psi(\mathbf{r}), \tag{2}$$

which is invariant in spatial rotation. Following [23], separating the angular variables from the wave functions

$$\Psi(\mathbf{r})=r^{-(D-1)/2}R_l(r)Y_{l_{D-1}\cdots l_1}(\theta_1\cdots\theta_{D-1}), \tag{3}$$

one obtains the radial Schrödinger equation as

$$\left[\frac{d^2}{dr^2}-\frac{l(l+D-2)+(D-1)(D-3)/4}{r^2}\right]R_l(r)$$
$$=\frac{2\mu}{\hbar^2}[E-V(r)]R_l(r), \tag{4}$$

which is a real equation.

For simplicity, we first study Eq. (4) with a cutoff potential

$$V(r)=0, \quad \text{when} \quad r\geqslant r_0, \tag{5}$$

where r_0 is a sufficiently large radius. The general case will be studied in Sec. VI. Similar to our previous works [20], we introduce a parameter λ for $V(r)$

$$V(r,\lambda)=\lambda V(r), \quad V(r,1)=V(r). \tag{6}$$

Accordingly, Eq. (4) can be modified as

$$\left[\frac{\partial^2}{\partial r^2}-\frac{(l-1+D/2)^2-1/4}{r^2}\right]R_l(r,\lambda)$$
$$=\frac{2\mu}{\hbar^2}[E-V(r,\lambda)]R_l(r,\lambda). \tag{7}$$

We now solve Eq. (7) in two regions and match the logarithmic derivatives of the radial functions at r_0

$$A_l(E,\lambda)\equiv\left[\frac{1}{R_l(r,\lambda)}\frac{\partial R_l(r,\lambda)}{\partial r}\right]_{r=r_0-}=\left[\frac{1}{R_l(r,\lambda)}\frac{\partial R_l(r,\lambda)}{\partial r}\right]_{r=r_0+}. \tag{8}$$

From Eq. (1) there is one convergent solution to Eq. (7) in the region $[0,r_0]$. When $V(r,0)=0$ this solution is

$$R_l(r,0)=(\pi kr/2)^{1/2}J_{l-1+D/2}(kr), \tag{9}$$

for $E>0$ and $k=(2\mu E)^{1/2}/\hbar$, and

$$R_l(r,0)=e^{-i(2l-2+D)\pi/4}(\pi\kappa r/2)^{1/2}J_{l-1+D/2}(i\kappa r), \tag{10}$$

for $E\leqslant 0$ and $\kappa=(-2\mu E)^{1/2}/\hbar$. $J_\nu(x)$ is the Bessel function and $R_l(r,0)$ in Eqs. (9) and (10) are real. A multiplied factor on $R_l(r,0)$ is not important.

In the region (r_0,∞), we have $V(r,\lambda)=0$. For $E>0$, the combination of two oscillatory solutions to Eq. (7) can always satisfy the matching condition (8) so that there is a continuous spectrum

$$R_l(r,\lambda)=(\pi kr/2)^{1/2}[\cos\delta_l(k,\lambda)J_{l-1+D/2}(kr)-\sin\delta_l(k,\lambda)N_{l-1+D/2}(kr)]\sim\cos\left[kr-\frac{(2l+D-3)\pi}{4}+\delta_l(k,\lambda)\right]\quad\text{when}\quad r\to\infty, \tag{11}$$

where $N_\nu(kr)$ is the Neumann function. Although $V(r,\lambda)$ does not depend on λ in the region (r_0,∞), through Eq. (8), $R_l(r,\lambda)$ and $\delta_l(k,\lambda)$ depend on λ. In fact, we can obtain from Eq. (8)

$$\tan\delta_l(k,\lambda)=\frac{J_{l-1+D/2}(kr_0)}{N_{l-1+D/2}(kr_0)}\times\frac{A_l(E,\lambda)-kJ'_{l-1+D/2}(kr_0)/J_{l-1+D/2}(kr_0)-1/(2r_0)}{A_l(E,\lambda)-kN'_{l-1+D/2}(kr_0)/N_{l-1+D/2}(kr_0)-1/(2r_0)}, \tag{12}$$

$$\delta_l(k)\equiv\delta_l(k,1), \tag{13}$$

where the prime denotes the derivative of the Bessel function, the Neumann function, and later the Hankel function with respect to their arguments. It is found from Eq. (12) that $\delta_l(k,\lambda)$ is determined up to a multiple of π due to the period of the tangent function. For convenience, we may use the convention for the phase shifts

$$\delta_l(k)=0,\quad\text{when}\quad V(r)=0, \tag{14}$$

which implies that $\delta_l(\infty)=0$ [24].

