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Number of quantal resonances

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Abstract
Based on extraction of resonances from quantal time delay, a theorem relating quantal time delay and the number of resonances below a certain energy is proved here. Several illustrations from quantum mechanics, neutron reflectometry and hadron resonances are presented.

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The physics of weakly-bound systems and resonances has been of great interest for the important role it plays in nuclear and particle physics. In particular, deriving reliable information about unstable and short-lived states leads to a deeper understanding in the theory of elementary particles in the case of hadron resonances [1] and hypernuclei [2], compound nuclear resonances [3] in (n, γ) and (p, γ) reactions and in the development of new models and theories in the active field of radioactive nuclei [4]. The research on halo nuclei is also intimately connected with the search for superheavy nuclei [5]. The structure of these elusive states is usually in the form of two-body, three-body or many-body resonances [6]. It would be interesting if we could infer from the phase-shift data for π–π or η–d or α–α scattering whether, respectively, a ρ-meson around $E = 770$ MeV is formed, or a hypernucleus or a resonant α-cluster [7] is formed. Clearly, we would like to be sure of our analysis by studying simple, non-trivial illustrations from quantum mechanics. In this paper, we present various illustrations to elucidate how resonant structures can be reliably extracted and understood.

The concept of central importance for our considerations is that of time delay. Time delay, $\mathcal{T}$, is defined as the difference between the density of states with and without interaction. This reduces to the following relation [5] between $\mathcal{T}$ and the S-matrix [8],

$$\mathcal{T} = -\tfrac{1}{2}\mathrm{i}\hbar\,\mathrm{Tr}\,S^{\dagger}\frac{\mathrm{d}S}{\mathrm{d}E} \tag{1}$$

for a general form of interaction. For central potentials, for the lth partial wave, $\mathcal{T}_l$ reduces to $\hbar\mathrm{d}\overline{\delta}_l/\mathrm{d}E$ where $\overline{\delta}_l$ is the difference between phase-shift $\delta_l(E)$ and hard-sphere scattering phase-shift $\delta_l^H(a, E)$ and where a is the range of interaction. For s-wave scattering, $\delta_l^H(a, E) = -ka$, where k is the wave number.

The complex-energy poles of time delay on an unphysical sheet like those of the S-matrix represent resonances. Consequently, the peaks in $\mathcal{T}(E)$ are signatures of resonances [9].

In a system where the number of single-particle states is modified in the presence of an impurity, the change in the states is related to the energy derivative of the phase-shift. The total change in the density of states leads to the Friedel sum rule, which is basically a statement of charge-neutrality [10]. On the other hand, an energy-integral of the phase-shift is shown to be connected to the energy of the impurity—Fumi's theorem. All the filled states contribute to the energy of the impurity via electron–impurity interactions.

In the context of nuclear physics, some recent works [11] treat the effect of the continuum by considering the contribution of narrow resonances. These narrow resonances are assumed to be like broadened bound states. This is, of course, not a valid assumption for broad resonances occurring in particle physics. When this assumption holds, the change in the single-particle continuum level density, $\delta\rho$, in the presence of a potential V is found by subtracting the free particle level density ρ_0 from the total level density, ρ:

$$\delta\rho = \rho(\epsilon) - \rho_0 = \sum_{l,j} \frac{(2j+1)}{\pi} \frac{\mathrm{d}\delta_{lj}}{\mathrm{d}\epsilon} \tag{2}$$

the last being due to Friedel [12]. The right-hand side of (2) is connected with time delay. We will consider an energy integral of time delay in this paper and illustrate it by a variety of physical situations of simple and advanced nature.

For a narrow resonance at energy E_0 of width Γ, time delay has a Lorentzian or a Breit–Wigner (B–W) form:

$$\tau(E) = \frac{\hbar\Gamma/2}{(E-E_0)^2 + \frac{\Gamma^2}{4}}. \tag{3}$$

Then, it follows that the number of resonances below E^* for a fixed partial wave is given by[1]

$$\begin{aligned} n_R &= \frac{1}{\pi}\int_0^{E^*} \left(\frac{\mathrm{d}\bar{\delta}(E)}{\mathrm{d}E}\right)\mathrm{d}E \\ &= N + \Delta, \qquad 0 < \Delta < 1. \end{aligned} \tag{4}$$

This is related to the approaches based on level-density [11, 13]. Since most of the methods fail to determine the absolute values of phase-shifts, therefore, the right-hand side of (4) would be different from the expression $[\bar{\delta}_l(E^*) - \bar{\delta}_l(0)]/\pi$. However, following somewhat more general considerations along the lines of [14], the spectral property of time delay implies that

$$\int_0^{E^*} \mathcal{T}(E)\mathrm{d}E = n_R h. \tag{5}$$

This is also valid for broad resonances, as shown in illustration IV. To appreciate (5), the following remarks are in order: (i) (5) is not Levinson's theorem; (ii) if the energy range includes bound states also, singularities will appear for bound states and non-zero widths appear for resonances, the shapes being Lorentzian only for narrow ones (see also comments at the end of illustration II).

