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Sum rules for the phase shift*

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It is observed that a number of phase-shift rules can be deduced from properties of the Jost function. The simplest of these is $\int_0^\infty (d\epsilon/\pi)[\delta_l(\epsilon) - \delta_l^{1B}(\epsilon)] = \sum_n \epsilon_{nl}$ where $\delta_l(\epsilon)$ is the phase shift, $\delta_l^{1B}(\epsilon)$ is the first Born approximation to the phase shift, and ϵ_{nl} is the nth bound-state energy with angular momentum l.

In this paper, a class of sum rules is derived for the phase shift in nonrelativistic potential scattering theory. These sum rules can be obtained quite simply from subtracted dispersion relations satisfied by the Jost function.

In the following analysis we restrict ourselves to the $l=0$ case, and furthermore require that the interaction potential $V(r)$ is well behaved and that the first Born phase shift,[1]

$$\delta_l^{1B}(k) = -\frac{2\mu}{\hbar^2} k \int_0^\infty dr\, r^2 V(r) j_l^2(kr), \quad \epsilon = \frac{\hbar^2 k^2}{2\mu}, \tag{1}$$

is well defined. If this is not the case, the δ_l^{1B} appearing in the simplest sum rule noted above should be replaced by the $|z| \to \infty$ limit of $-2\mu k \times \hbar^{-2} \langle k | T_l(z) | k \rangle$, where $T_l(z)$ is the partial-wave amplitude of the off-energy shell T matrix. For simplicity, singular potentials for which this generalization is necessary will not be considered here. For $l \neq 0$, explicit proof of at least the first sum rule is not difficult.

We will need explicitly only the first few terms in the Born series to a given order, for $l=0$. This series, for the nth-order Born sum is

$$\delta^{nB}(k) = \sum_{j=1}^{n} \delta_j^B(k), \tag{2}$$

with terms

$$\delta_1^B(k) = -\frac{1}{k} \int_0^\infty dr_1\, V(r_1) \sin^2 kr_1,$$
$$\delta_2^B(k) = \frac{1}{k^2} \int_0^\infty dr_1\, V(r_1) \sin^2 kr_1 \times \int_{r_1}^\infty dr_2\, V(r_2) \sin 2kr_2, \tag{3}$$
$$\vdots$$

The scattering state, asymptotic to $(1/r)\sin[kr - \delta(k)]$ as $r \to \infty$, is

$$\psi_{l=0}(k,r) = \frac{i}{2kr} \left(\frac{f(-k) f(k,r)}{|f(k)|} - \frac{f(k) f(-k,r)}{|f(k)|} \right),$$

where the coefficient $f(k) \equiv f(k,0)$ is the Jost function[2] and the function $f(k,r)$ satisfies the integral equation[2]

$$f(k,r) = e^{-ikr} + \frac{1}{k} \int_r^\infty \sin k(r'-r)\, V(r') f(k,r')\, dr'. \tag{4}$$

The $l=0$ partial-wave S matrix is given by the ratio $f(k)/f(-k)$, and a simple dispersion relation connects the phase shift $\delta(k)$ to the Jost function. This relation is[3]

$$f(k) = \exp\left[-\int_{-\infty}^\infty \frac{dk'}{\pi} \frac{\delta(k')}{k'-k+i\delta} + \sum_n \ln\left(1 + \frac{\kappa_n^2}{k^2}\right) \right], \tag{5}$$

where $\epsilon_n = -\kappa_n^2$ is the nth bound-state energy. The properties of these functions have been described extensively in the literature.[4] For our purpose here, everything necessary is contained in Eqs. (4) and (5), together with the definition of the Born series in (2) and (3). As is conventional, we take $\delta(-k) = -\delta(k)$ for real $k \neq 0$ and $\delta(k \to \infty) = 0$. $\delta(k=0^+) = \pi \sum_n (1)$ is a consequence of Levinson's theorem.[5]

