Perturbed Bound-State Poles in Potential Scattering. II

Y. S. Kim*

Department of Physics and Astronomy, University of Maryland, College Park, Maryland

AND

Kashyap V. Vasavada†

*Laboratory for Theoretical Studies, National Aeronautics and Space Administration,
Goddard Space Flight Center, Greenbelt, Maryland*

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The problem of maintaining the locality of the bound-state wave function is discussed in the S-matrix approach to the first-order energy shift. It is shown first that the nearby-singularity prescription in the Dashen-Frautschi formalism leads to the inclusion of unphysical terms coming from the nonlocal component of the wave function. It is pointed out that the infrared divergence of Dashen and Frautschi comes from this unphysical term. We then present an alternative method based on the Gelfand-Levitan formalism on the inverse-scattering problem. We discuss here an approximate solution of the Gelfand-Levitan equation that leads to a localized bound-state wave function. It is pointed out that this wave function gives the first-order energy shift without the infrared difficulty. Using soluble exponential potentials, we discuss numerical accuracies of this approach.

I. INTRODUCTION

IN a previous paper,[1] it was shown that the use of the Dashen-Frautschi[2] formula necessarily involves the solution of the unperturbed problem, and therefore the formula does not have general applicability. It was shown in the case of a soluble square-well potential that the disappearance of the infrared divergence is due to the fact that the bound-state wave function is localized (normalizable).

In applications of the Dashen-Frautschi formula, the solution of the unperturbed problem will in most cases have to go through various approximations. Although much effort has been made to understand the nature of the bound state in the past years, it still seems to be of prime importance to realize that the bound-state wave function is localized. And, it still seems to be essential to maintain the locality at every stage of approximation. In this paper we discuss first this locality problem in approximate evaluation of the Dashen-Frautschi dispersion integral. It is shown that the nearby-singularity approximation leads in general to a violation of the locality which is responsible for infrared difficulties.

As an alternative approach we suggest the use of the Gelfand-Levitan formalism on the inverse scattering problem.[3-6] We discuss here an approximate solution

of the Gelfand-Levitan equation which leads to a localized bound-state wave function. By taking the expectation value of the perturbing potential, one can then obtain the first-order energy shift without infrared difficulty.

In this approximation scheme, the bound-state wave function is constructed from the three bound-state parameters, namely, the binding energy, the residue of the bound-state pole, and the first derivative of the D function at the binding energy. Using soluble exponential potentials, we then compare the results of the present approximation scheme with the exact answers. Throughout the entire paper we restrict ourselves to the S-wave solution since the generalization to other partial waves seems straightforward.

In Sec. II, we discuss ambiguities in the approximate evaluation of the Dashen-Frautschi dispersion integral. In Sec. III, the Gelfand-Levitan formalism is outlined. We discuss then a one-pole-type approximation that leads to a localized bound-state wave function. In Sec. IV, we use soluble exponential potentials to discuss numerical accuracies of the present approximation scheme.

II. AMBIGUITIES IN THE DASHEN-FRAUTSCHI FORMALISM

Since the solution of the unperturbed problem will in general have to go through approximations, we regard these approximations as integral parts of the Dashen-Frautschi formalism. We show in this section that the nearby-singularity approximation leads in this case to a violation of the locality of the bound-state wave function.

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It is known in the previous paper[1] that the first-order energy shift δx_0 takes the form

$$\delta x_0 = -\frac{1}{R}\frac{1}{[D'(-x_0)]^2}\frac{1}{2\pi i}\int_C \frac{D^2(z)\delta A(z)dz}{z+x_0}. \quad (1)$$

We use here the notation of Ref. 1 except for $D(x)$, which stands here for the denominator Jost function. The contour C encloses the original pole at $z=-x_0$ and the perturbed pole at $x=-(x_0+\delta x_0)$. See Fig. 1. We assume that $D(z)$ and $\delta A(z)$ are such that the integrand decreases faster than z^{-1} at infinity.

