UWThPh-1985-6

INEQUALITIES FOR SCATTERING PHASE SHIFTS

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Abstract

A recently developed method, which was used to derive bounds on energy levels, is applied to continuous spectra and gives relations between scattering phase shifts of various angular momenta.

IN MEMORIAM PROF. VLADIMIR JURKO GLASER

I. Introduction

Motivated by quarkonium physics two of us started years ago a general study of nonrelativistic bound state problems. Early results were concerned with relations between low lying levels. Recently we succeeded in deriving more general results [1,2]. We have shown that the sign of the Laplacian of the potential determines the relative position of bound states with quantum numbers (ℓ,n) and $(\ell+1,n-1)$, where ℓ denotes the angular momentum and n the number of nodes of the wave function. A two step procedure was used to derive this result. In a first algebraic step we obtained a subsidiary potential such that the new $(\ell+1,n-1)$-th level was degenerate to the old (ℓ,n)-th level. In a second step using convexity properties and comparison theorems we were able to conclude that the old $(\ell+1,n-1)$-th level had to ly above or below the (ℓ,n)-th one depending on the sign of the Laplacian of the potential.

It is natural to ask for implications of that procedure to continuous spectra. Although there are some subtleties involved with dealing with non-normalizable solutions of the Schrödinger equation, we are able to derive relations between phase shifts of different angular momenta by following the above sketched procedure. Again the Laplacian of the potential determines the relationship between phase shifts of different angular momenta.

There are only a few general bounds on phase shifts and scattering length known [3,4,5], in chapter II we shall compare our results to an old result of Regge; there are a few more methods available to estimate energy levels and number of bound states [6]. It was in the context of such kind of questions that two of us had the chance to collaborate with Jurko Glaser [7,8]. But in addition we enjoyed his general interest in theoretical physics and learned a lot from his advices.

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II. General Considerations

We start from the Schrödinger operator with spherically symmetric potential

$$H_\ell = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r) \qquad (2.1)$$

and factorize H in the following way

$$H_\ell = A_\ell^- A_\ell^+ + E_\ell \,, \qquad A_\ell^\pm = \pm\frac{d}{dr} + g_\ell \,, \qquad g_\ell = -\frac{u_\ell'}{u_\ell} \qquad (2.2)$$

where u_ℓ denotes the solution of the Schrödinger equation $H_\ell u_\ell = E_\ell u_\ell$ for a suitable chosen energy E_ℓ, which fulfils the boundary condition $u_\ell(0) = 0$ and which is nonvanishing for $r \neq 0$. This last restriction amounts to choose

$$E_\ell \leq \inf \operatorname{spec} H_\ell \qquad (2.3)$$

and guarantees that g_ℓ in eq. (2.2) is non-singular.

We assume now that the potential is the sum of a Coulomb potential (which might be vanishing) and a short range potential

$$V(r) = -\frac{Z}{r} + V_{SR}(r) \qquad (2.4)$$

such that

$$\lim_{r\to 0} r^2 V_{SR}(r) > -\frac{1}{4} \,, \qquad \int_{r_0}^{\infty} dr \,|V_{SR}(r)| < \infty \,, \qquad V_{SR}(\infty) = 0 \,. \qquad (2.5)$$

The scattering wave function defined by

$$H_\ell \,\psi_{\ell,k} = k^2 \,\psi_{\ell,k} \,, \qquad \psi_{\ell,k}(0) = 0 \,, \qquad \psi_{\ell,k}(\varepsilon) > 0 \qquad (2.6)$$

has the asymptotic behaviour

$$\psi_{\ell,k}(r) \underset{r\to\infty}{\sim} \sin(kr - n \ln 2kr - \frac{\pi\ell}{2} + \eta_\ell + \delta_\ell) \,, \quad n = \frac{Z}{2k} \,, \qquad (2.7)$$

where η_ℓ denotes the Coulomb phase shift [9], which fulfils

$$\eta_\ell - \eta_{\ell+1} = \operatorname{arctg} \frac{Z}{2k(\ell+1)} \tag{2.8}$$

and δ_ℓ denotes the phase shift relative to the Coulomb one. As is usual [9] we define $\lim_{E\to\infty} \delta_\ell = 0$; this makes $\delta_\ell(E)$ unique for fixed ℓ by continuity in E.