We rewrite Eq. (5) in the form

$$f(k) = \exp[i\delta(k) + R(k)], \tag{6}$$

with

$$R(k) = \frac{2}{\pi} P \int_0^\infty dk' \frac{k'\delta(k')}{k^2 - k'^2} + \sum_n \ln\left(1 + \frac{\kappa_n^2}{k^2}\right), \tag{7}$$

and carry out a series of subtractions in this dispersion relation. Subtracting and adding $\delta_1^B(k')$, and using

$$\frac{1}{k^2 - k'^2} = \frac{1}{k^2} + \frac{k'^2}{k^2(k^2 - k'^2)},$$

we have

$$R(k)=\frac{2}{\pi}P\int_0^\infty dk'\,\frac{k'\delta_1^B(k')}{k^2-k'^2}+\frac{2}{\pi}P\int_0^\infty dk'\,\frac{k'}{k^2-k'^2}\left(\frac{k'^2}{k^2}\right)[\delta(k')-\delta_1^B(k')]$$
$$+\frac{2}{\pi k^2}\int_0^\infty dk'\,k'[\delta(k')-\delta_1^B(k')]+\sum_n\ln\left(1+\frac{\kappa_n^2}{k^2}\right). \quad (8)$$

Next, add and subtract $\delta_2^B(k')$ in the second term and repeat the entire manipulation. Continuation of this process produces, for example,

$$R(k)=R_1(k)+R_2(k)+\left\{R_3(k)+\frac{2}{\pi}P\int_0^\infty dk'\,\frac{k'}{k^2-k'^2}\left(\frac{k'^2}{k^2}\right)^2[\delta(k')-\delta^{3B}(k')]\right.$$
$$\left.+\sum_n\left[\ln\left(1+\frac{\kappa_n^2}{k^2}\right)-\frac{\kappa_n^2}{k^2}+\frac{1}{2}\,\frac{\kappa_n^4}{k^4}\right]\right\}+\frac{1}{k^2}I_1+\frac{1}{k^4}I_2, \quad (9)$$

where

$$R_j(k)=\frac{2}{\pi}P\int_0^\infty dk'\,\frac{k'}{k^2-k'^2}\left(\frac{k'^2}{k^2}\right)^{j-1}\delta_j^B(k') \quad (10)$$

and

$$I_j=2\int_0^\infty\frac{dk}{\pi}\,k(k^2)^{j-1}[\delta(k)-\delta^{jB}(k)]-\frac{1}{j}\sum_n(-\kappa_n^2)^j \quad (11)$$

define the terms $R_{1,2,3}$ and $I_{1,2}$. We have added terms to the bound-state sum (and subtracted them in defining $I_{1,2}$) so that the entire $\{\}$ term of Eq. (9) is of order k^{-6} for large k. Explicit evaluation of $R_1(k)$ and $R_2(k)$, using Eq. (3), gives

$$R_1(k)=\frac{1}{2k}\int_0^\infty dr_1\,V(r_1)\sin(2kr_1),$$
$$R_2(k)=-\frac{1}{k^2}\int_0^\infty dr_1\,V(r_1)\sin^2(kr_1)\times\int_{r_1}^\infty dr_2\,V(r_2)\cos(2kr_2). \quad (12)$$

The development of moment relations (sum rules) for the phase shift requires the asymptotic expansion of $f(k)$ for large k. This is to be done in two ways; first through the dispersion relation structure of Eqs. (6) and (9), and then directly from the integral equation (4).

First, consider the high-k behavior of $R(k)$. From the asymptotic evaluation of (12), we have

$$R_1(k)=(1/k^2)\tfrac{1}{4}V(r=0)-(1/k^4)\tfrac{1}{16}V''(r=0)+O(1/k^6),$$
$$R_2(k)=(1/k^4)\tfrac{1}{8}V^2(r=0)+O(1/k^6), \quad (13)$$

while $R_3(k)$, together with the remainder of the $\{\}$ term in Eq. (9), is of order k^{-6}. Consequently, we have

$$R(k)=C/k^2+D/k^4+O(1/k^6), \quad (14)$$

with

$$C\equiv I_1+\tfrac{1}{4}V(0),$$
$$D\equiv I_2-\tfrac{1}{16}V''(0)+\tfrac{1}{8}V^2(0). \quad (15)$$