Before attacking the problem of localized wave packet we first observe the following ambiguity in the approximation of retaining only nearby singularities.

Let us consider a function $g(z)$, which is analytic in the region enclosed by the contour C and decreases faster than z^{-1} at infinity. It is not difficult to construct such a function. We can consider, for example,

$$g(z) = A(a-b)/(z-a)(z-b), \quad (2)$$

where both a and b are outside the contour C, but a is near the bound-state poles and b is far away (see Fig. 1). A is an arbitrary constant. Since $g(z)$ is analytic in the region enclosed by C,

$$\delta x_0 = -\frac{1}{R}\frac{1}{[D'(-x_0)]^2}\frac{1}{2\pi i}\int_C \left[\frac{D^2(z)\delta A(z)}{z+x_0}+g(z)\right]dz. \quad (3)$$

As we have noted in the previous paper, the contour C can enclose all other singularities in the z plane, clockwise. We denote this contour by C'. Now, it is not difficult to see that

$$\int_C g(z)dz = \int_{C'} g(z)dz = 0. \quad (4)$$

The contour C', in this case, encloses both the nearby and faraway poles of $g(z)$. But according to the nearby singularity prescription, we are led to retain the pole at $z=a$ and discard that at $z=b$. Then we end up with the following ambiguity:

$$\delta x_0 = \delta x_0 - (A/R)[D'(-x_0)]^{-2}, \quad (5)$$

where A is still an arbitrary constant.

Even in general cases where $g(z)$ has other complicated singularities outside the contour C, the failure to enclose all those singularities leads to an addition of a nonzero number.

The above example calls for the removal of all the terms from the integrand of Eq. (3) whose over-all contribution to δx_0 is zero before employing any approximation method in evaluating the integral along the contour C'.

The next question to ask is whether there are such terms in Eq. (3) besides $g(z)$ which should not be there. The answer seems to be "yes". We recall from Ref. 1
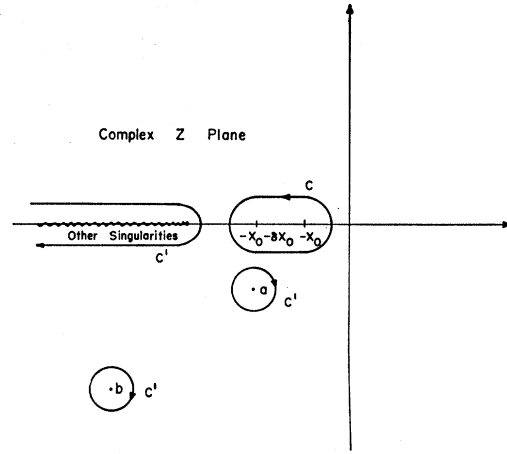

FIG. 1. Singularities and contours in complex energy plane.

that the nontrivial part of the integrand of Eq. (1) takes the form

$$D^2(x)\delta A(x) = (1/2ik)\{\delta f^{(+)}(x)f_0^{(-)}(x) - \delta f^{(-)}(x)f_0^{(+)}(x)\},$$

where

$$f_0^{(\mp)}(x) = f_0(\mp k) = 1+\frac{1}{k}\int_0^\infty \exp(\pm ikr)V_0(r)\phi(r)dr,$$

$$\delta f^{(\mp)}(x) = \frac{1}{k}\int_0^\infty \exp(\pm ikr)\delta V(r)\phi(r)dr$$

$$+\frac{1}{k}\int_0^\infty dr\,\exp(\pm ikr)V_0(r)\int_0^r I(r,r')\delta V(r')\phi(r')dr'.$$