The construction of time delay above using the complex energy eigenvalues may remind one of the potential scattering formalisms due to Kapur and Peierls [15]. To illustrate, with the s-wavefunction in the range of potential, the complex roots, $\mathcal{E}$, of $\hbar\partial u/\partial r(\mathcal{E}, r=a) = \mathrm{i}\sqrt{2m\mathcal{E}}u(\mathcal{E}, r)$ are taken as resonances here. However, in [15], $\sqrt{2m\mathcal{E}}$ is replaced by $\sqrt{2mE}$, where E is fixed. Moreover, Kapur–Peierls' formalism is designed to yield a non-unitary S-matrix.

At resonance, the phase-shift $\bar{\delta}(E) = \arctan\left(\frac{\Gamma/2}{E-E_0}\right)$, due to the presence of an inverse trigonometric function, has an essential ambiguity of $n\pi$ where n remains uncertain.

[1] For resonances with $\Gamma_j \ll E_j$, the S-matrix is $S(E) = \exp[2\mathrm{i}\bar{\delta}(E)] = \Pi_{j=1}^{N}(\frac{E-E_j-\mathrm{i}\Gamma_j/2}{E-E_j+\mathrm{i}\Gamma_j/2})$.

On the other hand, the ambiguity disappears in $\mathcal{T}(E)$ as one gets a purely algebraic expression, making the time delay unambiguous and hence more reliable than the phase-shifts themselves. The second derivative of $\bar{\delta}(E)$ reveals that on either side of $E = E_0$ the curvature changes sign and hence a point of inflection in the variation of $\bar{\delta}(E)$ is a necessary signature for the existence of a resonance.

Resonances which are complex energy Gamow–Siegert states of a potential generally arise when the potential is localized (e.g., short-range) or when there is a barrier of a finite width attached to the well. The square well represents the former when $l = 0$ and the latter when $l > 0$. However, for simplicity we present a s-wave square well potential [16] and a s-wave Dirac barrier potential $V_0\delta(r-a)$ [16] which represents the second situation. It is worth noting that illustrations III and IV are novel as they do not fall in the above categorization. Believing that a fundamental result is understood better in terms of diverse examples, we present them below.

1. Illustration I: square-well potential[2]

To begin with, we consider the most familiar potential $V(r < a) = -V_0$, $V(r \geqslant a) = 0$, as an example to illustrate our results on resonances. It may be noted that a reliable description of narrow resonances is important for separating the background. The s-wave S-matrix can be written as

$$S_0(E) = \frac{\mathrm{i}k \tan pa + p}{\mathrm{i}k \tan pa - p}. \tag{6}$$

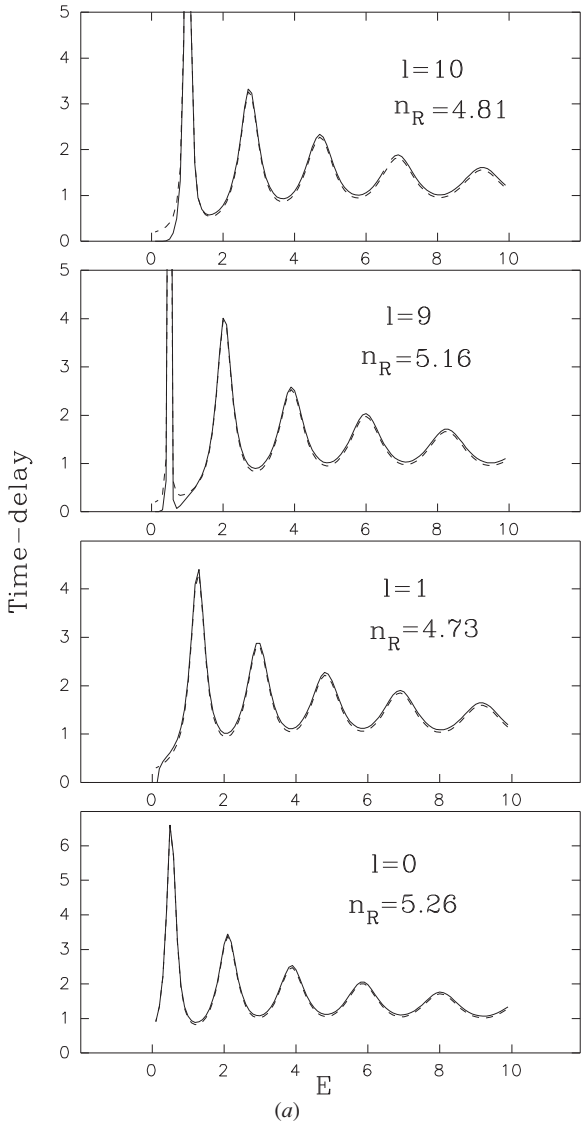
The complex poles (resonances) of $S_0(E)$, i.e., the roots of $\mathrm{i}k \tan pa = p$, are equivalent to demanding the outgoing wave, $u_0(r \geqslant a) = \mathrm{e}^{\mathrm{i}kr}$, instead of $u_0(r > a)$ as given above. The s-wave time delay for a square-well potential can be obtained as