Since the phase shift $\delta(k)$ will have an asymptotic expansion

$$\delta(k)=A/k+B/k^3+O(1/k^5), \quad (16)$$

we see from Eqs. (6), (14), and (16), that the Jost function has the expansion

$$f(k)=1+iA/k+(C-\tfrac{1}{2}A^2)/k^2+i[B-AC-(1/3!)A^3]/k^3$$
$$+[D+\tfrac{1}{2}C^2-AB-\tfrac{1}{2}CA^2+(1/4!)A^4]/k^4+\cdots. \quad (17)$$

Next, consider the integral equation (4) and its iteration. The direct iteration produces the series

$$f(k,r)=e^{-ikr}+\sum_{j=1}^\infty f_j(k,r), \quad (18)$$

where $f_j(k,r)$ represents the jth iterate. According to Eq. (4), we have

$$f_j(k,r)=\frac{1}{k}\int_r^\infty dr'\,\sin k(r'-r)V(r')f_{j-1}(k,r') \quad (19)$$

for $j\geq 1$, where $f_0(k,r')=e^{-ikr'}$. Each iterate can then be expanded for large k in a series of the form

$$f_j(k,r)=e^{-ikr}\sum_{n=0}^\infty\left(\frac{-i}{2k}\right)^{n+j}a_n^{(j)}(r), \quad (20)$$

so that the lowest-order term for the jth iterate is k^{-j}. Thus the complete sum for $f(k,r)$ is

$$f(k,r)=e^{-ikr}\left[1+\sum_{m=0}^\infty\left(\frac{-i}{2k}\right)^m b_m(r)\right],$$
$$b_m(r)=\sum_{\substack{j,n\text{ with}\\ j+n=m}}a_n^{(j)}(r). \quad (21)$$

In order to carry out the calculation to order k^{-4}, we need all terms $a_n^{(j)}$ for which $j+n\leq 4$. This includes 10 terms. After some computation, we find

$$a_0^{(1)}=U(r),\quad a_0^{(2)}=\tfrac{1}{2}U^2(r),\quad a_0^{(3)}=(1/3!)U^3(r),\quad a_0^{(4)}=(1/4!)U^4(r),$$
$$a_1^{(1)}=-V(r),\quad a_1^{(2)}=-W(r)-U(r)V(r),\quad a_1^{(3)}=-U(r)W(r)-\tfrac{1}{2}U^2(r)V(r),$$
$$a_2^{(1)}=-V'(r),\quad a_2^{(2)}=\tfrac{5}{2}V^2(r)-U(r)V'(r),$$
$$a_3^{(1)}=-V''(r), \tag{22}$$

with

$$U(r)\equiv\int_r^\infty V(r')\,dr',\qquad W(r)\equiv\int_r^\infty V^2(r')\,dr'. \tag{23}$$

The expansion for $f(k)=f(k,r=0)$ then takes the form

$$f(k)=1+(i/k)[-\tfrac{1}{2}b_1(0)]+(1/k^2)[-\tfrac{1}{4}b_2(0)]+(i/k^3)[\tfrac{1}{8}b_3(0)]+(1/k^4)[\tfrac{1}{16}b_4(0)]+\cdots, \tag{24}$$

with coefficients, from (21) and (22), given by

$$\begin{aligned}&b_1(0)=U(0),\quad b_2(0)=-V(0)+\tfrac{1}{2}U^2(0),\\&b_3(0)=-V'(0)-W(0)-U(0)V(0)+(1/3!)U^3(0),\\&b_4(0)=-V''(0)+\tfrac{5}{2}V^2(0)-U(0)V'(0)\\&\qquad-U(0)W(0)-\tfrac{1}{2}U^2(0)V(0)+(1/4!)U^4(0).\end{aligned} \tag{25}$$