Here $I(r,r')$ is the full Green's function for the unperturbed problem.[7] Now, the unperturbed wave function $\phi(r)$ can be written as[8]

$$\phi(r) = \phi_b(r)+\phi_i(r), \quad (6)$$

where $\phi_b(r)$ is the part that reduces to the bound-state wave function at the binding energy, and $\phi_i(r)$ is the part that vanishes at the same energy. $\phi_b(r)$ and $\phi_i(r)$ have the outgoing- and incoming-wave boundary conditions, respectively. We then write the integrand as

$$D^2(z)\delta A(z) = [D^2(z)\delta A(z)]_b+[D^2(z)\delta A(z)]_i, \quad (7)$$

where $[D^2(z)\delta A(z)]_i$ vanishes at $z=-x_0$ because of the disappearance of $\phi_i(r)$. Therefore

$$\int_C \frac{[D^2(z)\delta A(z)]_i}{z+x_0}dz = \int_{C'}\frac{[D^2(z)\delta A(z)]_i}{(z+x_0)}dz = 0. \quad (8)$$

[7] This Green's function satisfies the differential equation

$$(d^2/dr'^2)I(r,r')+[k^2-V_0(r')]I(r,r') = \delta(r-r').$$

There is a notational error for this quantity in the previous paper (see Ref. 1). This error, however, does not affect the conclusions contained therein.

[8] See, for instance, Eq. (22) of the present paper.

Thus, in order to guarantee the locality we should remove this term before making any approximations along the contour C'. Or, equivalently, we should estimate the contribution from this term before attaching any significance to the numerical result.

In the calculation of the proton-neutron mass difference by Dashen and Frautschi,[2] for instance, the infrared divergence, which should not appear in the problem of a localized bound-state wave function, comes from this incoming-wave component.

In the following sections, we shall discuss an approximation method that guarantees the locality of the bound-state wave function.

III. APPROXIMATION METHOD BASED ON THE GELFAND-LEVITAN FORMALISM

In this section we first outline the Gelfand-Levitan formalism on the inverse scattering problem.[3] This formalism enables us to construct wave functions from the scattering phase shifts and bound-state parameters for a given orbital angular momentum. (We are of course interested here in the S wave.) Then we discuss a one-pole-type approximation which gives a localized bound-state wave function.

Let us represent the regular solution of the Schrödinger equation as

$$\phi(r) = \sin kr + \int_0^r K(r,r') \sin kr' dr'. \qquad (9)$$

We already know one form of $K(r,r')$, that is,

$$K(r,r') = I(r,r') V_0(r').$$

But it is easy to see that the $K(r,r')$ function is not necessarily unique. One can in particular choose an energy-independent $K(r,r')$ function which satisfies the differential equation

$$\frac{\partial^2 K(r,r')}{\partial r^2} - \frac{\partial^2 K(r,r')}{\partial r'^2} = V_0(r) K(r,r'),$$

with the following boundary conditions[3]:

$$K(r,0) = 0,$$
$$dK(r,r)/dr = \tfrac{1}{2} V_0(r). \qquad (10)$$

Next, we consider the following spectral functions:

$$d\rho(x)/dx = C\delta(x+x_0), \qquad x<0,$$
$$d\rho(x)/dx = k/\pi f_0(k) f_0(-k), \quad x>0, \qquad (11)$$

with

$$\frac{1}{C} = \left[\frac{1}{x} \int_0^\infty \phi^2(r) dr \right]_{x \pm -x_0}, \qquad (12)$$

and

$$\frac{d\rho_0(x)}{dx} = 0 \quad x<0, \qquad \frac{d\rho_0(x)}{dx} = \frac{k}{\pi}, \quad x>0,$$

and consider also the function $g(s,t)$ determined by

$$g(s,t) = \int_{-\infty}^\infty \left(\frac{\sin ks}{k}\right)\left(\frac{\sin kt}{k}\right) d[\rho(x) - \rho_0(x)]. \qquad (13)$$

We have assumed that there is only one bound state. The spectral function $\rho_0(x)$ corresponds to that of the plane wave.

