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The S-matrix asymptotic behaviour in the case of singular potentials at high complex energies

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Abstract. The asymptotic behaviour of the S-matrix in the case of repulsive singular potential at the origin for large $|k|$ is presented in a more precise form. It is shown that the WKB method in the 'Langer' form yields explicit values of the first- and second-order terms of the S-matrix expansion.

Let us consider the S-wave Schrödinger equation

$$\varphi''+[k^2-V(r)]\varphi=0 \tag{1}$$

for a repulsive singular potential of the kind

$$V(r)=gr^{-m}+hr^{-\beta}+u(r) \tag{2}$$

where

$$\lim_{r\to 0} V(r)r^m=g>0 \tag{2}$$

and

$$U(r)r^2 \underset{r\to 0}{\to} 0; \qquad 2<\tfrac{1}{2}(m+2)<\beta<m.$$

There are a great number of works devoted to the definition of the S-matrix high-energy limit. Though it is generally recognised that the corresponding S-matrix has the form

$$S(k)=\exp\{-2i[a_1 g^{1/m}k^{1-(2/m)}+\tfrac{1}{4}\pi+o(1)]\} \tag{3}$$

the values of a_1, obtained by various methods (the variable phase method (Cologero 1964, 1967), WKB method (Limic 1962, Bertocchi *et al* 1965, Paliov and Rosendorff 1967) and the method integral equations (Jaffur 1967)) differ as was pointed out in the review by Frank *et al* (1971).

After the publication of this review much attention was paid in a number of articles to the potential

$$V(r)=gr^{-m}+l(l+1)/r^2.$$

The special case $m=4$ is exactly solvable and physically meaningful, it is used when the interaction of a charged particle with polarised matter is treated. We would like to draw attention to some papers on this problem: the solution of the scattering problem for singular potential (Rafe-Beketov and Kristov 1971); numerical results of phase shifts (Dolinsky 1974); the asymptotic behaviour of the S-matrix and the bound state energies for attractive singular potential (Adamen and Puzek 1979); the rigorous proof of the a_1 value (Fröman and Thylive 1979), which coincides exactly with that of Bertocchi *et al* (1965) and Paliov and Rosendorff (1967).

Interest in the S-matrix behaviour as $|k|\to\infty$ and $\theta=\arg k=\text{constant}\neq 0$ for the potentials which have the analytic S-matrix was stimulated by the problem of the validity of the dispersion relation. We recall now that the results of Limic (1962):

$$S(k) \underset{|k|\to\infty}{\sim} \exp(-2\mathrm{i}a_1 g^{1/m}k|k|^{-2/m}) = S_0(k) \tag{4}$$

and Jaffur (1967), Aly *et al* (1967)

$$S(k) \underset{|k|\to\infty}{\sim} \exp(-2\mathrm{i}a_1 g^{1/m}k^{1-(2/m)}) \tag{5}$$

are not in agreement. Details are given in the review by Frank *et al* (1971). Notice that the asymptotics given by Bertocchi *et al* (1965) are wrong because the condition

$$S_0^*(-k^*)S_0^{-1}(k) \xrightarrow[|k|\to\infty]{} 1 \tag{6}$$

is violated, which follows from the unitarity of the S-matrix:

$$S^*(-k^*) = S(k).$$

To clarify this discrepancy we consider only the problem of the S-matrix behaviour at large k. Using the WKB method it can be shown that (4) is true if a_1 is not a constant but a function of θ.

Consider a finite potential although the result is the same for any potential which decreases faster than the exponent

$$V(r) = \begin{matrix} gr^{-m} & r\leqslant 1 \\ 0 & r>1 \end{matrix} \qquad g>0. \tag{7}$$

Then the Jost solution $f(k, r)$ exists. It is a complete function provided that the variable r is fixed. Define the regular solution with the condition

$$\lim_{r\to 0} \sqrt{2}\, \varphi(k, r) g^{1/4} r^{-m/4} \exp\left(\frac{2g^{1/2}}{2-m}(1-r^{1-(m/2)})\right) = 1. \tag{8}$$

Its existence is proved in Limic (1962). Following the Poincaré theorem one can find that both the Jost solution and the Jost function, determined in terms of the Wronskion

$$f(k) = W\{f(k, r), \varphi(k, r)\},$$

constitute the complete function. In the case of a finite potential the equation

$$\varphi(k, r) = (1/2\mathrm{i}k)\{f(-k)f(k, r) - f(k)f(-k, r)\} \tag{9}$$

is valid in the complex k-plane besides the origin $k=0$. Define the asymptotic behaviour of the regular and Jost solutions as $|k|\to\infty$ and $0<\theta<\pi$. With that end in view make use of the WKB approximation for the regular solution

$$\varphi(k, r) = (1/\sqrt{2})[V(r)-k^2]^{-1/4} \exp\left\{[\mu(k, r) - \int_r^1 (V(t))^{1/2}\,\mathrm{d}t](1+\mathrm{o}(1))\right\}, \tag{10}$$