Comparison of Eqs. (17) and (24) now permits evaluation of the four constants A, B, C, and D. Thus we find the simple results

$$A=-\tfrac{1}{2}U(0),\quad B=-\tfrac{1}{8}[V'(0)+W(0)],\quad C=\tfrac{1}{4}V(0),\quad D=-\tfrac{1}{16}V''(0)+\tfrac{1}{8}V^2(0). \tag{26}$$

There are two pieces of information contained in (26). From a knowledge of A and B, we see [Eqs. (16) and (23)] that the high-k expansion of the phase shift is

$$\delta(k)=-\frac{1}{2k}\int_0^\infty V(r)dr-\frac{1}{(2k)^3}\left[V'(0)+\int_0^\infty V^2(r)dr\right]+\cdots, \tag{27}$$

an expansion which is equal to that of $\delta^{2B}(k)$ to this order in $1/k$. This asymptotic equality with the Born series is well known. It is clearly the asymptotic equality which makes the integrals in I_j [Eq. (11)] convergent. What appears more surprising is that the calculated values of C and D in Eq. (26) imply, from Eq. (15), that $I_1=I_2=0$. These two equations are the first two sum rules for the phase shift. In terms of energy rather than momentum these equations are

$$\int_0^\infty\frac{d\epsilon}{\pi}[\delta(\epsilon)-\delta^{1B}(\epsilon)]=\sum_n\epsilon_n, \tag{28}$$

$$\int_0^\infty\frac{d\epsilon}{\pi}\epsilon[\delta(\epsilon)-\delta^{2B}(\epsilon)]=\frac{1}{2}\sum_n\epsilon_n^2, \tag{29}$$

and it is clear that each I_j in the series can be evaluated by a higher-order expansion of the Jost function, following the method above. However, having gone through this explicit calculation, we can see immediately what has occurred.

The Born series, or coupling constant iteration for f and $\ln f$, can be generated from (18) and (19). From this series, we see that $R_1(k)+R_2(k)+\cdots$ is the Born series for $R(k)=\mathrm{Re}\ln f$ which accompanies that for $\mathrm{Im}\ln f=\delta(k)=\delta_1^B(k)+\delta_2^B(k)+\cdots$. Consequently,

$$R^{nB}(k)=\sum_{j=1}^{n}R_j(k) \tag{30}$$

is the equivalent of Eq. (2), and represents the nth Born approximation for $R(k)$. The inverse dispersion relation to Eq. (7) is[3]

$$\delta(k)=-(2/\pi)kP\int_0^\infty dk'\,\frac{R(k')}{k^2-k'^2}+i\sum_n\ln\left(\frac{1-i\kappa_n/k}{1+i\kappa_n/k}\right). \tag{31}$$

By adding and subtracting $R_1(k')$, the first term in (31) becomes

$$\delta_1^B(k)-\frac{2}{\pi}kP\int_0^\infty dk'\,\frac{R(k')-R_1(k')}{k^2-k'^2},$$

since

$$\delta_1^B(k)=-\frac{2}{\pi}kP\int_0^\infty dk'\,\frac{R_1(k')}{k^2-k'^2}$$

can be demonstrated directly. By using $1/(k^2-k'^2)=(1/k^2)+k'^2/[k^2(k^2-k'^2)]$, we then obtain

$$\delta(k)=\delta_1^B(k)-\frac{2}{\pi}kP\int_0^\infty dk'\,\frac{1}{k^2-k'^2}\,\frac{k'^2}{k^2}\,[R(k')-R_1(k')]-\frac{2}{\pi k}\int_0^\infty dk'\,[R(k')-R_1(k')]+i\sum_n \ln\left(\frac{1-i\kappa_n/k}{1+i\kappa_n/k}\right). \tag{32}$$