We follow now the mentioned first step and observe the algebraic relations

$$[A_\ell^-, A_\ell^+] = -2g_\ell' , \qquad [H_\ell, A_\ell^+] = -2g_\ell' A_\ell^+ \tag{2.9}$$

from which we deduce that A_ℓ^+ acts as a ladder operator mapping from wave functions with angular momentum ℓ to $\ell+1$: Define

$$\tilde{\psi}_{\ell+1,k} = -\frac{1}{k} A_\ell^+ \psi_{\ell,k} \tag{2.10}$$

we find that it is a scattering wave function for the operator

$$\tilde{H}_{\ell+1} = A_\ell^+ A_\ell^- = H_{\ell+1} + 2(g_\ell' - \frac{\ell+1}{r^2}) \tag{2.11}$$

with asymptotic behaviour

$$\tilde{\psi}_{\ell+1,k} \underset{r\to\infty}{\sim} \frac{1}{\cos \alpha_\ell} \sin(kr - n \ln 2kr - \frac{\pi(\ell+1)}{2} + \eta_\ell + \delta_\ell - \alpha_\ell) \tag{2.12}$$

where we introduced

$$\alpha_\ell = \operatorname{arctg} \frac{g_\ell(\infty)}{k} \ . \tag{2.13}$$

Observe that $g_\ell(\infty)$ behaves discontinuously as a function of the energy and is given by

$$g_\ell(\infty) = \begin{cases} \sqrt{|E_\ell|} & \text{if } E_\ell = \inf \operatorname{spec} H_\ell \\ -\sqrt{|E_\ell|} & \text{if } E_\ell < \inf \operatorname{spec} H_\ell \end{cases} \tag{2.14}$$

depending on whether E_ℓ belongs to a bound state wave function or not.

The phase shift for the new potential relative to the Coulomb one is given by

$$\tilde{\delta}_{\ell+1} = \delta_\ell + \eta_\ell - \eta_{\ell+1} - \alpha_\ell \,, \tag{2.15}$$

from which we deduce that

$$\tilde{\delta}_{\ell+1} \gtrless \delta_\ell \qquad \text{if} \quad g_\ell(\infty) \gtrless \frac{Z_\ell}{2(\ell+1)} \,. \tag{2.16}$$

Furthermore since an operator inequality between $\tilde{H}_{\ell+1}$ and $H_{\ell+1}$ implies an inequality between the phase shifts $\tilde{\delta}_{\ell+1}$ and $\delta_{\ell+1}$ we conclude that

$$\tilde{\delta}_{\ell+1} \lessgtr \delta_{\ell+1} \qquad \text{if} \quad g'_\ell(r) \gtrless \frac{\ell+1}{r^2} \tag{2.17}$$

provided we keep count of the nodes of $\tilde{\psi}_{\ell+1,k}$ and using monotonicity (2.28). Node counting is necessary in order to identify $\tilde{\delta}_{\ell+1}$ as the proper phase shift:

<u>LEMMA</u>: Nodes of $\psi_{\ell,k}$ and $\tilde{\psi}_{\ell+1,k}$ are interlaced; the first node after $r = 0$ belongs to $\psi_{\ell,k}$.

<u>PROOF</u>: From the definition (2.10) we get

$$(u_\ell \tilde{\psi}_{\ell+1,k})' = \frac{1}{k}(u'_\ell \psi_{\ell,k} - u_\ell \psi'_{\ell,k})' = \frac{k^2-E_\ell}{k} u_\ell \psi_{\ell,k} \,. \tag{2.18}$$

Integrating (2.18) between two zeros of $\tilde{\psi}$ shows that $\psi_{\ell,k}$ has to vanish in between. On the other hand

$$(\psi_{\ell,k}/u_\ell)' = -k(\tilde{\psi}_{\ell+1,k}/u_\ell) \tag{2.19}$$

implies, that there is a node of $\tilde{\psi}_{\ell+1,k}$ between two nodes of $\psi_{\ell,k}$, but not before the first node of ψ, since $(\psi/u)(r=0) \neq 0$.

Therefore we may summarize: If we find u_ℓ such that

$$g'_\ell(r) \gtrless \frac{\ell+1}{r^2} \quad \forall\, r \neq 0 \qquad \underline{\text{and}} \qquad g_\ell(\infty) \lessgtr \frac{Z}{2(\ell+1)} \tag{2.20}$$

the phase shifts to energy E are ordered according to $\delta_{\ell+1}(E) \gtrless \delta_\ell(E)$.

