Simple applications of fundamental solution method in 1D quantum mechanics
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Abstract

A method of fundamental solutions has been used to show its effectiveness in solving some well known problems of 1D quantum mechanics (barrier penetrations, over-barrier reflections, resonance states), i.e. those in which we look for exponentially small contributions to semiclassical expansions for considered quantities. Its usefulness for adiabatic transitions in two energy level systems is also mentioned.

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I. Introduction

The semiclassical methods belong to the most effective approximate methods in quantum theory [1]. Starting as the well known JWKB approximations [2] the methods have been successively developed in terms of the wave function formalism by Fröman and Fröman in one dimension and next extended to arbitrary finite dimension by Russian school of Maslov, Fedoriuk and collaborators [3, 4, 5]. Parallelly, a formulation of the semiclassical methods relied on the Feynman path integral formalism in quantum mechanics [6] has been developed by Gutzwiller [7].

As it is well known semiclassical series expansions most frequently are asymptotic expansions i.e. the corresponding series are divergent [8]. Therefore these series to be used have to be abbreviated. This is usually done keeping only few first terms of the series. However the best results are obtained if these abbreviations are done at the least terms of the series.

Nevertheless, in general, even in the best cases there are still some discrepancies left between the abbreviated series and the approximated quantities. It is well known that a source for these discrepancies is related with additional, “exponentially small” contributions which are lost when the main semiclassical series are constructed. Therefore, in order to improve accuracy of the semiclassical methods it is necessary to recover these tiny contributions [9, 10, 11], [12]–[15].

Sometimes it is unavoidable. Namely there are cases when the main contributions are built uniquely from these exponentially small objects, i.e. the corresponding semiclassical series vanish identically in these cases. The well known examples of the latter situation are all barrier penetration amplitudes [1]. Therefore there is a need for a systematic way of semiclassical expansions containing also their exponentially small elements.

One of ways used for this goal is the technique of Borel resummation of semiclassical series [16]. To use, however, the latter one has to have solutions of the Schrödinger equation which can be semiclassically expanded and which can be also recovered from their expansions by the method of Borel resummation. In other case the problem of exponentially small contributions can not be well defined.

An existence of solutions with Borel summable semiclassical expansions is not common - only limited sets of them can have this property. In fact, an existence of such solutions is well established only in 1D quantum mechanics [17]. This is why a discussion which follows is limited to one dimension.

A solution of a stationary Schrödinger equation which semiclassical expansion is Borel summable to the solution itself is called a fundamental solution.

For a given one dimensional potential there is a definite (finite or infinite) set of fundamental solutions [11, 17, 18].

In the next section a construction of fundamental solutions is described.
II. Fundamental solutions and their properties

1. Fundamental solutions

Let us describe shortly basic lines in defining fundamental solutions [3, 4, 17, 18]. In the following we shall limit ourselves to one dimensional potentials $V(x, \bar{h})$ which have unique complex extensions both into $x$- and $\bar{h}$-planes and which are meromorphic on the $x$-plane while having the following asymptotic expansions in $\Re \bar{h} > 0$ for $\Re \bar{h} \to +\infty$:

$$V(x, \bar{h}) \sim V_0(x) + \bar{h}V_1(x) + \bar{h}^2V_2(x) + \ldots$$  \hspace{1cm} (1)

Let us put $q(x, \bar{h}) = V(x, \bar{h}) - E$, where $E$ is an energy of the quantum system and let $Z$ denote a set of all the points of the $x$-plane at which $q(x, \bar{h})$ has its single or double poles. Let $\delta(x)$ be a meromorphic function of $x$, the unique singularities of which are double poles at the points collected by $Z$ with coefficients at all the poles equal to $1/4$ each. (The latter function can be constructed in general with the help of the Mittag-Leffler theorem [19]).

Consider now a function

$$\tilde{q}(x, \bar{h}) = q(x, \bar{h}) + \bar{h}^2\delta(x)$$ \hspace{1cm} (2)

A presence and a role of the $\delta$-term in (2) are explained below. This term contributes to (2) if and only when a corresponding function $q(x, \bar{h})$ contains simple or second order poles. (Otherwise a corresponding $\delta$-term is put to zero). It is called a Langer term [17, 18, 20].

The Stokes graph corresponding to a function $\tilde{q}(x, \bar{h})$ consists now of Stokes lines emerging from roots (turning points) of $\tilde{q}(x, \bar{h})$. Stokes lines satisfy one of the following equations:

$$\Re \int_{x_i}^x \sqrt{\tilde{q}(\xi, \bar{h})}\, d\xi = 0$$ \hspace{1cm} (3)

with $x_i$ being a root of $\tilde{q}(x, \bar{h})$. We shall assume further a generic situation when all roots $x_i$ are simple.

Stokes lines which are not closed end at these points of the $x$-plane (i.e. have the latter points as their boundaries) for which the action integral in (3) becomes infinite. Of course such points are singular for $\tilde{q}(x, \bar{h})$ and they can be its finite poles or its poles lying at infinity.