III. BOUND STATES

There is only one convergent solution to Eq. (7) in the region (r_0,∞) for $E\leqslant 0$

$$R_l(r,\lambda)=e^{i(l+D/2)\pi/2}(\pi\kappa r/2)^{1/2}H^{(1)}_{l-1+D/2}(i\kappa r)\sim e^{-\kappa r}\quad\text{when}\quad r\to\infty, \tag{15}$$

where $H^{(1)}_\nu(x)$ is the Hankel function of the first kind. In fact, $R_l(r,\lambda)$ in Eq. (15) does not depend on λ. The matching condition (8) may be satisfied only for some discrete E, where the bound states appear. Therefore, there exists a discrete spectrum for $E\leqslant 0$.

It is worth paying some attention to the solutions with $E=0$. If $A_l(0,1)$ (zero momentum and $\lambda=1$) is equal to $(3-2l-D)/(2r_0)$, it matches a solution

$$R_l(r,1)=r^{(3-2l-D)/2},\quad r\in(r_0,\infty), \tag{16}$$

from which we know the solution describes a bound state for $l>2-D/2$ and a half bound state for $l\leqslant 2-D/2$.

IV. STURM-LIOUVILLE THEOREM

Since Eq. (7) is a Sturm-type equation, there exists SLT, which shows that the logarithmic derivative of wave functions is monotonic with respect to E [25] and provides a powerful tool for proving the Levinson theorem. Denote by $\overline{R}_l(r,\lambda)$ the solution to Eq. (7) for the energy $\overline{E}$

$$\left[\frac{\partial^2}{\partial r^2}-\frac{(l-1+D/2)^2-1/4}{r^2}\right]\overline{R}_l(r,\lambda)=\frac{2\mu}{\hbar^2}[\overline{E}-V(r,\lambda)]\overline{R}_l(r,\lambda). \tag{17}$$

Multiplying Eq. (7) and Eq. (17) by $\overline{R}_l(r,\lambda)$ and $R_l(r,\lambda)$, respectively, and calculating their difference, we have

$$\frac{\partial}{\partial r}\left\{R_l(r,\lambda)\frac{\partial \overline{R_l}(r,\lambda)}{\partial r}-\overline{R_l}(r,\lambda)\frac{\partial R_l(r,\lambda)}{\partial r}\right\}$$

$$=-\frac{2\mu}{\hbar^2}(\overline{E}-E)\overline{R_l}(r,\lambda)R_l(r,\lambda). \tag{18}$$

From the boundary condition, both solutions $R_l(r,\lambda)$ and $\overline{R_l}(r,\lambda)$ vanish at the origin. Integrating Eq. (18) from 0 to r_0, we obtain

$$\frac{1}{\overline{E}-E}\left[R_l(r,\lambda)\frac{\partial \overline{R_l}(r,\lambda)}{\partial r}-\overline{R_l}(r,\lambda)\frac{\partial R_l(r,\lambda)}{\partial r}\right]_{r=r_0-}$$

$$=-\frac{2\mu}{\hbar^2}\int_0^{r_0}\overline{R_l}(r,\lambda)R_l(r,\lambda)dr.$$

Taking the limit as $\overline{E}$ to E, we have

$$\frac{\partial A_l(E,\lambda)}{\partial E}=\frac{\partial}{\partial E}\left[\frac{1}{R_l(r,\lambda)}\frac{\partial R_l(r,\lambda)}{\partial r}\right]_{r=r_0-}$$

$$=-\frac{2\mu}{\hbar^2 R_l(r_0,\lambda)^2}\int_0^{r_0}R_l(r,\lambda)^2dr<0. \tag{19}$$