Equation (32) is the analog of Eq. (8). If we repeat this process of subtraction, we have the analog of Eq. (9), i.e.,

$$\delta(k)=\delta_1^B(k)+\delta_2^B(k)+\left\{\delta_3^B(k)-\frac{2}{\pi}kP\int_0^\infty dk'\,\frac{1}{k^2-k'^2}\left(\frac{k'^2}{k^2}\right)^2[R(k)-R^{3B}(k)]\right.$$
$$\left.+i\sum_n\left[\ln\left(\frac{1-i\kappa_n/k}{1+i\kappa_n/k}\right)+2\frac{i\kappa_n}{k}+\frac{2}{3}\left(\frac{i\kappa_n}{k}\right)^3\right]\right\}-\frac{2}{k}J_1-\frac{2}{k^3}J_2, \tag{33}$$

where

$$\delta_j^B(k)=-\frac{2}{\pi}kP\int_0^\infty dk'\,\frac{1}{(k^2-k'^2)}\left(\frac{k'^2}{k^2}\right)^{j-1}R_j(k') \tag{34}$$

and

$$J_j=\int_0^\infty\frac{dk}{\pi}\,(k^2)^{j-1}[R(k)-R^{jB}(k)]+\frac{(-1)^j}{2j-1}\sum_n\kappa_n^{2j-1}. \tag{35}$$

We have added terms to the bound-state sum (and subtracted them in defining $J_{1,2}$) so that the entire $\{\ \}$ term of Eq. (33) is of order k^{-5} for large k. Note that Eqs. (10) and (34) are consistent for any j. That is, insertion of (10) into (34) leads to the identity $\delta_j^B(k)=\delta_j^B(k)$.

If (33) is expanded for large k, the first two terms $\delta_1^B(k)+\delta_2^B(k)$ give the correct asymptotic expansion to order k^{-3}. The $\{\ \}$ term of (33) is of order k^{-5}, hence $J_1=J_2=0$. This gives two sum rules on $R(k)=\mathrm{Re}\ln f(k)$ analogous to those ($I_1=I_2=0$) on the phase shift $\delta(k)=\mathrm{Im}\ln f(k)$.

It is now clear that continued subtraction in both equations (9) and (33) will give the result that $I_j=J_j=0$ for all fixed j. This depends on the fact that $\delta^{jB}(k)$ and $R^{jB}(k)$ give correctly the asymptotic values of $\delta(k)$ and $R(k)$ to terms of order k^{-2j+1} and k^{-2j}, respectively. The two sets of sum rules, in terms of energy integrals and bound states $\epsilon_n=-\kappa_n^2$, are

$$\int_0^\infty\frac{d\epsilon}{\pi}\,\epsilon^{j-1}[\delta(\epsilon)-\delta^{jB}(\epsilon)]=\frac{1}{j}\sum_n(\epsilon_n)^j, \tag{36}$$

$$\int_0^\infty\frac{d\epsilon}{\pi}\,\epsilon^{j-3/2}[R(\epsilon)-R^{jB}(\epsilon)]=-\frac{2(-1)^j}{2j-1}\sum_n(-\epsilon_n)^{j-1/2}. \tag{37}$$

We emphasize that $\delta^{jB}(\epsilon)$ and $R^{jB}(\epsilon)$ refer to the *sums* of the first j terms in the Born series for $\delta(\epsilon)$ and $R(\epsilon)$, respectively [Eqs. (2) and (30)]. An immediate and somewhat surprising consequence of (36), when there are no bound states, is that $\delta(\epsilon)$ must have values both greater than and less than the first Born approximation $\delta^{1B}(\epsilon)$; i.e., the integrated $[\delta(\epsilon)-\delta^{1B}(\epsilon)]$ is zero.

