Perturbative Scattering Phase Shifts in One-Dimension:
Closed-form results

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Abstract

A simple closed form expression is obtained for the scattering phase shift perturbatively to any given order in effective one-dimensional problems. The result is a hierarchical scheme, expressible in quadratures, requiring only knowledge of the zeroth order solution and the perturbation potential.

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Since most quantum mechanical problems cannot be solved exactly, perturbation theory is a useful tool. Standard perturbation theory relies on the use of the Green function or the spectral summation over the intermediate states. Variants of the standard perturbation theory were introduced by Schrödinger [1], Podolsky [2], Sternheimer [3] and Dalgarno and Lewis [4]. Originally, the Dalgarno–Lewis method was introduced as a means of calculating sum rules. Another useful variation of perturbation theory was introduced by Wentzel [3] and later by Price [5] and by Polikanov [6]. However, this method was overlooked until its rediscovery by Aharonov and Au [8] and more or less about the same time by Turbiner [9]. This method has now come to be widely known as “Logarithmic Perturbation Theory” or LPT for short.

LPT has many advantages. In one-dimensional problems, it becomes possible to obtain perturbative solutions to all order in a hierarchical scheme, for the energies and wave functions for the bound states [7–9] and for the phase shifts in scattering states [10]. A few modifications of LPT to handle the presence of zeros in the wave functions in excited bound states were given by Au et al. [11].

In three-dimensions, the zeros of excited bound states appear as nodal surfaces. A variation of LPT to address this difficulty was given by Au [12]. In this method, the bound state wave function is written as \( F \exp(-G) \), and a perturbation expansion is carried out only on \( F \). In the absence of any nodes, the zeroth order function \( F_0 \) can be set equal to unity as the information on the unperturbed wave function can be totally absorbed into \( G \).

This is then equivalent to writing the perturbed wave function as a scalar function times the unperturbed wave function. When confined only to the first order correction, this method yields the equivalent of the Dalgarno–Lewis method. Henceforth, we refer this method of writing the perturbed wave function as a product of the unperturbed wave function and a scalar function as the Dalgarno–Lewis Perturbation Theory (DLPT for short). The difficulties associated with the presence of zeros in the wave function when using DLPT are also discussed in reference [12].

In Eq. (1.25) of Ref. [12], the hierarchical structure of DLPT is displayed explicitly.
for a multidimensional system. For one-dimensional system, this hierarchy can be trivially integrated twice to give the perturbative solutions in quadrature to reproduce the results of Kim and Sukhatme [13]. Recently, Nandi et. al. [14] applied DLPT to the scattering phase shifts in one-dimension and rederived the results of Au et. al. [10] obtained via LPT.

The equivalence of DLPT and LPT was first discussed by Au and Aharonov [15], and  subsequently by many other authors [16]. In the absence of nodal difficulties, this equivalence can be expected simply from the well defined mapping between the wave function and its logarithm. From the Wronskian conditions, one can easily see that the scattering wave function in one-dimension with the expected asymptotic behavior is free from zeros and hence its logarithm is regular. It follows from the above that LPT and DLPT should produce the same perturbative scattering phase shifts.

In this letter, we apply DLPT to the scattering problem in one-dimension and derive a closed form expression for the perturbative correction to the phase shift to any order. This is an improvement over earlier works where the calculational procedures were laid out, but no such closed form results were available.