Each such a singularity $z_k$ of $\tilde{q}(x, \bar{h})$ defines a domain called a sector. This is the connected domain of the $x$-plane bounded by Stokes lines and $z_k$ itself. The latter is also a boundary for Stokes lines or an isolated boundary point of a sector (as it is in the case of the second order pole).

In each sector the LHS in (3) is only positive or only negative. Consider now the Schrödinger equation:

$$\Psi''(x) - \bar{h}^{-2}q(x)\Psi(x) = 0$$ \hspace{1cm} (4)
corresponding to a potential \( V(x, \hbar) \) and energy \( E \) (we have put a mass \( m \) in \((\text{I})\) to be equal to \( 1/2 \)).

Following Fröman and Fröman \([3]\) and Fedoriuk \([4]\) (see also \([17, 18]\)) in each sector \( S_k \) having a singular point \( z_k \) at its boundary one can define a solution to \((\text{I})\) having the following Dirac form:

\[
\Psi_k(x) = \tilde{q}^{-\frac{1}{4}}(x) e^{\frac{\pi}{\hbar} W(x)} \chi_k(x) \quad k = 1, 2, \ldots
\]

where:

\[
\chi_k(x) = 1 + \sum_{n \geq 1} \left( -\frac{\sigma \hbar}{2} \right)^n \int_{z_k}^x d\xi_1 \int_{z_k}^{\xi_1} d\xi_2 \cdots \int_{z_k}^{\xi_{n-1}} d\xi_n \omega(\xi_1)\omega(\xi_2)\cdots\omega(\xi_n)
\]

\[
\times \left( 1 - e^{-\frac{2\pi}{\hbar} (W(x) - W(\xi_1))} \right) \left( 1 - e^{-\frac{2\pi}{\hbar} (W(\xi_1) - W(\xi_2))} \right) \cdots \left( 1 - e^{-\frac{2\pi}{\hbar} (W(\xi_{n-1}) - W(\xi_n))} \right)
\]

with

\[
\omega(x) = \frac{\delta(x)}{\tilde{q}^{\frac{1}{2}}(x, \hbar)} - \frac{1}{4} \frac{\tilde{q}''(x, \hbar)}{\tilde{q}^{\frac{1}{2}}(x, \hbar)} + \frac{5}{16} \frac{\tilde{q}'(x, \hbar)}{\tilde{q}^{\frac{3}{2}}(x, \hbar)}
\]

and

\[
W(x) = \int_{x_i}^x \sqrt{\tilde{q}(\xi, \hbar)} d\xi
\]

where \( x_i \) is a root of \( \tilde{q}(x, \hbar^2) \) lying at the boundary of \( S_k \).

In \((\text{I})\) and \((\text{II})\) a sign \( \sigma (= \pm 1) \) and an integration path are chosen in such a way to have:

\[
\sigma \Re (W(\xi_j) - W(\xi_{j+1})) \geq 0
\]

for any ordered pair of integration variables (with \( \xi_0 = x \)). Such a path of integration is then called canonical.

The Langer \( \delta \)-term appearing in \((\text{I})\) and \((\text{II})\) is necessary to make all integrals in \((\text{I})\) converging when \( z_k \) is a first or a second order pole of \( \tilde{q}(x, \hbar^2) \) or when solutions \((\text{II})\) are to be continued to such poles. As it follows from \((\text{I})\) each such a pole \( z_k \) demands a contribution to \( \delta(x) \) of the form \( (2(x - z_k))^{-2} \), what has been already assumed in the corresponding construction of \( \delta(x) \).

A domain \( D_k(\supset S_k) \) where \( \chi_k(x) \) can be represented by \((\text{I})\) with canonical integration paths is called canonical.

2. Standard semiclassical expansion \([21]\)

Let us note that the \( \chi \)-factors entering the Dirac forms \((\text{I})\) are the solutions of the following two second order linear differential equations obtained by the substitution \((\text{II})\) into the Schrödinger equation \((\text{I})\):

\[
\tilde{q}^{-\frac{1}{4}}(x) \left( \tilde{q}^{-\frac{1}{4}}(x) \chi(x) \right)'' + \frac{2\sigma}{\hbar} \chi'(x) + \tilde{q}^{-\frac{1}{4}}(x) \delta(x) \chi(x) = 0
\]
Eqs. (10) provide us with a general form of semiclassical expansions for a \( \chi \)-factors if such expansions exists. Namely, assuming the latter we can substitute into (10) the semiclassical expansion for \( \chi \):

\[
\chi(x) \sim \sum_{n \geq 0} \left( -\frac{\sigma \hbar}{2} \right)^n \kappa_n(x)
\]

(11)
to get the following recurrent relations for \( \kappa_n(x) \):

\[
\kappa_n(x) = C_n + \int_{x_n}^x \tilde{D}(y)\kappa_{n-1}(y)dy \quad , \quad n \geq 1
\]