$$\mathcal{T}_0(E) = \hbar \frac{V_0 \tan pa + apk^2 \sec^2 pa}{2pk(p^2 + k^2 \tan^2 pa)}. \tag{7}$$

Relevant complex poles of the S-matrix, $(E_j - \mathrm{i}\Gamma_j/2)$, such that $E_j, \Gamma_j > 0$, are known to be the resonant energies. With the help of *Find Root* by *Mathematica*, by taking $2m = 1 = \hbar$, and fixing the values of V_0 and a, we find the resonant energies (e.g., poles of (6), for $l = 0$). We then construct the time delay as a sum of Lorentzians as these resonances are narrow. The solid lines in figure 1 display the exact values of $\mathcal{T}_l(E)$ for $l = 0, 1, 9, 10$ for a square-well potential ($V_0 = 5, a = 10$) up to an energy $E = 10$. The dashed lines show the time delay as calculated using the first fifteen complex energies $E_j - \mathrm{i}\Gamma_j/2$. Excellent reproduction of the time delay can be seen to testify to the representation of the time delay by a sum over Lorentzians for a localized potential possessing resonances. We check that E_j are the energies where the peaks in time delay occur. Further, we check that Γ_j is nothing but twice the inverse of the height of the jth peak. The values of the integral of the time delay up to $E = 10$, n_R (4), are mentioned in each part of figure 1(a) which can be verified to give the number of resonances as depicted by the number of peaks in $\mathcal{T}_l(E)$.

Interestingly, in the above calculations when $l = 9, 10$, we find that the *first* complex roots $E = 0.384\,99$–$0.479\,894\,\mathrm{i} = E_A$ and $E = 0.541\,725$–$0.574\,161\,\mathrm{i} = E_B$ respectively do not show up as peaks in $\mathcal{T}_l(E)$. Moreover, if they are included in the summation (4), they spoil the reproduction of the time delay at other energies. Similarly, when $V_0 = 5$ and $a = 2$, we find that $E_1 = 0.023\,387$–$0.542\,466\,\mathrm{i} = E_C$ and $E_2 = 9.383\,65$–$4.430\,07\,\mathrm{i}$ are the poles of

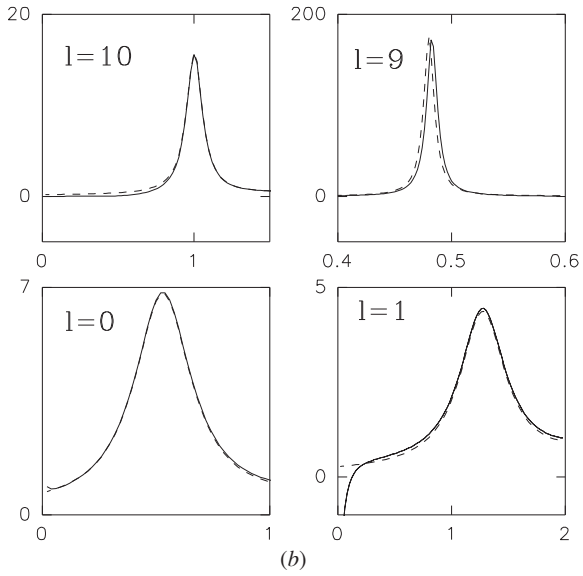
[2] For a square barrier, we find resonances above the top of the barrier using time delay and verify our result for the number of resonances.