A somewhat more awkward form of the sum rules can be obtained by explicit integration of the Born terms, subtracting and adding the asymptotic limit necessary in each integral. Thus, by using Eqs. (3) and (12), we may show that the first two sum rules in each set become

$$\frac{2}{\pi}\int_0^\infty dk\,k\left(\delta(k)+\frac{1}{2k}U(0)\right)=-\sum_n\kappa_n^2+\tfrac{1}{4}V(0), \tag{38}$$

$$\frac{2}{\pi}\int_0^\infty dk\,k^3\left(\delta(k)+\frac{1}{2k}U(0)+\frac{1}{(2k)^3}[V'(0)+W(0)]\right)$$
$$=\frac{1}{2}\sum_n\kappa_n^4+\tfrac{1}{8}V^2(0)-\tfrac{1}{16}V''(0), \tag{39}$$

$$\frac{1}{\pi}\int_0^\infty dk\,R(k)=\sum_n\kappa_n+\tfrac{1}{4}U(0), \tag{40}$$

$$\frac{1}{\pi}\int_0^\infty dk\,k^2\left(R(k)-\frac{1}{(2k)^2}V(0)\right)$$
$$=-\frac{1}{3}\sum_n\kappa_n^3+\tfrac{1}{16}[V'(0)+W(0)], \tag{41}$$

where $U(0)$ and $W(0)$ are defined in Eq. (23). Equations (38) and (39) can be verified explicitly for cases where the phase shift and bound states are known for a given local potential. For a nonlocal potential, or for $l\neq 0$, the appropriate equation to verify is (36). For example, when $l\neq 0$, the quantity $\frac{1}{4}V(0)$ in (38) is in general multiplied by the coefficient

$$C_l=(-1)^l\left[\frac{1}{2}\left(\frac{(l+2)!}{l!}+\frac{l!}{(l-2)!}\right)-\frac{(l+1)!}{(l-1)!}\right].$$

Equation (38), which relates the potential at the origin and its integral over all space to the phase-shift and bound-state eigenvalues, has been previously obtained by Newton,[6] and the first sum rule is simplest to verify in this form[7] (see Appendix).

When no bound states are present, we know that the phase shift uniquely determines the potential. However, in the presence of bound states there can be a variety of different potentials with identical phase shifts and bound-state energies. Bargmann has shown,[8] by explicit construction of $f(k)$, that two of the Eckart potentials,

$$V_i(r, \sigma_i, \beta_i, \lambda_i) = -\sigma_i \lambda_i^2 \beta_i e^{-\lambda_i r}(1+\beta_i e^{-\lambda_i r})^{-2},$$
$$\lambda_i > 0, \quad \beta_i > -1 \tag{42}$$

will have the same $f(k)$, and hence the same $\delta(k)$, $R(k)$, and ϵ_n. Specifically, Bargmann shows that the potentials $V_1(r, 6, 1, \lambda_1)$ and $V_2(r, 2, 3, 2\lambda_1)$ have identical Jost functions, and he observes that these potentials have common values at the origin and common integrals over r [$V(0)$ and $U(0)$ equal], although their shapes are quite different.

The sum rules make clear the necessary relation between potential parameters. If $\delta(k)$, $R(k)$, and ϵ_n are identical for two potentials, then it is clear from our equations (38)–(41) that $V(0)$, $U(0)$, $V''(0)$, and $[W(0)+V'(0)]$ must also be identical for these two potentials. Applying these restrictions to the Eckart potential of the form (42), we find that (except for the trivial solution $\sigma_1 = \sigma_2$, $\beta_1 = \beta_2$, $\lambda_1 = \lambda_2$) we must have

$$\beta_2 = 4 - \beta_1, \quad \lambda_2 = [(5-\beta_1)/(1+\beta_1)]\lambda_1,$$
$$\sigma_2 = (\sigma_1\beta_1)/(4-\beta_1). \tag{43}$$

Thus, if $(\sigma_1, \beta_1, \lambda_1) = (6, 1, \lambda_1)$, we are required to have Bargmann's choice $(\sigma_2, \beta_2, \lambda_2) = (2, 3, 2\lambda_1)$ for the second potential.

I would like to thank Walter Kohn for many helpful comments and suggestions during the course of this analysis.