where

$$\mu(k, r) = \int_0^{r_0} [(V(t) - k^2)^{1/2} - (V(t))^{1/2}]\, dt$$

and $V(r_0) = k^2$, here we mean the positive imaginary branch of the square root, i.e. $k = i\rho$, $\rho > 0$. This formula is true for pure imaginary k as well as for complex values ($\mathrm{Im}\, k > 0$). We now are concerned with the first two order terms of the expansion

$$\begin{aligned}\mu(k, r) - \int_r^1 (V/t))^{1/2}\, dt &= \int_0^{r_0} [(V(t) - k^2)^{1/2} - (V(t))^{1/2}]\, dt + \int_{r_0}^{r} [(V(t) - k^2)^{1/2} + ik]\, dt \\ &\quad - ik(r - r_0) - \int_{r_0}^{1} (V(t))^{1/2}\, dt. \end{aligned} \tag{11}$$

The first integral can be written in the form:

$$\int_0^{r_0} [(V(t) - k^2)^{1/2} - (V(t))^{1/2}]\, dt \underset{\substack{|k| \to \infty \\ 0 < \theta < \pi}}{\sim} g^{1/m} |k|^{1-(2/m)} \mathscr{C}(\theta),$$

where

$$\mathscr{C}(\theta) = (1/m) \int_1^{\infty} [(\xi - e^{2i\theta})^{1/2} - \sqrt{\xi}]^{-1} \xi^{-[1+(1/m)]}\, d\xi.$$

The second integral is:

$$\int_{r_0}^{r} [(V(t) - k^2)^{1/2} + ik]\, dt \underset{\substack{|k| \to \infty \\ 0 < \theta < \pi}}{\sim} -ig^{1/m} a(\theta) k |k|^{-2/m},$$

where

$$a(\theta) = 1 + (1/m) \int_0^1 [1 - (1 - e^{-2i\theta}\xi)^{1/2}] \xi^{1-(1/m)}\, d\xi,$$

and the third integral is:

$$\int_{r_0}^{1} (V(t))^{1/2}\, dt \underset{\substack{|k| \to \infty \\ 0 < \theta < \pi}}{\sim} \frac{2g^{1/m}}{(2-m)} |k|^{1-(2/m)}.$$

Substituting these formulae into (11) and (11) into (10), we obtain

$$\varphi(k, r) \underset{\substack{|k| \to \infty \\ 0 < \theta < \pi}}{\sim} \exp\{-ikr + ia(\theta) k |k|^{-2/m} g^{1/m} - g^{1/m}[\mathscr{C}(\theta) + 2/(m-2)] |k|^{1-(2/m)}\}. \tag{12}$$

Using (12) and (9) we have

$$f(k) \underset{\substack{|k| \to \infty \\ 0 < \theta < \pi}}{\sim} \exp(g^{1/m} C(\theta) |k|^{1-(2/m)}),$$

$$S(k) \underset{\substack{|k| \to \infty \\ 0 < \theta < \pi}}{\sim} \exp\{g^{1/m} |k|^{1-(2/m)} [C(-\theta) - C(\theta)]\},$$

where

$$C(\theta)=\exp[i(\tfrac{1}{2}\pi+\theta)]a(\theta)+\mathscr{C}(\theta)+2/(m-2).$$

This result coincides with that of Rafe-Beketov and Khristov (1971) if $\theta=0$. Consider now the asymptotic behaviour of the S-matrix in the case of the potentials sum given by (1), where $U(r)$ involves the centrifugal barrier term as well.

It follows from (1) and the conditions of theorem (2.6.1) of Rafe-Beketov and Khristov (1971) that

$$\delta_l(k)\underset{k\to\infty}{\sim}-k+\int_{r_0(k)}^{1}(k^2-gt^{-m}-ht^{-\beta})^{1/2}\,dt+(l+\tfrac{1}{2})\tfrac{1}{2}\pi+o(1). \qquad (12)$$

Here $r_0(k)$ is the turning point, i.e. the point where the integrand becomes zero. Obviously at large k just one turning point exists. One can easily obtain the expansion

$$r_0\underset{k\to\infty}{\sim}g^{1/m}k^{-2/m}-(h/m)g^{(1-\beta)/m}k^{2(\alpha-m-1)/m}+o(k^{2(\beta-m-1)/m}). \qquad (13)$$

Transforming the integral term in (12) by expanding the integrand in powers:

$$\int_{r_0(k)}^{1}(k^2-gt^{-m}-ht^{-\beta})^{1/2}\,dt$$
$$=k-r_0(k)+\sum_{n=1}^{\infty}(-1)^n\binom{\frac{1}{2}}{n}k^{-2n+1}\sum_{s=0}^{h}\binom{n}{s}g^{n-s}h^s$$
$$\times\frac{r_0^{-mn+(m-\beta)s+1}-1}{-mn+(m-\beta)s+1}.$$