(*a*)

Figure 1. (*a*) Time delay, $\mathcal{T}(E)$, for a square-well potential ($V_0 = -5, a = 10$) for four values of angular momentum $l = 0, 1, 9, 10$. The solid lines are the exact calculation and the dashed lines represent a sum of Lorentzians using the first 15 resonances (poles of S-matrix on an unphysical sheet). Interestingly, in the case of $l = 9, 10$ the very first complex energies $E_A = 0.384\,99 - 0.479\,84\mathrm{i}$ and $E_B = 0.541\,725 - 0.574\,161\mathrm{i}$, respectively are not included (see text for details). Note that the values of n_R agree with the number of peaks in all the plots of time delay, illustrating (4). (*b*) The first peaks corresponding to figure 1(*a*) are separated out and shown for clarity.

$S_0(E)$ (6). We find that E_1 does not lead to a peak in $\mathcal{T}_0(E)$, whereas E_2 shows up as a broad peak in $\mathcal{T}_0(E)$. Note that in these examples $\Gamma_j > E_j$ and the corresponding B–W profile appears only partly for energies $E > 0$, most of it creeps into the negative energy regime. We rule out E_A, E_B, E_C as resonances by studying the corresponding wavefunctions. The



(*b*)

Figure 1. (Continued.)

wavefunctions at energies equal to the real part of these complex energies for the $l = 0$ case show scattering state-like behaviour whereas the localization within $r < a$ is inhibited.

2. Illustration II: repulsive Dirac delta s-wave barrier

The Dirac delta barrier, $V_0\delta(r - a)$, $V_0 > 0$ in the three-dimensional Schrödinger equation [16], even in s-wave, supports the Gamow–Siegert states. The poles of the S-matrix can be worked out to be the complex roots of $k \cot ka - aV_0 = \mathrm{i}k$, a condition which one also gets by using the outgoing wave boundary condition at $r = a$. The s-wave quantal time delay can be found as

$$\mathcal{T}_0(E) = \hbar \frac{aV_0 \tan^2 ka + ak^2 \sec^2 ka}{2[k^2 \tan^2 ka + (k + aV_0 \tan ka)^2]}. \tag{8}$$

For $V_0 = 10$ and $a = 1$, we find the first four poles of the S-matrix and construct the time delay as a sum of Lorentzians (shown as dotted lines in figure 2). Even with only five poles, the $\mathcal{T}_0(E)$ (8) (solid line) is excellently reproduced by the dotted line in figure 2. By an integration of time delay up to energy $E = 170$, we get the value of the integral $n_R = 4.0114$, correctly indicating four resonances or metastable states. In the limit of $V_0 \to \infty$, we get $E_j \to \frac{j^2\pi^2\hbar^2}{2ma^2}$ and $\Gamma_j \to 0$ these states will be the bound states of a particle contained between two rigid walls of width a. Thus, for large values of V_0 one gets Dirac delta like spikes in $\mathcal{T}_0(E)$ at energies $E = E_j$.

3. Illustration III

While studying the reflectometry of the polarized neutrons from magnetized superconductors, Zhang and Lynn [17] arrived at a novel result wherein a single, pronounced, parameter-dependent dip occurs in the reflectivity. In terms of simple quantum mechanics this means that the reflectivity, $R(E)$, of the potential-step barrier, $V(x > 0) = V_1 + V_2(1 - \mathrm{e}^{-x/a})$,

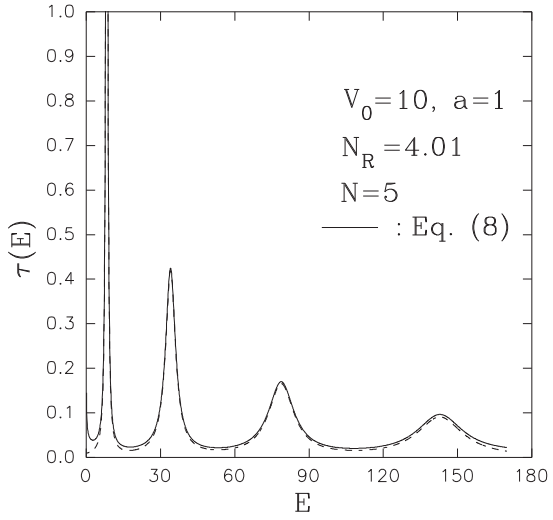


Figure 2. Excellent reproduction of the time delay (8) by a sum of Lorentzians for the Dirac delta potential by using just the first five complex energies (resonances). A value of n_R close to 4 illustrates the existence of four resonances up to $E = 170$.