Here it is interesting to quote an old result of Regge [3]. By going over to complex angular momenta he derived the result that quite general

$$\frac{d\delta_\ell}{d\ell} < \frac{\pi}{2} \qquad \text{and} \qquad \delta_{\ell+1} - \delta_\ell < \frac{\pi}{2} . \tag{2.21}$$

There is an elementary proof, which shows that (2.21) follows from the positivity of the centrifugal term. One starts from the Schrödinger equation for angular momentum ℓ

$$\psi''_{\ell,k} = \frac{\ell(\ell+1)}{r^2}\,\psi_{\ell,k} + (V - k^2)\psi_{\ell,k} . \tag{2.22}$$

Integrating the derivative of the Wronskian for two different ℓ's, we [illegible]

$$(\psi_{L,k}\,\psi'_{\ell,k} - \psi_{\ell,k}\,\psi'_{L,k})(R) = \int_0^R dr\,\frac{\psi_{\ell,k}\psi_{L,k}}{r^2}\,[\ell(\ell+1) - L(L+1)] , \tag{2.23}$$

$$k\sin(\delta_L - \delta_\ell - \frac{(L-\ell)\pi}{2}) = -\int_0^\infty dr\frac{\psi_{\ell,k}\psi_{L,k}}{r^2}\,[L(L+1) - \ell(\ell+1)] \tag{2.24}$$

using the well-known asymptotic behaviour of $\psi_{\ell,k}$. In the limit $L \to \ell$:

$$k(\frac{d\delta_\ell}{d\ell} - \frac{\pi}{2}) = -(2\ell+1)\int_0^\infty \frac{dr}{r^2}\,\psi^2_{\ell,k} . \tag{2.25}$$

From the above remark it is obvious how one can generalize Regge's result to include a Coulomb term. We obtain instead of (2.25) using the asymptotic behaviour (2.7)

$$k(\frac{d\delta_\ell}{d\ell} + \frac{d\eta_\ell}{d\ell} - \frac{\pi}{2}) = -(2\ell+1)\int_0^\infty \frac{dr}{r^2}\,\psi^2_{\ell,k}(r) \tag{2.26}$$

and finally

$$\delta_{\ell+1} - \delta_\ell < \frac{\pi}{2} + \operatorname{arctg}\frac{Z}{2k(\ell+1)} . \tag{2.27}$$

In the same manner we generalize the monotonicity of δ_ℓ in V for long range potentials: Let $V^{(\alpha)} = V + \alpha W$, $W \geq 0$. Then

$$k\,\frac{d\delta_\ell^{(\alpha)}}{d\alpha} = -\int_0^\infty dr\,W(r)\,\psi^2_{\ell,k}(r) \leq 0 . \tag{2.28}$$

Note that Regge's inequality is the analogue of $E_{n,\ell} < E_{n,\ell+1}$.

III. Derivation of Bounds

A) The Case $\Delta V > 0$

This means that $Z(r) = r^2V'(r)$ is monotonously increasing. Observe that, if $Z = \lim_{r\to\infty} Z(r)$ is positive there are infinitely many bound states of H_ℓ; if Z is zero or negative no bound states occur, since $V(\infty) = 0$.

For $Z > 0$ we choose $E_\ell = \inf \operatorname{spec} H_\ell$ and (following our procedure of Ref. [2]) get from $\Delta V > 0$ that (for fixed R)

$$V(r) \geq V(R) + Z(R)(\frac{1}{R} - \frac{1}{r}) . \tag{3.1}$$

From the Min-Max-principle we deduce that

$$E_\ell \geq V(R) + \frac{Z(R)}{R} - (\frac{Z(R)}{2(\ell+1)})^2 =: f(R) \tag{3.2}$$

an inequality which we shall use several times in the following.

For the case $Z \leq 0$ we choose $E_\ell = -(Z/2(\ell+1))^2$ and observe that (3.2) holds too, since $f(R)$ is an increasing function of R and equality in (3.2) is obtained for $R \to \infty$.