Substituting this into (12) and taking into account (13) we get:

$$\delta_l(k)\underset{k\to\infty}{\sim}a_1g^{1/m}k^{1-2/m}+a_2g^{(1-\alpha)/m}hk^{(2\beta-m-2)/m}+o(k^{(2\beta-m-2)/m}) \qquad (14)$$

where

$$a_1=a(0)=1-\sum_{n=1}^{\infty}(-1)^n\binom{\frac{1}{2}}{n}\frac{1}{mn-1}$$

$$a_2=\frac{1}{m}-\sum_{n=1}^{\infty}(-1)^n\binom{\frac{1}{2}}{n}\left(\frac{1}{m}-\frac{n}{mn-(m-\alpha)-1}\right).$$

It can be seen from (14) that if $\alpha<\frac{1}{2}(m+2)$ the second order term of the expansion equals $(l+\frac{1}{2})\pi/2$.

Appendix

In the Appendix we prove formula (10) for $|k|\to\infty$, $0<\theta\equiv\arg k<\pi$. Let us start from the equation

$$y''-[-k^2+gr^{-m}+Q(r,k)]y=[u(r)-Q(r,k)]y \qquad (A1)$$

where

$$Q(r,k)=\frac{5}{16}\frac{g^2m^2r^{-2m-2}}{(gr^{-m}-k^2)^2}-\frac{gm(m-1)r^{-m-2}}{4(gr^{-m}-k^2)}$$

$$U(r)=\begin{matrix} 0 & r<1 \\ -gr^{-m} & r\geqslant 1. \end{matrix}$$

This equation coincides with equation (2), provided the potential is taken in the form (7). The functions

$$\chi_{1,2}(k,r)=(1/\sqrt{2})(gr^{-m}-k^2)^{-1/4}\exp\left(\pm\int_x^1(gt^{-m}-k^2)^{1/2}\,\mathrm{d}t\right)$$

are independent solutions of the equation (A1) with the RHS equal to zero ($k=\mathrm{i}\rho$, $\rho>0$). It is easy to see that

$$W(\chi_1,\chi_2)=1,\qquad \lim_{r\to 0}\mathrm{e}^{\mu(k,1)}\chi_2(k,r)\chi_2^{-1}(0,r)=1$$

where

$$\mu(k,r)=\int_0^r((gt^{-m}-k^2)^{1/2}-(gt^{-m})^{1/2})\,\mathrm{d}t.$$

Hence the function

$$\phi(k,r)=\varphi(k,r)\,\mathrm{e}^{-\mu(k,1)}/\chi_2(k,r)$$

is a solution of the integral equation

$$\phi(k,r)=1+\int_0^r R(k,r,t)\phi(k,t)\,\mathrm{d}t \tag{A2}$$

where

$$R(k,r,t)=\{\chi_2(k,t)\chi_1(k,t)-[\chi_1(k,r)/\chi_2(k,r)]\chi_2^2(k,t)\}[u(t)-Q(k,t)].$$

The quantity $gt^{-m}-k^2$ takes the complex values at $0<\theta<\pi$ and $0<t<\infty$ except the negative ones and zero. So we may choose the branch of $(gt^{-m}-k^2)^{1/2}$ with positive real part, i.e. at $\theta=\frac{1}{2}\pi$. Consequently

$$\left|\frac{\chi_1(k,x)}{\chi_2(k,x)}\chi_2^2(k,t)\right|=\exp\left(-2\int_t^x(g\xi^{-m}-k^2)^{1/2}\,\mathrm{d}\xi\right)<1$$

when $0<t<x$ and

$$|R(k,r,t)|<\frac{5}{16}\frac{g^2m^2t^{-2m-2}}{|gt^{-m}-k^2|^{5/2}}+\frac{1}{4}\frac{gm(m+1)t^{-m-2}}{|gt^{-m}-k^2|}+\frac{|U(t)|}{|gt^{-m}-k^2|}\equiv F(k,t). \tag{A3}$$

Obviously $F(k,t)\in L(0,a)$ for $a>0$ and

$$\lim_{\substack{|k|\to\infty\\ 0<\theta<\pi}}\int_0^a F(x,t)\,\mathrm{d}t=0. \tag{A4}$$

Now we use the following lemma (Titchmarsh 1946).

The equation

$$f(x)=p(x)+\int_0^x k(x,t)f(t)\,\mathrm{d}t \qquad 0\leqslant x\leqslant a$$

for

$$|p(x)|<C, \qquad |k(x,t)|<k(t)\in L(0,a) \qquad (0\leqslant t\leqslant x\leqslant a)$$

possesses a single solution and

$$|f(x)|\leqslant C\exp\left[\int_0^x k(t)\,\mathrm{d}t\right].$$

From (A2) and (A3) we get

$$\phi(k,x)\xrightarrow[\substack{|k|\to\infty\\ 0<\theta<\infty}]{} 1.$$

This convergence is uniform with respect to $x\in[0,a]$. Hence

$$\varphi(x,k)=\chi_1(k,x)\,\mathrm{e}^{\mu(k,1)}[1+\mathrm{o}(1)].$$

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