$V(x \leqslant 0) = 0$, as a function of energy shows a *single*, pronounced, spike-like minimum at an energy slightly above the step, for certain sets of parameters, (V_1, V_2, a). Usually when a semi-infinite potential is smooth, $R(E)$ is a smoothly converging function of energy. A discontinuity of the derivative at a point in a semi-infinite potential turns out to be the essence [18, 19] of this novel reflectivity. An interesting claim [20] that the energy ($E = E_d$) at which this reflectivity minimum occurs corresponds to a 'half-bound state' has been refuted by the help of several model potentials [19]. Let us take the case of an exponential step where $r(E) = \sqrt{R(E)}\,\mathrm{e}^{\mathrm{i}\theta(E)}$ is given by

$$r(E) = \frac{\mathrm{i}kJ_{-2\mathrm{i}pa}(2qa) + qJ'_{-2\mathrm{i}pa}(2qa)}{\mathrm{i}kJ_{-2\mathrm{i}pa}(2qa) - qJ'_{-2\mathrm{i}pa}(2qa)} \tag{9}$$

where $p = \frac{\sqrt{2m(E-V_1-V_2)}}{\hbar}$ and $q = \sqrt{\frac{2mV_2}{\hbar^2}}$. Whenever $2qa$ is close [17] to the zeros of $J_0(z)$, a single pronounced minimum exists in $R(E)$. More precisely, when $V_1 = V_2 = 1$ and $a = 1.31(2m = 1 = \hbar)$ the dip in reflectivity occurs at $E = 2.0445 = E_d$ [18]. We find that the reflection time delay, $\frac{\mathrm{d}\theta}{\mathrm{d}E}$, possesses a single dip at $E = E_d$, confirming the existence of a resonance there (see figure 3). Since the contention is regarding the dip in reflectivity, we have calculated the reflection-phase-shift (θ) and its derivative. Eventually, the integration (4) of time delay over a long range of energy (from $E = 2$ to $E = 4$, 6, 10) divided by π has been checked to yield a number very close to 1. Thus, the composite semi-infinite potential steps [18, 19] are a new type of model potential which are neither localized nor is there a well attached to a barrier. They, however, possess a single resonance. We also find that the low energy, single minimum in reflectivity of the composite potential wells [19] such as $V(x) = -V_0 \exp(-|x|/a)$ is nothing but a resonance.

4. Illustration IV

Usually, narrow resonances are treated as elementary particles [21]. However, even relatively broader resonances like the excited state of a nucleon called $\Delta^{++}(1232)$ are treated as particles.

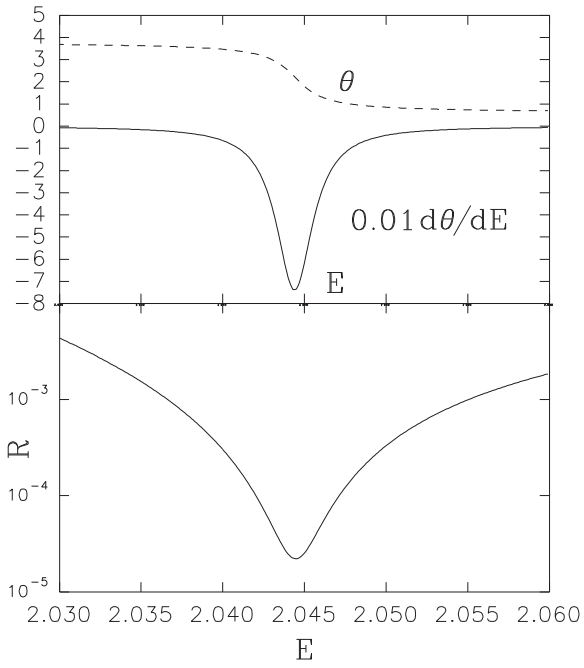


Figure 3. An instance of reflectivity, $R(E)$, dip in the exponential semi-infinite potential step when $V_1 = V_2 = 1$ and $a = 1.31$. At $E = 2.0445$ there occurs a dip in $R(E)$ and $\mathcal{T}(E)$ and the (reflection) phase-shift, $\theta(E)$ displays a point of inflection. The value of n_R from $E = 2$ up to $E = 4, 6, 10$ has been found to be very close to 1.