(12)
where a linear operator \( \tilde{D}(x) \) is given by:

\[
\tilde{D}(x) = \tilde{q}^{-\frac{1}{4}}(x, \hbar) \frac{d^2}{dx^2} \tilde{q}^{-\frac{1}{4}}(x, \hbar) + \tilde{q}^{-\frac{1}{4}}(x, \hbar) \delta(x)
\]

(13)
and

\[
\kappa_0(x) \equiv C_0
\]

and where \( x_n, \quad n \geq 1 \), are arbitrary chosen regular points of \( \omega(x) \) and \( C_n, \quad n \geq 0 \), are arbitrary constants. It is, however, easy to show that choosing all points \( x_n \) to be the same, say \( x_0 \), merely redefines constants \( C_n \). Assuming this we get for \( \kappa_n(x) \):

\[
\kappa_n(x) = \sum_{k=0}^{n} C_{n-k} I_k(x, x_0)
\]

(14)
where

\[
I_0(x, x_0) \equiv 1
\]

and

\[
I_n(x, x_0) = \int_{x_0}^x d\xi_n \tilde{D}(\xi_n) \int_{x_0}^{\xi_n} d\xi_{n-1} \tilde{D}(\xi_{n-1}) \cdots \int_{x_0}^{\xi_3} d\xi_2 \tilde{D}(\xi_2) \int_{x_0}^{\xi_2} d\xi_1 \omega(\xi_1)
\]

(15)

\[
n = 1, 2, \ldots
\]

Substituting (14) into (11) we get finally for the considered semiclassical expansion:

\[
\chi(x, \hbar) \sim \chi^{as}(x, \hbar) \equiv \sum_{n \geq 0} \left( -\frac{\sigma \hbar}{2} \right)^n C_n \sum_{k \geq 0} \left( -\frac{\sigma \hbar}{2} \right)^k I_k(x, x_0)
\]

(16)
The form (16) is called a standard form for the expansion (11). The formula (16) can be applied to fundamental solutions \( \chi \)-factors \( \chi_k(x, \hbar) \) of (8). In this case however, due to the explicit form (8) of these factors, their asymptotic
expansions in corresponding canonical domains $D_k$ can be found directly from (3) to be:

$$\chi_k(x, \hbar) \sim \chi_k^{as}(x, \hbar) = 1 + \sum_{n \geq 1} \left( -\frac{\sigma_k \hbar}{2} \right)^n \kappa_{k,n}(x)$$

$$\kappa_{k,n}(x) = I_n(x, z_k)$$

(17)

where $z_k$ is a singular point in a corresponding sector $S_k$ where the solution (3) is defined.

The latter formula can be brought to the standard form (16) by noticing that the following identity holds:

$$\chi_{k,n}(x) = \sum_{p=0}^{n} \chi_{k,p}(x_0) I_{n-p}(x, x_0)$$

(18)

so that we get

$$\chi^{as}(x, \hbar) = \chi^{as}(x_0, \hbar) \sum_{k \geq 0} \left( -\frac{\sigma \hbar}{2} \right)^k I_k(x, x_0)$$

(19)

i.e. a "constant" $C(\hbar) \equiv \sum_{n=0}^{\infty} \left( -\frac{\sigma \hbar}{2} \right)^n C_n$ coincides with $\chi^{as}(x_0, \hbar)$ in this case.

3. Borel summability of semiclassical expansions [21]

The standard semiclassical expansions (16) can be tried to be Borel summed. Necessary and sufficient conditions for that have been formulated by Watson-Nevanlinna-Sokal theorem [16]. In this respect, the following two important facts have been shown for the case of 1D quantum mechanics with meromorphic potentials [21]:

1. Fundamental solution semiclassical expansions as defined by (17) are Borel summable to these solutions themselves;

2. Fundamental solutions are the unique ones with the above property, i.e. each semiclassical series (17) which can be Borel summed (such a summation always provides us with a solution to the Schrödinger equation (4)) is always summed to some fundamental solution (up to a multiplicative constant).

III. Examples of applications of fundamental solutions

Let us make a general statement that having for a given one dimensional problem a complete set of the corresponding fundamental solutions we can get an answer, exact as well as approximate, for any basic quantum mechanical question one can put for this problem. A typical list of them is, as one knows, the following:
1. Quantization of bound states

2. One dimensional scattering amplitudes: reflection and transmission coefficients

3. Quantization of resonant states

However, each time whenever higher dimensional problems can be reduced to one dimensional ones the above questions can be solved effectively also for such cases. Typical here are problems with spherical or other symmetries among which the Coulomb or Yukawa potentials are well known examples.