When $E=\hbar^2k^2/(2\mu)$ is larger than zero and tends to zero, we have

$$A_l(E,\lambda)=A_l(0,\lambda)-c^2k^2+\cdots,\quad c^2\geqslant 0. \tag{20}$$

Similarly, from the boundary condition that $R_l(r,\lambda)$ tends to zero at infinity for $E\leqslant 0$, we have

$$\frac{\partial}{\partial E}\left[\frac{1}{R_l(r,\lambda)}\frac{\partial R_l(r,\lambda)}{\partial r}\right]_{r=r_0+}$$

$$=\frac{2\mu}{\hbar^2 R_l(r_0,\lambda)^2}\int_{r_0}^{\infty}R_l(r,\lambda)^2dr$$

$$>0. \tag{21}$$

This is another form of SLT [25]. As E increases, the logarithmic derivative of the radial function at r_0- decreases monotonically, but that at r_0+ for $E\leqslant 0$ increases monotonically. For $E\leqslant 0$, because both sides of Eq. (8) are monotonic as E changes, the variation of $A_l(0,\lambda)$ as λ changes determines the number of bound states.

V. LEVINSON THEOREM

In this section we will show from SLT that both $\delta_l(0,\lambda)$ and n_l are related with the variation of $A_l(0,\lambda)$. We first study the relation between n_l and $A_l(0,\lambda)$ when the potential changes. For $E\leqslant 0$, from SLT the logarithmic derivative of the radial function at r_0 is monotonic with respect to E. From Eq. (15) we obtain the logarithmic derivative

$$\left(\frac{1}{R_l(r,\lambda)}\frac{\partial R_l(r,\lambda)}{\partial r}\right)_{r=r_0+}$$

$$=\frac{i\kappa H^{(1)}_{l-1+D/2}(i\kappa r_0)'}{H^{(1)}_{l-1+D/2}(i\kappa r_0)}-\frac{1}{2r_0}$$

$$=\begin{cases}\dfrac{3-2l-D}{2r_0} & \text{when}\quad E\sim 0\\ -\infty & \text{when}\quad E\to-\infty,\end{cases} \tag{22}$$

which does not depend on λ. On the other hand, when $\lambda=0$ we obtain from Eq. (10)

$$A_l(E,0)=\left(\frac{1}{R_l(r,0)}\frac{\partial R_l(r,0)}{\partial r}\right)_{r=r_0-}$$

$$=\frac{i\kappa J'_{l-1+D/2}(i\kappa r_0)}{J_{l-1+D/2}(i\kappa r_0)}-\frac{1}{2r_0}$$

$$=\begin{cases}\dfrac{2l-1+D}{2r_0} & \text{when}\quad E\sim 0\\ \infty & \text{when}\quad E\to-\infty.\end{cases} \tag{23}$$

It is evident from Eqs. (22) and (23) that when $\lambda=0$ and as E increases from $-\infty$ to 0, there is no overlap between two variant ranges of two logarithmic derivatives such that there is no bound state except for the case of $l=0$ and $D=2$ where a half bound state occurs at $E=0$.

Second, we study the relation between $\delta_l(0,\lambda)$ and $A_l(0,\lambda)$ when the potential changes. The $\delta_l(0,\lambda)$ is the limit of $\delta_l(k,\lambda)$ as k tends to zero. Therefore, we are interested in $\delta_l(k,\lambda)$ at a sufficiently small momentum k, $k\ll 1/r_0$. In this case we obtain from Eq. (12)

$$\tan\delta_l(k,\lambda)=\frac{-\pi(kr_0)^{2l-2+D}}{2^{2l-2+D}\Gamma(l+D/2)\Gamma(l-1+D/2)}\frac{A_l(l,\lambda)-(2l-1+D)/(2r_0)}{A_l(0,\lambda)-c^2k^2-\dfrac{3-2l-D}{2r_0}\left[1-\dfrac{2(kr_0)^2}{(2l+D-3)(2l+D-4)}\right]}, \tag{24a}$$