The $K(r,r')$ function then satisfies the following integral equation:

$$K(r,r') + g(r,r') + \int_0^r dt\, K(r,t) g(r',t) = 0. \qquad (14)$$

Therefore, if the denominator Jost function $f_0(-k)$ and the bound-state parameters x_0 and C are given, we can determine $g(s,t)$ by evaluating the integral of Eq. (13), $K(r,r')$ by solving the integral equation of Eq. (14), $\phi(r)$ by Eq. (9), and $V_0(r)$ by Eq. (10).

We now adopt the following approximation scheme. For the negative energy we take the exact spectral function

$$d\rho(x)/dx = C\delta(x+x_0), \quad x<0, \qquad (15)$$

and for the continuous positive-energy spectrum we take the plane-wave approximation

$$d\rho(x)/dx = d\rho_0(x)/dx, \quad x>0. \qquad (16)$$

Then, as was pointed out in Ref. 3, the Gelfand-Levitan integral equation can be solved in the following simple way. We observe first that the $g(r,s)$ function takes the simple form

$$g(r,s) = C \sinh \alpha r \sinh \alpha s / x_0, \qquad (17)$$

where $\alpha = (x_0)^{1/2}$. The integral equation of Eq. (14) becomes

$$C[\sinh \alpha r \sinh \alpha s/x_0] + K(r,s)$$
$$+ C \int_0^r dt\, K(r,t) \left[\frac{\sinh \alpha s \sinh \alpha t}{x_0}\right] = 0. \qquad (18)$$

For this integral equation we have the following solution.

$$K(r,s) = -C[\sinh \alpha r \sinh \alpha s/x_0]$$
$$\times \left[1 + \frac{C}{x_0} \int_0^r \sinh^2 \alpha t\, dt\right]^{-1}, \qquad (19)$$

which gives the wave function

$$\phi(r) = \sin kr - C[\sinh \alpha r]\left[1 + \frac{C}{x_0} \int_0^r \sinh^2 \alpha t\, dt\right]^{-1}$$
$$\times \int_0^r dt \frac{\sinh \alpha t \sin kt}{x_0}. \qquad (20)$$

At the binding energy $k=i\alpha$, the above wave function becomes

$$\phi_b(r)=i\left[1+\frac{C}{x_0}\int_0^r \sinh^2\alpha t\, dt\right]^{-1}\sinh\alpha r. \quad (21)$$

We now see that this wave function decreases as $\exp(-\alpha r)$ for large r and that the locality of the bound-state wave function is manifestly maintained in this approximation. As we can see by integration,

$$\int_0^\infty dr \sinh^2\alpha r\left[1+\frac{C}{x_0}\int_0^r \sinh^2\alpha t dt\right]^{-2}=\frac{x_0}{C},$$

the approximate wave function of Eq. (21) satisfies the normalization condition of Eq. (12).

Our remaining task is to relate the constant C to the bound-state parameters. For this purpose we follow the steps outlined in Ref. 5. We first observe that the regular solution $\phi(r)$ can be written as a linear combination of the Jost solutions.

$$\phi(r)=(1/2i)[f_0(k)f_0(r,-k)-f_0(-k)f_0(r,k)]. \quad (22)$$

The Jost solutions $f_0(r,-k)$ and $f_0(r,k)$ satisfy outgoing- and incoming-wave boundary conditions, respectively. Furthermore

$$f_0(0,\pm k)=f_0(\pm k). \quad (23)$$

Now at the binding energy $k=i\alpha$, the above equation reduces to

$$\phi_b(r)=(1/2i)f_0(i\alpha)f_0(r,-i\alpha). \quad (24)$$

We note here that $\phi_b(r)$ is proportional to $f_0(r,-i\alpha)$ and $\phi_b'(0)=i\alpha$. Thus

$$\phi_b=[i\alpha/f_0'(0,-i\alpha)]f_0(r,-i\alpha). \quad (25)$$

Multiplying Eq. (24) by Eq. (26), one obtains

$$[\phi_b(r)]^2=\frac{\alpha f_0(i\alpha)}{2f_0'(0,-i\alpha)}[f_0(r,-i\alpha)]^2. \quad (26)$$