APPENDIX–TWO EXAMPLES

A classic example,[8] for which everything necessary is known and very simple, is the Eckart potential of Eq. (42), with $(\sigma, \beta, \lambda) = (2, \beta, 2\alpha)$. Thus, with $\hbar = 2\mu = 1$, we take

$$V(r) = -8\beta\alpha^2 e^{-2\alpha r}(1+\beta e^{-2\alpha r})^{-2}, \tag{A1}$$

for which there is one bound state for $l=0$ with $\epsilon_0 = -\kappa^2$, and

$$\kappa = \alpha(\beta-1)/(\beta+1), \tag{A2}$$

with the very simple Jost function

$$f(k) = (k+i\kappa)/(k-i\alpha), \tag{A3}$$

so that $R(k)$ and $\delta(k)$ are given by

$$R(k) = \ln\left(\frac{k^2+\kappa^2}{k^2+\alpha^2}\right)^{1/2};$$
$$\delta(k) = \tan^{-1}(\kappa/k) + \tan^{-1}(\alpha/k). \tag{A4}$$

For this potential,

$$V(0) = 2(\kappa^2 - \alpha^2),$$
$$V'(0) = 4\kappa(\kappa^2-\alpha^2),$$
$$V''(0) = 4(\kappa^2-\alpha^2)(3\kappa^2-\alpha^2), \tag{A5}$$
$$U(0) = \int_0^\infty dr\, V(r) = -2(\kappa+\alpha),$$
$$W(0) = \int_0^\infty dr\, V^2(r) = \tfrac{4}{3}(\kappa+\alpha)^2(2\alpha-\kappa),$$

where we have eliminated the parameter β by using (A2). Insertion of (A4) and (A5) in the sum rules (38)–(41) now gives

$$\frac{2}{\pi}\int_0^\infty dk\, k\left(\tan^{-1}\frac{\kappa}{k} + \tan^{-1}\frac{\alpha}{k} - \frac{\kappa+\alpha}{k}\right) = -\tfrac{1}{2}(\kappa^2+\alpha^2), \tag{A6}$$

$$\frac{2}{\pi}\int_0^\infty dk\, k^3\left(\tan^{-1}\frac{\kappa}{k} + \tan^{-1}\frac{\alpha}{k} - \frac{\kappa+\alpha}{k} + \frac{\kappa^3+\alpha^3}{3k^3}\right) = \tfrac{1}{4}(\kappa^4+\alpha^4), \tag{A7}$$

$$\frac{1}{\pi}\int_0^\infty dk\, \ln\left(\frac{k^2+\kappa^2}{k^2+\alpha^2}\right)^{1/2} = \tfrac{1}{2}(\kappa-\alpha), \tag{A8}$$

$$\frac{1}{\pi}\int_0^\infty dk\, k^2\left[\ln\left(\frac{k^2+\kappa^2}{k^2+\alpha^2}\right)^{1/2} - \frac{\kappa^2-\alpha^2}{2k^2}\right] = -\tfrac{1}{6}(\kappa^3-\alpha^3), \tag{A9}$$

and each of these is verified by elementary integration.

For a second example, consider the usual T matrix theory for the general nonlocal potential. The potential term in the Schrödinger equation becomes $\int d^3r' \langle \vec{r}|V|\vec{r}'\rangle \varphi(\vec{r}')$, and $\langle \vec{r}|V|\vec{r}'\rangle \Rightarrow V(r)\delta(\vec{r}-\vec{r}')$ takes us back to the local case. The off-shell T matrix for this interaction satisfies the equation

$$\langle \vec{k}|T(z)|\vec{k}'\rangle = \langle \vec{k}|V|\vec{k}'\rangle + \int \frac{d^3q}{(2\pi)^3}\langle \vec{k}|V|\vec{q}\rangle \times \left[1\Big/\left(z - \frac{\hbar^2 q^2}{2\mu}\right)\right]\langle \vec{q}|T(z)|\vec{k}'\rangle, \tag{A10}$$

for complex z, where

$$\langle \vec{k}|V|\vec{k}'\rangle = \int d^3r\, d^3r'\, e^{-i\vec{k}\cdot\vec{r}}\langle \vec{r}|V|\vec{r}'\rangle e^{i\vec{k}'\cdot\vec{r}'} \tag{A11}$$

is the Fourier transform of $\langle \vec{r}|V|\vec{r}'\rangle$.