when $l>2-D/2$,

$$\tan\delta_l(k,\lambda)=\frac{-\pi(kr_0)^2}{4}\times\frac{A_l(0,\lambda)-3/(2r_0)}{A_l(0,\lambda)-c^2k^2+\frac{1}{2r_0}[1+2(kr_0)^2\ln(kr_0)]},\tag{24b}$$

when $l=2-D/2$ ($D=4$ and $l=0$ or $D=2$ and $l=1$),

$$\tan\delta_l(k,\lambda)=-(kr_0)\frac{A_l(0,\lambda)-1/r_0}{A_l(0,\lambda)-c^2k^2+k^2r_0},\tag{24c}$$

when $l=(3-D)/2$ ($D=3$ and $l=0$), and

$$\tan\delta_l(k,\lambda)=\frac{\pi}{2\ln(kr_0)}\times\frac{A_l(0,\lambda)-c^2k^2-\frac{1}{2r_0}[1-(kr_0)^2]}{A_l(0,\lambda)-c^2k^2-\frac{1}{2r_0}\left[1+\frac{2}{\ln(kr_0)}\right]},\tag{24d}$$

when $l=1-D/2$ ($D=2$ and $l=0$). Likewise, we can also obtain from Eq. (12) that $\delta_l(k,\lambda)$ increases monotonically as $A_l(E,\lambda)$ decreases

$$\left.\frac{\partial\delta_l(k,\lambda)}{\partial A_l(E,\lambda)}\right|_k=\frac{-8r_0\cos^2\delta_l(k,\lambda)}{\pi\{[2r_0A_l(E,\lambda)-1]N_{l-1+D/2}(kr_0)-2kr_0N'_{l-1+D/2}(kr_0)\}^2}\leqslant 0,\tag{25}$$

where $k=(2\mu E)^{1/2}/\hbar$.

Since Eq. (7) is analogous to that of two-dimensional (2D) case [20], the analysis is very similar to that of [20]. The reader is strongly suggested to refer to our previous works [20]. Repeating the proof carried out in [20], we can obtain the nonrelativistic Levinson theorem in D dimensions for noncritical cases

$$\delta_l(0)=n_l\pi.\tag{26a}$$

Similarly, for the critical case $l=2-D/2$ and $l=(3-D)/2$, it should be modified as

$$\delta_l(0)=\begin{cases}(n_m+1)\pi, & \text{when } l=1,\quad D=2,\quad\text{or } l=0,\quad D=4\\ (n_m+1/2)\pi, & \text{when } l=0,\quad D=3,\end{cases}\tag{26b}$$

when a half bound state occurs. The Levinson theorem given in Eq. (26) coincides with the previous results in 2D and 3D.

VI. DISCUSSION

We now discuss the general case where the potential $V(r)$ has a tail at $r>r_0$. Let r_0 be so large that only the leading term in $V(r)$ is concerned in the region (r_0,∞)

$$V(r)\sim\frac{\hbar^2}{2\mu}br^{-n},\quad\text{when}\quad r\to\infty,\tag{27}$$

where b is a nonvanishing constant and n is a positive constant, not necessarily to be an integer. From Eq. (1), n should be larger than 3. However, we are also interested in the modification of the Levinson theorem for $n=2$, in which Newton [2] found two examples where the Levinson theorem is violated.

When $n=2$, we define

$$\nu^2=(l-1+D/2)^2+b.\tag{28}$$

Equation (7) thus becomes

$$\frac{\partial^2R_l(r,\lambda)}{\partial r^2}+\left[\frac{2\mu E}{\hbar^2}-\frac{\nu^2-1/4}{r^2}\right]R_l(r,\lambda)=0,\quad r\geqslant r_0.\tag{29}$$