Since fundamental solutions are immanently related to JWKB and, wider, semiclassical expansions then they give rice to following further applications:

4. JWKB formulae for wave functions, energy levels, scattering amplitudes and matrix elements

5. Exactness of JWKB formulae for energy level quantization

6. Exponential asymptotics in semiclassical expansions

We know also that a time evolution of two energy level systems can always be rephrased as the stationary Schrödinger equation with a time as the corresponding independent variable. Therefore the method of fundamental solutions can be applied also to:

7. Adiabatic transitions in two energy level systems

To illustrate some of these applications we shall consider a potential of the form

\[ V(x) = \frac{x^2 - 1}{(x^2 + 1)^2} \]

Fig.1 A potential \( V(x) = \frac{x^2 - 1}{(x^2 + 1)^2} \)

This potential is shown on Fig.1. It has two maxima at the points \( x_{\pm}^{\text{max}} = \pm \sqrt{3} \) with a value \( V(\pm \sqrt{3}) = \frac{1}{8} \) and a minimum at \( x^{\min} = 0 \) with a value \( V(0) = -1 \). It has also two real roots at \( x_{\pm}^{\text{root}} = \pm 1 \) and two second order poles at \( x_{\pm}^{\text{pole}} = \pm i \). Therefore, depending on its energy \( E \), a particle can be bounded by this potential for \(-1 < E < 0\), can form resonant states for \( 0 < E < \frac{1}{8}\) and can scatter for \( 0 < E \), penetrating both the barriers for \( 0 < E < \frac{1}{8}\) or being “softly” reflected in its over-barrier scattering for \( E > \frac{1}{8}\).

For describing all the above possibilities in terms of fundamental solution method we have to draw first Stokes graphs corresponding to these cases. Since the potential
considered has two second order poles it has to acquire two additional Langer terms, one for each pole, so that we have to draw Stokes graphs for the following $\tilde{q}$-function:

$$\tilde{q}(x, \bar{h}) = \frac{x^2 - 1}{(x^2 + 1)^2} - \frac{\bar{h}^2}{4} \left( \frac{1}{(x - i)^2} + \frac{1}{(x + i)^2} \right) - E$$ \hspace{1cm} (20)

Depending on an energy $E$ these graphs are shown on figures 2-4. They corresponds to different states of a particle and we consider them consecutively.

1$^\circ$ Bound states: $-1 < E < 0$

Fig.2 shows the “first” sheet (from an infinite number of them) of a Riemann surface on which fundamental solutions are defined. A number of the latter is also infinite. $S_1, S_3, S_\bar{3}, S_2$ denote the corresponding sectors lying on the “first” sheet, so that there are four fundamental solutions defined on this sheet: $\Psi_1(x), \Psi_3(x), \Psi_\bar{3}(x) = \bar{\Psi}_3(\bar{x}), \Psi_2(x)$, corresponding to the respective sectors.

The solutions $\Psi_1(x)$ and $\Psi_2(x)$ vanishing at infinities of the respective sectors $S_1, S_2$ (i.e. at $\pm\infty$ respectively) can represent two branches of a corresponding bound state wave function. To do this they have to coincide (up to a constant) with each other, i.e. we have:

$$\Psi_1(x) \equiv C\Psi_2(x)$$ \hspace{1cm} (21)

Writing (21) first for $x = x_+^{\text{pole}} \in S_3$ and next for $x = x_-^{\text{pole}} \in S_3$ we find:

$$C = \frac{\chi_{1\rightarrow3}(\bar{h}, E)}{\chi_{2\rightarrow3}(\bar{h}, E)} e^{-\frac{i}{\hbar} \int_K \sqrt{q(x, \bar{h}, E)} dx} = -\frac{\chi_{1\rightarrow3}(\bar{h}, E)}{\chi_{2\rightarrow3}(\bar{h}, E)} e^{\frac{i}{\hbar} \int_K \sqrt{q(x, \bar{h}, E)} dx}$$ \hspace{1cm} (22)

where an integration contour $K$ is shown on Fig.2 and $\chi_{1\rightarrow3}$, etc. mean integrations in (6) performed between singular points of the corresponding sectors along canonical paths.

From (22) we get immediately the following quantization condition for energy levels:

$$e^{-\frac{i}{\hbar} \int_K \sqrt{q(x, \bar{h}, E)} dx} = -\frac{\chi_{1\rightarrow3}(\bar{h}, E)\chi_{2\rightarrow3}(\bar{h}, E)}{\chi_{1\rightarrow3}(\bar{h}, E)\chi_{2\rightarrow3}(\bar{h}, E)} \hspace{1cm} (23)$$

with its obvious JWK $B$-limit:

$$e^{-\frac{i}{\hbar} \int_K \sqrt{q(x, \bar{h}, E^{JWK B})} dx} = -1$$ \hspace{1cm} (24)

2$^\circ$ Scattering amplitudes - reflection and transmission coefficients: $0 < E < \frac{1}{8}$
A corresponding graph is shown on Fig.3. We assume the plane wave is incoming from the left. It reflects mainly from the barriers but also penetrates them both but with much smaller amplitude. Therefore for $x$ sufficiently close to $+\infty$ there is only outgoing plane wave while for $x$ sufficiently close to $-\infty$ there are two waves: incoming and reflected.