Next, we write the Schrödinger equation for the Jost solution $f_0(r,-k)$,

$$-f_0''(r,-k)+V_0(r)f_0(r,-k)=k^2f_0(r,-k),$$

and differentiate the above equation with respect to k. Then

$$-\dot{f}_0''(r,-k)+V_0(r)\dot{f}_0(r,-k)$$
$$=2kf_0(r,-k)+k^2\dot{f}(r,-k),$$

where

$$\dot{f}_0(r,-k)=(\partial/\partial k)f_0(r,-k).$$

Applying a canonical procedure to the above two equations and integrating over r at the binding energy $k=i\alpha$, we arrive at

$$2i\alpha\int_0^\infty f_0^2(r,-i\alpha)dr=-\dot{f}_0(0,-i\alpha)f'(0,-i\alpha). \quad (27)$$

By Eq. (26) and the relation

$$\dot{f}_0(0,-i\alpha)=2i\alpha D'(-x_0),$$

Eq. (17) becomes

$$\frac{1}{C}=\frac{1}{x_0}\int_0^\infty |\phi_b(r)|^2 dr=\frac{1}{2\alpha}f_0(i\alpha)D'(-x_0). \quad (28)$$

On the other hand, $f_0(i\alpha)$ is related to the residue of the bound-state pole R by

$$f_0(i\alpha)=-2\alpha D'(-x_0)R. \quad (29)$$

Therefore

$$1/C=-R[D'(-x_0)]^2. \quad (30)$$

We have shown above that the constant C can be determined by the three bound-state parameters R, x_0, and $D'(-x_0)$. Now, the determination of the wave function is complete. One can then obtain the first-order energy shift by taking the expectation value of the perturbing potential:

$$\delta x_0=-\frac{C}{x_0}\int_0^\infty |\phi(r)|^2\delta V(r)dr. \quad (31)$$

Finally, let us make a few remarks about the nature of the present approximation. As was pointed out in the previous paper, the Born approximation is not expected to be valid along the continuous energy spectrum. Accordingly, we are not ready here to assert that the wave function of Eq. (21) is very accurate. However, this wave function satisfies the correct boundary conditions at $r=0$ and $r=\infty$. Furthermore, our experience in variational method assures us that the energy shift of Eq. (31) is not too sensitive to the exact shape of the wave function. Thus the numerical accuracy of Eq. (31) depends crucially on the position of the peak of the wave function, which is in turn determined by the parameter C. We shall discuss this point in the following section. Although it is another crude approximation, the present method is a definite improvement over that of Dashen and Frautschi, and may perhaps be the first step toward a more complete and satisfactory procedure.

IV. NUMERICAL ANALYSIS

In order to investigate numerical accuracies of the present approximation scheme, we discuss here soluble exponential potentials.