The partial-wave expansion

$$\langle \vec{r}|V|\vec{r}'\rangle = \sum_{l,m} Y_l^m(\hat{r})Y_l^{m*}(\hat{r}')\langle r|V_l|r'\rangle \tag{A12}$$

results in

$$\langle \vec{k}|\, V \text{ or } T(z)|\vec{k}'\rangle = (4\pi)^2 \sum_{l,m} Y_l^m(\hat{k})Y_l^{m*}(\hat{k}')\langle k|\, V_l \text{ or } T_l(z)|k'\rangle, \tag{A13}$$

with

$$\langle k|\, V_l|k'\rangle = \int_0^\infty dr\,dr'\,r^2 j_l(kr)\langle r|\, V_l|r'\rangle r'^2 j_l(k'r') \tag{A14}$$

and

$$\langle k|T_l(z)|k'\rangle = \langle k|\, V_l|k'\rangle + \frac{2}{\pi}\int_0^\infty q^2 dq\left(\frac{\langle k|\, V_l|q\rangle}{z-\hbar^2 q^2/2\mu}\right)\langle q|T_l(z)|k'\rangle. \tag{A15}$$

Bound states $\epsilon_{nl}=z$ appear as poles on the negative real axis of the T matrix, while the full scattering amplitude is

$$f(\vec{k},\vec{k}') = -\frac{2\mu}{\hbar^2}\,\frac{1}{4\pi}\langle\vec{k}|\,T\left(\frac{\hbar^2 k'^2}{2\mu}+i\delta\right)|\vec{k}'\rangle$$

and

$$e^{i\delta_l(k)}\sin\delta_l(k) = -\frac{2\mu}{\hbar^2}\,k\,\langle k|T_l\left(\frac{\hbar^2 k^2}{2\mu}+i\delta\right)|k\rangle \tag{A16}$$

gives the phase shift. The first Born phase shift is given by

$$\delta_l^{1B}(k) = -(2\mu/\hbar^2)\,k\,\langle k|\, V_l|k\rangle.$$

The classic model problem in T-matrix theory is that of the separable potential $\langle r|\, V_l|r'\rangle = A_l f_l(r) f_l(r')$, a form which also quarantees separability in k space. The solution to (A15) can then be constructed explicitly. To make that solution even simpler, consider the cutoff attractive potential

$$\langle k|\, V|k'\rangle = -\frac{\hbar^2}{2\mu}\,\lambda\,\frac{1}{(kk')^{1/2}}\,\Theta(\bar{k}-k)\Theta(\bar{k}-k') \tag{A17}$$

for fixed l. Then

$$\delta^{1B}(\epsilon) = \lambda\Theta(\bar{\epsilon}-\epsilon),\quad \bar{\epsilon}\equiv\hbar^2\bar{k}^2/2\mu \tag{A18}$$

is the Born phase shift. From the (now trivial) solution to Eq. (A15), we then find the single bound state (λ positive only)

$$\epsilon_0 = -\frac{\bar{\epsilon}}{e^{\pi/\lambda}-1}, \tag{A19}$$

together with the phase shift [using (A16)],

$$\delta(\epsilon) = \tan^{-1}\left\{\lambda\Big/\left[1-\frac{\lambda}{\pi}\ln\left(\frac{\bar{\epsilon}}{\epsilon}-1\right)\right]\right\}\Theta(\bar{\epsilon}-\epsilon). \tag{A20}$$

The first sum rule [Eq. (36) with $j=1$] now reads

$$-\frac{\bar{\epsilon}}{e^{\pi/\lambda}-1} = \int_0^{\bar{\epsilon}}\frac{d\epsilon}{\pi}\left(\tan^{-1}\left\{1\Big/\left[1-\frac{\lambda}{\pi}\ln\left(\frac{\bar{\epsilon}}{\epsilon}-1\right)\right]\right\}-\lambda\right), \tag{A21}$$

and again this can be verified by direct integration.

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[1]Hereafter, $2\mu=\hbar=1$.

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