The outgoing wave can be represented by the fundamental solution $\Psi_1(x)$ since at $x$ close to $+\infty$ it becomes a plane wave with positive momentum.

Similarly, the solution $\Psi_2(x)$ can represent the incoming wave while the solution $\Psi_3(x)$ - the reflected one.

It is clear that to solve our problem we have to find a relation:

$$\Psi_2(x) = R\Psi_2(x) + T\Psi_1(x)$$  \hspace{1cm} (25)

where the reflection amplitude $R$ and the transmission one $T$ have to be expressed only in terms of fundamental solution factors.

Note, that (25) expresses not only a physical fact but also a mathematical one that every solution of the Schrödinger equation is a linear combination of another two if the latter are linear independent and the linear independence of any two fundamental solutions is their basic property.

As previously, Eq.(25) has to be valid for any $x$ and therefore it means that the rhs of (25) is an analytic continuation of $\Psi_2(x)$. However, we have to perform this analytic continuation being constrained that it goes entirely along canonical paths. Such a continuation ensures keeping the full control over the semiclassical properties of the amplitudes $R$ and $T$. This continuation can be done in many ways but the simplest one is to take the solution $\Psi_1(x)$ (instead of $\Psi_2(x)$) and to continue it canonically to the sector $S_2$ or $S_3$.

There are two groups of sectors in Fig.2 such that in each group its sectors can contact canonically with each other. These are $S_1, S_1, S_3, S_3$ and $S_2, S_2, S_3, S_3$. Therefore continuing $\Psi_1(x)$ we express it first by a linear combination of $S_3, S_3$ and next the latter two solutions - as linear combinations of $S_2, S_2$. We get:

$$\Psi_1(x) = \alpha_{\frac{1}{2} \rightarrow 3} \Psi_3(x) + \alpha_{\frac{1}{2} \rightarrow 3} \Psi_3(x)$$

$$\Psi_3(x) = \alpha_{\frac{3}{2} \rightarrow 2} \Psi_2(x) + \alpha_{\frac{3}{2} \rightarrow 2} \Psi_2(x)$$  \hspace{1cm} (26)

where

$$\Psi_3(x) = \overline{\Psi_3(x)}$$

and $x$ goes to a singular point $z_k$ of the sector $S_k$ along a canonical path.
Finally we get
\[ \Psi_1(x) = \left( \alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2 + \alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2 \right) \Psi_2(x) + \left( \alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2 + \alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2 \right) \Psi_2(x) \] (28)

Comparing (28) with (25) we obtain:
\[ R = \frac{\alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2 + \alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2}{\alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2 + \alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2} \]
\[ T = \frac{1}{\alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2 + \alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2} \] (29)

All \( \alpha \)-coefficients in the above formulae can be easily expressed in terms of the three factors constituting the Dirac form (5) of fundamental solutions to get:
\[ R = i \chi_{\frac{1}{3}} \to 3 \chi_{\frac{3}{2}} \to 2 + \chi_{\frac{1}{3}} \to 3 \chi_{\frac{3}{2}} \to 2 \int_{x_1}^{x_2} \sqrt{\tilde{q}(x)} dx \]
\[ T = - \frac{\chi_{\frac{3}{2}} \to 3}{\chi_{\frac{1}{3}} \to 3 \chi_{\frac{3}{2}} \to 2 + \chi_{\frac{1}{3}} \to 3 \chi_{\frac{3}{2}} \to 2} e^{i \frac{1}{h} \int_{x_1}^{x_2} \sqrt{q(x)} dx} e^{i \frac{1}{h} \oint K_{2} \sqrt{\tilde{q}(x)} dx} \] (30)

A semiclassical limit which follows from (31) is immediate:
\[ R^{JWKB} = i \]
\[ T^{JWKB} = - \frac{1}{2 \cos \left( \frac{1}{h} \int_{x_1}^{x_2} \sqrt{q(x)} dx \right)} e^{i \frac{1}{h} \oint K_{2} \sqrt{\tilde{q}(x)} dx} \] (31)

The JWKB formula for \( T \) seems to suggest a singular behaviour of this amplitude for energies for which cosine in its denominator is close to zero. This is, in fact, a situation closely related to the problem discussed in the next point and, as one knows, describes so called resonant scattering. Of course, in the last case the above JWKB-formula for \( T \) has to be modified leading us to its Breit - Wigner form.

3° Resonant states - resonance widths: \( 0 < E < \frac{1}{8} \)

For the energy range as given above the potential considered gives rise to resonant states to exist. A condition for their existence follows directly from Eq. (28) as a demand for the solution \( \Psi_2(x) \) not to contribute to this equation, i.e. resonant wave functions can have only branches \( outgoing \) to both infinities of the real \( x \)-axis. Therefore a corresponding condition takes the form:
\[ \alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2 + \alpha_{\frac{1}{3}} \to 3 \alpha_{\frac{3}{2}} \to 2 = 0 \] (32)
i.e. resonant energies have to be singular points (poles) for both the amplitudes $R$ and $T$.