Since for a pure Coulomb potential $V(r) = -\bar{Z}/r$ the appropriate g_ℓ of eq. (2.2) becomes

$$g_{\ell,\bar{Z}}(r) = -\frac{\ell+1}{r} + \frac{\bar{Z}}{2(\ell+1)} \tag{3.3}$$

we may rewrite (3.2) as

$$g^2_{\ell,\bar{Z}}(R) \geq (\frac{\ell+1}{R})^2 + V(R) - E_\ell . \tag{3.4}$$

Next, we distinguish two cases: If the r.h.s. of (3.4) is negative, the Riccati equation for $g_\ell(r)$

$$g'_\ell(r) = g^2_\ell(r) - \frac{\ell(\ell+1)}{r^2} - V(r) + E_\ell \tag{3.5}$$

taken at $r = R$ shows already that

$$g_\ell'(R) \geq \frac{\ell+1}{R^2} . \qquad (3.6)$$

If the r.h.s. of (3.4) is nonnegative we define two Coulomb potentials $B_\pm/r$ with $B_- < B_+$ by

$$g_{\ell,B_\pm}^2(R) = \left(-\frac{\ell+1}{R} + \frac{B_\pm}{2(\ell+1)}\right)^2 = \left(\frac{\ell+1}{R}\right)^2 + V(R) - E_\ell . \qquad (3.7)$$

If $Z > 0$ there exist infinitely many bound states and we follow our steps of Ref. [2]. For the new situation with $Z \leq 0$ we get first $Z(R) \leq 0$ for all R since $Z' \geq 0$. Using again (3.2) to bind the r.h.s. of (3.7) shows that $Z(R) \leq B_-$ from which we get

$$V(r) - E_\ell \geq \left(\frac{B_-}{2(\ell+1)}\right)^2 - \frac{B_-}{r} \quad \text{for} \quad r \leq R . \qquad (3.8)$$

Now we compare the original Schrödinger equation with wave function u_ℓ to another one with potential B_-/r and wave function u_- and get

$$\frac{u_\ell'(R)}{u_\ell(R)} - \frac{u_-'(R)}{u_-(R)} = \int_0^R dr \, \frac{u_\ell(r)u_-(r)}{u_\ell(R)u_-(R)} \left[V(r) - E_\ell + \frac{B_-}{r} - \left(\frac{B_-}{2(\ell+1)}\right)^2\right] \geq 0. \quad (3.9)$$

Therefore $g_\ell(R) \leq g_{\ell,B_-} \leq 0$ which implies $g_\ell^2(R) \geq g_{\ell,B_-}^2(R)$ and finally $g_\ell'(R) \geq (\ell+1)/R$, which allows to formulate

<u>THEOREM 1</u>: Let $V(r)$ fulfil conditions (2.5). Suppose $\Delta V \geq 0$ for $r \neq 0$ and let $\delta_\ell(E)$ denote the scattering phase shift relative to the Coulomb potential $-Z/r$. The $\delta_\ell(E)$ are then monotonous in ℓ:

$$\delta_{\ell+1}(E) \geq \delta_\ell(E) . \qquad (3.10)$$

Moreover, if $Z < 0$ we choose E_ℓ to be the ground state energy; since then $\sqrt{E_\ell} \leq Z/2(\ell+1)$ we get

$$\delta_{\ell+1}(E) \geq \delta_\ell(E) + \operatorname{arctg} \frac{Z}{2k(\ell+1)} - \operatorname{arctg} \frac{\sqrt{|E_\ell|}}{k} , \quad E = k^2 . \qquad (3.11)$$

B) The Case $\Delta V \leq 0$

This means that $Z(r)$ is monotonously decreasing. For $Z \geq 0$ we choose $E_\ell = \inf \operatorname{spec} H_\ell$, for $Z \leq 0$ we take $E_\ell = \min\{-(Z/2(\ell+1))^2, \inf \operatorname{spec} H_\ell\}$. From $\Delta V \leq 0$ we get

$$V(r) \leq V(R) + Z(R)\left(\frac{1}{R} - \frac{1}{r}\right) \tag{3.12}$$

and deduce for $Z(R) > 0$ that

$$\inf \operatorname{spec} H_\ell \leq V(R) + \frac{Z(R)}{R} - \left(\frac{Z(R)}{2(\ell+1)}\right)^2 =: h(R) . \tag{3.13}$$

Since $h(R)$ is monotonously decreasing for $Z(R) \leq 0$, and $h(\infty) = - (Z(\infty)/2(\ell+1))^2$, we get in any case that

$$E_\ell \leq V(R) + \frac{Z(R)}{R} - \left(\frac{Z(R)}{2(\ell+1)}\right)^2 \tag{3.14}$$

and

$$g_\ell(\infty) \geq \frac{Z}{2(\ell+1)} . \tag{3.15}$$

We rewrite (3.14) in analogy to (3.4) as

$$g_{\ell,Z}^2(R) \leq \left(\frac{\ell+1}{R}\right)^2 + V(R) - E = g_{\ell,B_\pm}^2(R) . \tag{3.16}$$

(3.16) has always solutions $B_\pm$ with $B_- \leq Z(R) \leq B_+$.