Here we would like to demonstrate that the time delay calculated from the available [22] elastic scattering phase-shifts of π^+ and p $(P33)$ yields a peak at $E = 1218$ MeV of width $\Gamma = 129$ MeV (see figure 4) corresponding to the formation of the well-known baryon resonance called the Δ-resonance which has mass as 1232 MeV and width as 120 MeV. This result can also be found in [23] where there is a more detailed study on unflavoured baryon resonances. The integration (4) of time delay in the energy range given in figure 4 divided by π yields 0.87 instead of unity, simply because the resonance data are truncated at the lower energies. This illustration, in addition to [23] shows that (4) and (5) are also valid for non-central interactions and for broad resonances with lifetimes $\sim 10^{-23}$ s. It should also be noted that one is in a relativistic regime with energies of the order of GeV. The concept of time delay holds in the relativistic regime because of its connection with the S-matrix (1) [24].

Hitherto, the energy-integral of the first derivative of phase-shift over a large range of energy is supposed to either vanish [25] or yield the number of bound states [21] via the well-known result in (10). In such a confusing scenario, we have brought out the correct meaning of the energy-integral mentioned above. We have revealed that the integral (4) does not vanish and it yields the number of resonances possessed by a potential. Since time and energy are conjugate variables, (5) can be interpreted as an analogue of the Bohr–Sommerfeld quantization. This is also a quantum analogue of some results in classical scattering theory obtained 20 years ago by Narnhofer and Thirring [26].

Finally, we would like to make some observations on Levinson's theorem in its original form that relates the phase-shift at zero energy to the number of bound states, n_B, possessed

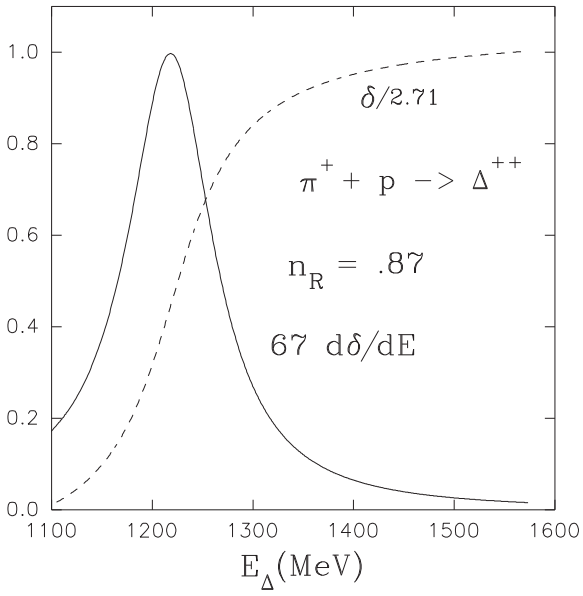


Figure 4. The well known baryon resonance, Δ^{++} [1], is demonstrated as a peak in time delay in the phase-shift data [24] of the scattering : $\pi^+ + \mathrm{p} \rightarrow \Delta^{++}$. We get $M_\Delta = 1218$ MeV and $\Gamma_\Delta = 129$ MeV, whereas the standard values are $M_\Delta = 1232$ MeV and $\Gamma_\Delta = 120$ MeV. The value of n_R we get is 0.87.

by an attractive potential: $n_B = \delta_l(0)/\pi$ [8].[3] However, it is very often written as [8, 21, 27][4]

$$n_B = [\delta_l(0) - \delta_l(\infty)]/\pi. \tag{10}$$

It is important to note that (10) seems to relate the negative energy bound states to the phase-shift at an infinitely positive energy. This is basically done to provide a reference at infinite energy where the phase-shift is assumed to be zero. Although for short-range potentials, $\delta_l(\infty)$ is zero, this is not generally true (see footnote 4). In a specific calculation, one may find $\delta_l(0)$ and $\delta_l(\infty)$ with ambiguous factors of, say, $m_1\pi$ and $m_2\pi$ with m_1, m_2 as two arbitrary, uncontrollable integers, having nothing to do with the potential. To obtain phase-shifts free of such ambiguities (modulo π), one needs to employ special methods like the variable phase approach [28] and an integral representation of phase-shift found recently [29].

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[3] For the case when the edge of the potential separating bound and scattering states ($E = 0$) possesses a 'half-bound state' one writes $n_B = \delta_l(0)/\pi - 1/2$.
[4] $\delta(\infty)$ does not vanish for several classes of potentials (see e.g. appendix III in [28]).

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