In terms of $\chi$-factors this condition reads:

$$e^{-\frac{2}{h} \int_{x_1}^{x_2} \sqrt{q(x)} dx} = -\frac{\chi_{1\to3} \chi_{2\to3}}{\chi_{1\to3} \chi_{2\to3}}$$

(33)

Eq. (33) is very similar to (24). The main difference between these formulae lies, however, in energies for which they can be satisfied. For the latter these energies are real (and negative), for the former the corresponding energies can be only complex.

To see this let us note that $\alpha$-coefficients are, in general, not independent. Despite this limitation follows from the fact that among any four fundamental solutions which can communicate canonically with themselves only a pair of them are linear independent. This limitation leads to the following identity:

$$\alpha_{\frac{j}{2}\to k} = \alpha_{\frac{j}{2}\to t} + \alpha_{\frac{j}{2}\to j} \alpha_{\frac{j}{2}\to k}$$

(34)

for each quartet $i, j, k, l$.

For the case considered there are, as we have already mentioned, two groups of fundamental solutions, each containing four of them, related to the sectors $S_1, S_1, S_3, S_3$ and $S_2, S_2, S_3, S_3$. Therefore there are the following two identities for corresponding $\alpha$-coefficients:

$$\alpha_{\frac{1}{2}\to 3} = \alpha_{\frac{1}{2}\to 3} + \alpha_{\frac{1}{2}\to 1} \alpha_{\frac{1}{2}\to 3}$$

(35)

$$\alpha_{\frac{2}{2}\to 3} = \alpha_{\frac{2}{2}\to 3} + \alpha_{\frac{2}{2}\to 2} \alpha_{\frac{2}{2}\to 3}$$

which can be written by $\chi$-factors as:

$$\chi_{1\to3} \chi_{1\to3} = \chi_{1\to3} \chi_{1\to3} - \chi_{3\to3} e^{-\frac{i}{2} \oint_{K_1} \sqrt{q(x)} dx}$$

(36)

$$\chi_{2\to3} \chi_{2\to3} = \chi_{2\to3} \chi_{2\to3} - \chi_{3\to3} e^{\frac{i}{2} \oint_{K_2} \sqrt{q(x)} dx}$$

The last equations are written, by assumption, for a complex energy $E$. However, for a real one they take the forms:

$$|\chi_{1\to3}|^2 = |\chi_{1\to3}|^2 - \chi_{3\to3} e^{-\frac{i}{2} \oint_{K_1} \sqrt{q(x)} dx}$$

(37)

$$|\chi_{2\to3}|^2 = |\chi_{2\to3}|^2 - \chi_{3\to3} e^{\frac{i}{2} \oint_{K_2} \sqrt{q(x)} dx}$$

Now, we use the last identities to show that putting $E = E_0 - i\frac{\Gamma}{2}$ we get a width $\Gamma$ as exponentially small quantity in comparison with $E_0$. To see this let us write the "quantization" condition (33) in the following form:

$$e^{-\frac{2}{h} \int_{x_1}^{x_2} \sqrt{q(x)} dx} = -e^{i\phi_{1\to3} + i\phi_{2\to3} - i\phi_{1\to3} - i\phi_{2\to3}} \left| \frac{\chi_{1\to3} \chi_{2\to3}}{\chi_{1\to3} \chi_{2\to3}} \right|$$

(38)
where \( \phi_{1\rightarrow3}, \phi_{2\rightarrow3}, \phi_{1\rightarrow3}, \phi_{2\rightarrow3} \) are phases of the corresponding \( \chi \)-factors.

We now put

\[
-\frac{2}{i\hbar} \int_{-x_1}^{x_1} \sqrt{\tilde{q}(x, E_0)} dx = (2k + 1)\pi + \phi_{1\rightarrow3} + \phi_{2\rightarrow3} - \phi_{1\rightarrow3} - \phi_{2\rightarrow3}
\]

(39)

so that we get

\[
-\frac{2}{\hbar} \int_{-x_1}^{x_1} \sqrt{\tilde{q}(x, E_0 - \frac{\Gamma}{2})} dx + \frac{2}{\hbar} \int_{-x_1}^{x_1} \sqrt{\tilde{q}(x, E_0)} dx = \frac{1}{2} \ln \left| \frac{\chi_{1\rightarrow3}\chi_{2\rightarrow3}}{\chi_{1\rightarrow3}\chi_{2\rightarrow3}} \right|_{E = E_0 - \frac{\Gamma}{2}}(40)
\]