If $\nu^2<0$, there are infinite number of bound states. We will not discuss this case as well as the case with $\nu=0$ here. When $\nu^2>0$, we take $\nu>0$. Some formulas given in the previous sections can be obtained through replacing $(l-1+D/2)$ by ν. Equation (22) becomes

$$\left(\frac{1}{R_l(r,\lambda)}\frac{\partial R_l(r,\lambda)}{\partial r}\right)_{r=r_0+}=\frac{i\kappa H_\nu^{(1)}(i\kappa r_0)'}{H_\nu^{(1)}(i\kappa r_0)}-\frac{1}{2r_0}=\begin{cases}\frac{1-2\nu}{2r_0} & \text{when}\quad E\sim 0\\ -\infty & \text{when}\quad E\to-\infty.\end{cases}\tag{30}$$

The scattering solutions (11) in the region (r_0,∞) become

$$R_l(r,\lambda)=\sqrt{\frac{\pi kr}{2}}\{\cos\eta_l(k,\lambda)J_\nu(kr)-\sin\eta_l(k,\lambda)N_\nu(kr)\}$$
$$\sim\sin\left(kr-\frac{\nu\pi}{2}+\frac{\pi}{4}+\eta_l(k,\lambda)\right),\quad \text{when}\quad r\to\infty. \tag{31}$$

The $\delta_l(k)$ can be thus calculated from $\eta_l(k,1)$

$$\delta_l(k)=\eta_l(k,1)+(2l-2+D-2\nu)\pi/4. \tag{32}$$

$\eta_l(k,\lambda)$ satisfies

$$\tan\eta_l(k,\lambda)=\frac{J_\nu(kr_0)}{N_\nu(kr_0)}\times\frac{A_l(E,\lambda)-kJ'_\nu(kr_0)/J_\nu(kr_0)-1/(2r_0)}{A_l(E,\lambda)-kN'_\nu(kr_0)/N_\nu(kr_0)-1/(2r_0)}, \tag{33}$$

and it increases monotonically as $A_l(E,\lambda)$ decreases

$$\left.\frac{\partial\eta_l(k,\lambda)}{\partial A_l(E,\lambda)}\right|_k=\frac{-8r_0\cos^2\eta_l(k,\lambda)}{\pi\{[2r_0A_l(E,\lambda)-1]N_\nu(kr_0)-2kr_0N'_\nu(kr_0)\}^2}\leqslant 0. \tag{34}$$

For a sufficiently small k, the asymptotic formulas of $\tan\eta_l(k,\lambda)$ can be obtained from Eq. (24) through replacing l by $\nu+1-D/2$, except for the cases of $0<\nu<1/2$ and $1/2<\nu<1$. For the latter cases we have

$$\tan\eta_l(k,\lambda)=\frac{-\pi(kr_0)^{2\nu}}{2^{2\nu}\nu\Gamma(\nu)^2}\times\frac{A_l(0,\lambda)-(\nu+1/2)/r_0}{A_l(0,\lambda)-c^2k^2-\dfrac{1-2\nu}{2r_0}+\dfrac{2\pi\cot(\nu\pi)}{r_0\Gamma(\nu)^2}\left(\dfrac{kr_0}{2}\right)^{2\nu}}. \tag{35}$$

Repeating the proof of the Levinson theorem (26), we obtain the modified Levinson theorem for the noncritical cases

$$\delta_l(0)=(4n_l+2l-2+D-2\nu)\pi/4. \tag{36a}$$

For the critical case where $A_l(0,1)=(-\nu+1/2)/r_0$, the modified Levinson theorem (26a) holds for $\nu>1$, but it should be revised for $0<\nu\leqslant 1$ as

$$\delta_l(0)=(4n_l+2l-2+D+2\nu)\pi/4. \tag{36b}$$

When $n>2$, for any arbitrarily given small ϵ, one can always find a sufficiently large r_0 such that $|V(r)|<\epsilon/r^2$ in the region (r_0,∞). Since $\nu^2=(l-1+D/2)^2+\epsilon\sim(l-1+D/2)^2$, the Levinson theorem (26) holds for this case. It is easy to check, similar to that done in [20], that two examples in $D=3$ pointed out by Newton (see pages 438–439 in [2]), where the Levinson theorem (26) is violated, satisfy the modified Levinson theorem (36).

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