The unperturbed wave function \( \psi_0(x) \) is given by the Schroedinger equation
\[
-\frac{1}{2}\psi''_0(x) + V(x)\psi_0(x) = \frac{1}{2}k^2\psi_0(x),
\]
for a particle with energy \( \frac{1}{2}k^2 \). In our notation \( \hbar = m = 1 \). Similarly, \( \psi(x) \), the perturbed wave function, is given by
\[
-\frac{1}{2}\psi''(x) + V(x)\psi(x) + \lambda U(x)\psi(x) = \frac{1}{2}k^2\psi(x),
\]
with \( \lambda U(x) \) the perturbing potential. Both Schrodinger equations are subjected to the boundary condition at infinity.
\[
\psi_0(x) = \psi(x) = \exp(-ikx), \quad \text{as} \quad x \to \infty.
\]
Then the phase shifts are defined as their respective phases at \( x = 0 \).
\[
\exp(-2i\delta_0) = \frac{\psi^*_0(0)}{\psi_0(0)}, \quad \exp(-2i\delta) = \frac{\psi^*(0)}{\psi(0)}.
\]
The Wronskian condition,
\[ \psi_0(x)\psi_0''(x) - \psi_0^*(x)\psi_0'(x) = 2ik, \]  
(5)
prevents \( \psi_0(x) \) from having any node, and ensures that the ratio
\[ f(x) = \psi(x)/\psi_0(x) \]  
(6)
is well-defined. The perturbative correction, in terms of \( f(x) \), is given by
\[ \psi_0(x)f''(x) + \lambda\psi_0'(x)f'(x) - 2\lambda U(x)\psi_0(x)f(x) = 0. \]  
(7)
where one can perform a perturbative expansion on \( f(x) \),
\[ f(x) = f_0(x) + \lambda f_1(x) + \lambda^2 f_2(x) + \ldots, \]  
(8)
with \( f_0(x) \equiv 1 \) identically. Performing this expansion on Eq. (7), one gets to zeroth order,
\[ \lambda^0 : \quad \psi_0(x)f_0''(x) + 2\psi_0'(x)f_0'(x) = 0 \]  
(9a)
and to the \( n \)th order,
\[ \lambda^n : \quad \psi_0(x)f_n''(x) + 2\psi_0'(x)f_n'(x) = 2U(x)\psi_0(x)f_{n-1}(x), \quad n \geq 1. \]  
(9b)
The first one vanishes identically as \( f_0(x) \equiv 1 \), while the second one can be recasted in the form
\[ (\psi_0^2(x)f_n'(x))' = 2U(x)\psi_0^2(x)f_{n-1}(x), \]  
(10)
which can be integrated from infinity to give in a hierarchical scheme:
\[ f_n(x) = \int_x^\infty dy \frac{1}{\psi_0^2(y)} \int_y^\infty dz 2U(z)\psi_0^2(z) f_{n-1}(z). \]  
(11)
As a result, one can apply it recursively to obtain \( f_n(x) \) of arbitrarily high order.

Relation (11) can be solved in terms of the zeroth order information. The Wronskian condition (5) can be rewritten as
\[ \psi_0^2(x)\left(\frac{\psi_0^*(x)}{\psi_0(x)}\right)' = \rho(x)q'(x) = 2ik, \]  
(12)
where the definitions of \( \rho(x) \) and \( q(x) \) are identical to that in Ref. \[10,11\].

\[
\rho(x) = \psi_0^2(x), \quad q(x) = \frac{\psi_0^*(x)}{\psi_0(x)} - \frac{\psi_0^*(0)}{\psi_0(0)}.
\] (13)

Then relation (11) becomes, upon using these two relations:

\[
f_n(x) = \int_x^\infty dz \ 2U(z) \ \rho(z) \ f_{n-1}(z) \ \int_x^z dy \ \frac{1}{\rho(y)}
= \frac{1}{ik} \int_x^\infty dz \ 2U(z) \ \rho(z) \ f_{n-1}(z) (q(z) - q(x)) = J[f_{n-1}](x),
\] (14)

with

\[
J[g](x) = \frac{1}{ik} \int_x^\infty dz \ 2U(z) \ \rho(z) (q(z) - q(x)) \ g(z).
\] (15)

So one can apply Eq. (14) iteratively and gets

\[
f_n(x) = \underbrace{J[J[\cdots J[1] \cdots]}}_{\text{n times}}(x).
\] (16)

After obtaining the expressions for \( f_n(x) \), the only remaining task is to express \( \delta_n \) in terms of these \( f_n \)'s. Recall that the phase shift corrections \( \delta_n \) are naturally defined by

\[
\delta = \delta_0 + \lambda \delta_1 + \lambda^2 \delta_2 + \cdots.
\] (17)