We now expand both the sides of (40) into the Taylor series around \( E_0 \) abbreviating the latters on the first terms. We get

\[
\frac{i}{\hbar} \frac{d}{dE_0} \int_{-x_1}^{x_1} \sqrt{\tilde{q}(x, E_0)} dx = \frac{1}{2} \ln \left( \left| \frac{\chi_{1\rightarrow3}\chi_{2\rightarrow3}}{\chi_{1\rightarrow3}\chi_{2\rightarrow3}} \right|_{E = E_0}^2 - \frac{i}{2} \frac{d}{dE_0} \left| \frac{\chi_{1\rightarrow3}\chi_{2\rightarrow3}}{\chi_{1\rightarrow3}\chi_{2\rightarrow3}} \right|_{E = E_0}^2 \right)
\]

(41)

Next, using (38), we obtain

\[
\frac{2}{\hbar} \int_{-x_1}^{x_1} \frac{1}{\sqrt{\tilde{q}(x, E_0)}} dx = \ln \left( 1 + \frac{\chi_{3\rightarrow3}}{\chi_{1\rightarrow3}} \right) \left( 1 + \frac{\chi_{3\rightarrow3}}{\chi_{2\rightarrow3}} \right) \left( 1 + \frac{\chi_{3\rightarrow3}}{\chi_{2\rightarrow3}} \right)
\]

(42)

It follows from (43) that, up to higher order terms in exponentials, \( \Gamma \) is given by

\[
\Gamma = \frac{\hbar}{2} \int_{-x_1}^{x_1} \frac{1}{\sqrt{\tilde{q}(x, E_0)}} dx \left( \frac{\chi_{3\rightarrow3}(E_0)}{|\chi_{1\rightarrow3}(E_0)|^2} + \frac{\chi_{3\rightarrow3}(E_0)}{|\chi_{2\rightarrow3}(E_0)|^2} \right) e^{\frac{i}{\hbar} \int_{K_1} \sqrt{q(x, E_0)} dx}
\]

(43)

Finally, in a JWKB limit we get

\[
\Gamma_{JWKB} = \frac{2\hbar}{T} e^{\frac{i}{\hbar} \int_{K_2} \sqrt{q(x, E_0)} dx}
\]

(44)

where \( T \) is a classical period of a particle moving between the two barriers.

40. **Over barrier scattering amplitudes;** \( \frac{1}{8} < E \)

A Stokes graph corresponding to this case is shown on Fig.4. A scattering wave function is represented as previously by the fundamental solution \( \Psi_2 \), a reflected one - by \( \Psi_2 \) and a transmitted one - by \( \Psi_1 \). As in the previous case these solutions are related by Eq. (25) and the reflection and transmission amplitudes are given again by Eqs. (39). A difference which has to appear between these two cases lies of course in
formulae expressing $\alpha$-coefficients by corresponding $\chi$-factors. For the case considered we get according to Fig. 4:

\[
R = i \frac{\chi_{1 \rightarrow 3 \chi_{2 \rightarrow 3}} + \chi_{1 \rightarrow 3 \chi_{2 \rightarrow 3}}}{\chi_{1 \rightarrow 3 \chi_{2 \rightarrow 3}} + \chi_{1 \rightarrow 3 \chi_{2 \rightarrow 3}} e^{\frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{\tilde{q}(x)} dx}} e^{\frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{\tilde{q}(x)} dx} \quad (45)
\]

\[
T = \frac{\chi_{3 \rightarrow 3 e^{-\frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{\tilde{q}(x)} dx}}}{\chi_{1 \rightarrow 3 \chi_{2 \rightarrow 3}} + \chi_{1 \rightarrow 3 \chi_{2 \rightarrow 3}} e^{\frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{\tilde{q}(x)} dx}} e^{\frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{\tilde{q}(x)} dx}
\]

Fig. 4 Stokes graph corresponding to energy range $\frac{1}{8} < E$

where an integration between the points $x_1, -\bar{x}_1$ can run along the Stokes line linking these points. Therefore the corresponding integral is purely imaginary.

On the other hand, an integral between the points $\bar{x}_1, x_1$ is real and negative since it can be taken along the anti-Stokes line linking these points.

JWKB approximations to the above amplitudes follows immediately to be:

\[
R_{JWKB} = i e^{\frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{\tilde{q}(x)} dx}
\]

\[
T_{JWKB} = e^{-\frac{1}{\hbar} \int_{x_1}^{-x_1} \sqrt{\tilde{q}(x)} dx}
\]

(46)

b) Particle in a Coulomb field

Let $R_l(r), \ l = 0, 1, ...$, denote radial parts of the Coulomb wave functions corresponding to subsequent orbital momentum numbers. As it is well known functions $\Psi^{(l)}(r) = r R_l(r), \ l = 0, 1, ...$, satisfy then Schrödinger equations (4) with respective potentials $V_l(r) = -\frac{\alpha}{r} + \frac{\hbar^2 (l + \frac{1}{2})^2}{2 r^2}, \ l = 0, 1, ...$, shown in Fig. 5, and with boundary conditions $\Psi^{(l)}(0) = 0, \ l = 0, 1, ...$ .