First, for the exponential potential

$$V_0(r)=-V_0\exp(-mr), \quad V_0>0, \quad (32)$$

we solve the Schrödinger equation and obtain the exact wave function and the Jost functions. The parameters m and V_0 are chosen in such a way that this potential will give only one bound state. We then calculate the bound-state parameters x_0, R, and $D'(-x_0)$ and con-
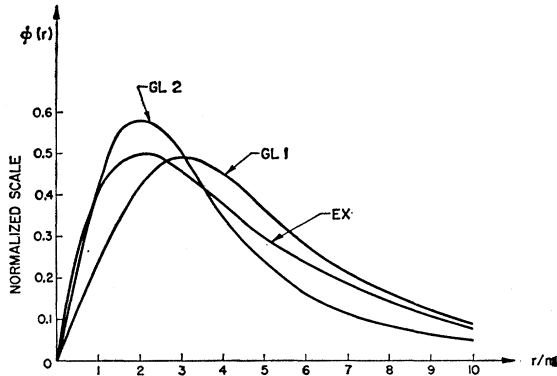
FIG. 2. Exact (EX), approximate (GL1), and adjusted (GL2) wave functions. These curves are drawn in a normalized scale for $V_0 = 2.47m^2$, $\alpha = 0.25m$, and $m = 1$.
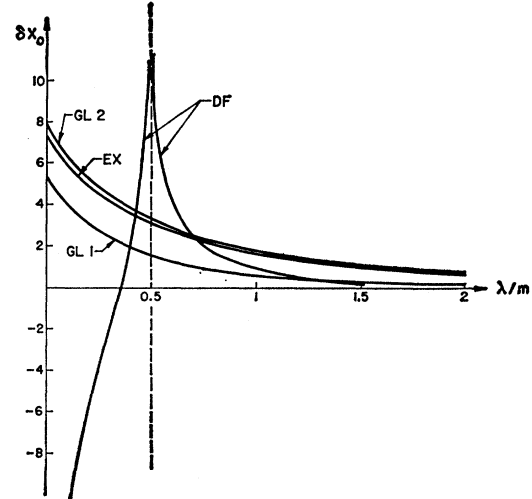

FIG. 3. Exact (EX), approximate (GL1), and adjusted (GL2) values for the energy shift δx_0. δx_0 is measured in the unit of (gx_0/m). These curves were also plotted for $V_0 = 2.47m^2$, $\alpha = 0.25m$, and $m = 1$. The Dashen-Frautschi (Born approximation) curve (DF) was calculated from Eqs. (19) and (20) of Ref. 1. The singularity at $\lambda = 2\alpha$ (0.5 in this case) is caused by the fact that the contour C is pinched by the pole $z = -x_0$ and the approaching singularity of the perturbed amplitude $A'(z)$ at $z = (\frac{1}{2}\lambda)^2$.

struct the approximate wave function according to the procedure described in the preceding section. Both the exact and approximate wave functions are plotted in Fig. 2. It is seen there that the approximate wave function takes the maximum value at a larger value of r than the exact wave function. This is, of course, due to the Born approximation of the continuous positive-energy spectrum.

In order to study a possible wider applicability of the attractive functional form of Eq. (21), we replace the constant C by a larger value $\bar{C}$ in such a way that the new approximate wave function will have its peak at the same place as the exact solution. We call this new approximate form the adjusted wave function. Then, the inclusion of the continuous positive-energy spectrum will effectively correspond to this adjustment.

Next, we introduce a small perturbing potential of the form

$$\delta V(r) = -(g/r) \exp(-\lambda r), \qquad (33)$$

TABLE I. The ratio $(r_{max}{}^{GL1})/(r_{max}{}^{EX})$ is given for several different combinations of V_0 and m. $(\delta x_0)_{EX}$ and $(\delta x_0)_{GL1}$ are also given at $\lambda = 0$ (again in units of $gx_0 m^{-1}$). The binding energy is fixed at $(x_0)^{1/2} = 0.25$.

V_0	m	$(r_{max}{}^{GL1})/(r_{max}{}^{EX})$	$(\delta x_0)_{EX}$	$(\delta x_0)_{GL1}$
2.47	1	1.54	7.36	5.32
1.76	0.8	1.71	6.65	4.30
1.17	0.6	2.21	5.84	2.92
0.69	0.4	2.06	4.87	2.54

and take the expectation values

$$\delta x_0 = -(\Phi, \delta V(r)\Phi)$$

using the exact, approximate, and adjusted wave functions. As is shown in Fig. 3, the energy shift for the adjusted wave function is very close to the exact value. The energy shift corresponding to the approximate wave function differs by a factor of 1.5–2.5 for $0 \leq \lambda \leq m$.

As is indicated in Table I, we would expect for all range-depth ratios that the approximate energy shift is smaller than the exact value roughly by a factor of 2. It would be extremely interesting to see whether one can improve this accuracy by including contributions from the positive-energy spectrum.

ACKNOWLEDGMENTS