From the definitions of \( f(x) \) and \( \delta \), it is easy to see that

\[
\delta - \delta_0 = \text{Im} \ \log f(0).
\] (18)

Performing an expansion in powers of \( \lambda \), one can express \( \delta_n \) as a function of the \( n \)-th derivative of \( \log f(0) \),

\[
\delta_n = \text{Im} \ \frac{1}{n!} \left( \frac{d^n}{d\lambda^n} \log f(0) \right)_{\lambda=0}.
\] (19)

Now we have obtained the correction of \( f(x) \) to arbitrary order by Eq. (16), and expressed \( \delta_n \) in terms of \( f(0) \) by Eq. (19). One only need to combine these two pieces of knowledge to get a closed form expression of \( \delta_n \). This can be most conveniently achieved by the lemma below.
Lemma: If $g = g(f(\lambda))$ and $f(\lambda) = 1 + \lambda f_1 + \lambda^2 f_2 + \ldots$, then
\[
\frac{1}{n!} \left. \frac{d^n g}{d\lambda^n} \right|_{\lambda=0} = \sum_{\{i_p\}_n} \frac{1}{i_1!i_2! \ldots i_n!} g^{(j)} f_{i_1} f_{i_2} \ldots f_{i_n},
\]
where $\{i_p\}_n = \{(i_1, i_2, \ldots, i_n)\}$ is the set of $n$ non-negative integers satisfying
\[
\sum_{p=1}^n p i_p = n,
\]
$j$ is defined by $j = \sum_{p=1}^n i_p$, and $g^{(j)} = \left. \frac{d^j g}{df^j} \right|_{f=1}$.

The proof is straightforward, just perform the double Taylor expansion and collect terms of the same order in $\lambda$. For our purpose, $g = \log f$ and hence $g^{(j)} = (-1)^{j-1}(j - 1)!$. This leads us to the central result of this paper,
\[
\delta_n = \text{Im} \sum_{\{i_p\}_n} (-1)^{j-1} \frac{(j - 1)!}{i_1!i_2! \ldots i_n!} f_{i_1} f_{i_2} \ldots f_{i_n},
\]
where $f_n \equiv f_n(0)$ is given in Eq. (16).

Physical results should be independent of which perturbative scheme one chooses to work with, and the $\delta_n$ obtained above should agree with the standard Rayleigh–Schroedinger results as well as those from LPT. The agreement of LPT with the Rayleigh–Schroedinger theory on phase shifts was demonstrated explicitly in Ref. [10] up to order $\lambda^4$. We shall demonstrate below that Eq. (22) also reproduces exactly the same expressions for $\delta_n$ given by LPT.

For any given $n$, we are going to enumerate all the non-negative integer $n$-plet $(i_1, i_2, \ldots, i_n)$ which satisfy the condition $\sum_{p=1}^n p i_p = n$. Each of these $n$-plet is going to give a term in Eq. (22). The integral expressions for $f_n(0)$’s are substituted in, and the rest are just simplifications.

For $n = 1$, there is only one element in $\{i_p\}$, namely (1). Then Eq. (22) gives
\[
\delta_1 = \text{Im} \int_0^\infty dx U(x) \rho(x) q(x) = -\frac{1}{k} \text{Re} \int_0^\infty dx U(x) \rho(x) q(x).
\]
Note that \( q(0) = 0 \). This agrees with the LPT result (Eq. (26) in Ref. [10]). In the notation defined in Ref. [10], with

\[
I[F_1, F_2, \ldots, F_n] = \int_0^\infty dx_1 \int_0^\infty dx_2 \int_0^\infty dx_n F_1(x_1) F_2(x_2) \cdots F_n(x_n),
\]

the result is

\[
\delta_1 = -\frac{1}{k} \text{Re} I[U \rho q].
\]  

This notation will facilitate the presentation of higher order results.