Next we distinguish two cases: If $g_\ell(R) \leq 0$ we take B_- and get

$$\left(\frac{B_-}{2(\ell+1)}\right)^2 - \frac{B_-}{r} \geq V(r) - E_\ell \quad \text{for} \quad \underline{r \leq R} . \tag{3.17}$$

Comparing again the Schrödinger equations to potential V with wave function u_ℓ to that with $-B_-/r$ and wave function u_- we get

$$\frac{u_\ell'(R)}{u_\ell(R)} - \frac{u_-'(R)}{u_-(R)} = \int_0^R dr\, \frac{u_\ell(r)u_-(r)}{u_\ell(R)u_-(R)} \left(V(r) - E_\ell + \frac{B_-}{r} - \left(\frac{B_-}{2(\ell+1)}\right)^2\right) \leq 0 \tag{3.18}$$

and the chain of inequalities

$$0 \geq g_\ell(R) \geq g_{\ell,B_-}(R) \Rightarrow g_\ell^2(R) \leq g_{\ell,B_-}^2(R) \Rightarrow g_\ell'(R) \leq \frac{\ell+1}{R^2} , \qquad (3.19)$$

which solves the problem in that case. Suppose next that $g_\ell(R) > 0$, then we take B_+/r as comparison potential for which we get

$$\left(\frac{B_+}{2(\ell+1)}\right)^2 - \frac{B_+}{r} \geq V(r) - E_\ell \quad \text{for} \quad r \geq R . \qquad (3.20)$$

If u_+ denotes the wave function for the potential $-B_+/r$ we get

$$\frac{u_\ell'(R)}{u_\ell(R)} - \frac{u_+'(R)}{u_+(R)} = \int_R^\infty dr \frac{u_\ell(r)u_+(r)}{u_\ell(R)u_+(R)}\left(\left(\frac{B_+}{2(\ell+1)}\right)^2 - \frac{B_+}{r} - V(r) + E_\ell\right) \geq 0, \quad (3.21)$$

and the chain of inequalities

$$g_\ell(R) \leq g_{\ell,B_+}(R) \Rightarrow g_\ell^2(R) \leq g_{\ell,B_+}^2(R) \Rightarrow g_\ell'(R) \geq \frac{\ell+1}{R^2} \qquad (3.22)$$

provided the integral in (3.21) is convergent. This is the case since if $E_\ell = 0$, u_ℓ, although not L^2, grows less than any exponential, and if $E_\ell = -(Z/2(\ell+1))^2$, u_ℓ behaves like $u_\ell(r) \underset{r\to\infty}{\sim} \exp(|Z|r/2(\ell+1))$ whereas $u_{B_+}(r) \underset{r\to\infty}{\sim} \exp(-B_+r/2(\ell+1))$ and since $B_+ > Z(R) \geq Z$ the convergence of the integral in (3.21) is guaranteed.

This allows us to formulate finally

THEOREM 2: Let $V(r)$ fulfil conditions (2.5). Suppose $\Delta V \leq 0$ for $r \neq 0$ and let $\delta_\ell(E)$ denote the scattering phase shift relative to the Coulomb potential $-Z/r$. Then

$$\delta_{\ell+1}(E) \leq \delta_\ell(E) . \qquad (3.23)$$

Moreover, if the ground state energy for angular momentum ℓ is lower than $-(Z/2(\ell+1))^2$ and $Z \leq 0$, or if $Z > 0$ we get

$$\delta_{\ell+1}(E) \leq \delta_\ell(E) + \operatorname{arctg}\frac{Z}{2k(\ell+1)} - \operatorname{arctg}\frac{\sqrt{|E_\ell|}}{k}, \qquad E = k^2 . \qquad (3.24)$$

Note that theorem 1 and Regge's inequality eq. (2.21) allows to bracket $\delta_{\ell+1} - \delta_\ell$, while in the case of theorem 2 Regge's inequality becomes superfluous.

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