Fig. 5 Coulomb potential corrected by centrifugal term

To apply the fundamental solution formalism to two problems considered in this case, i.e. to bound states ($E < 0$) and to a scattering problem ($E > 0$) the additive Langer term $\frac{\hbar^2}{4m} \frac{(l + \frac{1}{2})^2}{r^2}$ has to be introduced to each potential $V_l(r)$ to give $V_l(r) = -\frac{\alpha}{r} + \frac{\hbar^2 (l + \frac{1}{2})^2}{2 r^2}, \ l = 0, 1, ...$ . Then figures 6 and 7 show respective Stokes graphs corresponding to the above two problems.

Fig. 6 Coulomb Stokes graph corresponding to energy range $E < 0$

1° Bound state energies: $E < 0$
Fig. 6 shows the Stokes graph corresponding to this case. The fundamental solutions \( \Psi_1^{(l)}(r) \) and \( \Psi_3^{(l)}(r) \) corresponding to the sectors \( S_1 \) and \( S_3 \) respectively are those which satisfy necessary boundary conditions: the first one vanish at \( r = +\infty \), the second - at \( r = 0 \). Therefore, identifying them with each other we obtain a wave function of a bound state and a condition for energies of this state. We have:

\[
\Psi_1^{(l)}(r) = C_l \Psi_3^{(l)}(r)
\]  

\[
C_l = \frac{e^{-\frac{i}{\hbar} \int \sqrt{V_1 - E} dx}}{\chi_{2\rightarrow 3}} = -\frac{e^{\frac{i}{\hbar} \int \sqrt{V_1 - E} dx}}{\chi_{2\rightarrow 3}}
\]

Fig. 7 Coulomb Stokes graph corresponding to energy range \( E > 0 \)

The last equation provides us simultaneously with the corresponding quantization condition. If we perform necessary integrations in the \( \chi \)-factors contained in this equation along the negative real \( r \)-axis then we note that both these factors are real. On the other hand they are mutually complex conjugated. Therefore, they have to cancel each other, so that we get the following net result for the quantization condition in the Coulomb potential:

\[
\frac{i}{\hbar} \int \sqrt{V_1 - E} dx = (2k + 1)\pi, \quad k = 0, 1, ...
\]

The above formula is a famous JWKB formula of Langer which appeared to be exact. As we can see this is not accidental.

2° Coulomb scattering: \( E > 0 \)

This situation is represented by Fig. 7 where the solution \( \Psi_1^{(l)}(r) \) describes an incoming wave while \( \Psi_1^{(l)}(r) \) - an outgoing one. It is now sufficient only to write such a combination of both these wave functions to make it vanishing at \( r = 0 \). But this property is the one of the solution \( \Psi_3^{(l)}(r) \), i.e. the combination mentioned has to be proportional to the last solution. But it means that to find a corresponding scattering amplitude \( S_l \) it is enough to express \( \Psi_1^{(l)}(r) \) as a linear combination of \( \Psi_1^{(l)}(r) \) and \( \Psi_3^{(l)}(r) \). We get from Fig. 7:

\[
\Psi_1^{(l)}(r) = \frac{\chi_{1\rightarrow 3}^{(l)}}{\chi_{1\rightarrow 3}} \Psi_1^{(l)}(r) + \frac{1}{\chi_{1\rightarrow 3}} \Psi_3^{(l)}(r)
\]

It follows from (49) that

\[
S_l = \frac{\chi_{1\rightarrow 3}^{(l)}}{\chi_{1\rightarrow 3}} = e^{2ie_1^{(l)}}
\]
where $\phi_{1 \rightarrow 3}^{(l)}$ is a phase of $\chi_{1 \rightarrow 3}^{(l)}$. Its JWKB approximation follows directly from (50) to be:

$$
\phi_{1 \rightarrow 3}^{(l), \text{JWKB}} = \frac{\hbar}{2} \int_{0}^{\infty} \omega(r) r dr
$$

$$
\omega(r) = \frac{1}{4r^2 \tilde{q}^2(r, \hbar)} - \frac{1}{4 \tilde{q}^2(r, \hbar)} + \frac{5}{16} \frac{\tilde{q}''(r, \hbar)}{\tilde{q}^2(r, \hbar)} + \frac{5}{16} \frac{\tilde{q}''(r, \hbar)}{\tilde{q}^3(r, \hbar)}
$$

(51)

$$
\tilde{q}(r, \hbar) = -\frac{\alpha}{r} + \frac{\hbar^2 (l + \frac{1}{2})^2}{r^2}, \quad l = 0, 1, ...
$$

where an integration path is anyone which does not coincide with any of the real half axes.

IV. Conclusions

As we have demonstrated the method of fundamental solutions appears to be very effective in solving any well defined problem of one-dimensional Schrödinger equation. It provides us both with exact solutions of such problems and immediately with their semiclassical approximations, including also exponentially small corrections to main semiclassical series.

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