Less trivial is the case \( n = 2 \), where \((i_1, i_2)\) can be either \((0, 1)\) or \((2, 0)\). Eq. (21) then gives

\[
\delta_2 = \text{Im}(f_2 - \frac{1}{2} f_1^2).
\]  

In particular,

\[
f_2 = \frac{-1}{k^2} \int_0^\infty dx \ U(x) \ \rho(x) \ q(x) \ \int_x^\infty dy \ U(y) \ \rho(y) \ (q(y) - q(x))
\]

\[
= \frac{1}{k^2} I[U \rho q^2, U \rho] - \frac{1}{k^2} I[U \rho q, U \rho]
\]

\[
= \frac{1}{k^2} I[U \rho q^2, U \rho] + \frac{1}{2} f_1^2.
\]

As a result, we have reproduced Eq. (31) in Ref. [10]:

\[
\delta_2 = \frac{1}{k^2} \text{Im} I[U \rho q^2, U \rho].
\]  

The \( n = 3 \) is more cumbersome but still straightforward. In this case \((i_1, i_2, i_3)\) can be \((0, 0, 1), (1, 1, 0)\) and \((3, 0, 0)\). Hence

\[
\delta_3 = \text{Im}(f_3 - f_1 f_2 + \frac{1}{3} f_1^3).
\]  

After expanding out the \( f_n \)'s and some changes of variables, the result can be casted into the form

\[
\delta_3 = \frac{2}{k^3} \text{Re} I[U \rho q^2, U \rho q, U \rho],
\]
which has been reported in Eq. (33) of Ref. [10].

Similar exercises can be done with even higher \( n \). We do not think, however, that it is instructive to present those higher order calculations in full details. We just want to report that the \( \delta_4 \) expression also agrees with that from LPT. The possible \((i_1, i_2, i_3, i_4)\)'s are \( (0, 0, 0, 1), (1, 0, 1, 0), (0, 2, 0, 0), (2, 1, 0, 0) \) and \( (4, 0, 0, 0) \). Note that the number of elements in \( \{i_p\}_n \) is increasing faster than \( n \).

The central result of this article is Eq. (22), which is a closed form expression for \( \delta_n \), obtained for the first time, and expressible in terms of only zeroth order and on-shell informations. We have also explicitly checked that the results for \( n \leq 4 \) agree with those from LPT. Admittedly, the results are still not as simple as one would like to see. There are two sources of complexity of the results. Firstly, the cardinality of \( \{i_p\}_n \) is growing with \( n \). It is easy to see that combinatorically this is the same as the number of inequivalent irreducible representations of the symmetric group \( S_n \) [17]. Graphically, this is equal to the number of ways of drawing different Young diagrams with \( n \) boxes. The other complication is that each \( f_n \), expressed as iterated \( J[\cdot\cdot] \)'s, breaks down to many terms of the form \( I[\cdot\cdot] \)'s. As a result, we expect the higher order results to grow more and more messy.

Still, this drawback is compensated by another nice feature of the scheme, namely the freedom to choose the unperturbed system. Since only on-shell information is needed in our scheme, it is much easier to find a “unperturbed” state which approximates the exact system than in the case of the Rayleigh–Schrodinger scheme, in which off-shell information is also needed and one needs to solve the “unperturbed” system completely. As discussed in Ref. [10], one expects \( \delta_n \) converges quickly as long as “Levinson criterion” (the unperturbed and perturbed system should have the same number of bound states) is satisfied. Hence the first several terms in the perturbation series should suffice to give a good approximation of the exact \( \delta \), and the higher order terms are seldom needed in practice.

In conclusion, we have obtained the perturbative correction to the scattering phase shift of any effectively one-dimensional Schrodinger problem. The result can be expressed in closed form and only on-shell information is needed. With a suitable choice of the “un-
perturbed” system, the perturbation series converges rapidly. We have also demonstrated explicitly that our results agree with the conventional LPT results up to the fourth order in the expansion series.

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