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Integral Equations For The Jost Solutions And Decaying Resonance States

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Scattering states ($\Psi = \psi$) are defined as solutions of (partial) Schrödinger equation

$$\left\{ \frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + p^2 - U(r) \right\} \Psi_l(p,r) = 0, \quad (1)$$

which obey boundary conditions at the origin and at the infinity [1, 2]

$$\psi_l(p,r)|_{r=0} = 0; \quad \psi_l(p,r)|_{r\to\infty} \cong \hat{j}_l(pr) + p f_l(p) \hat{h}_l^{+}(pr), \quad (2)$$

where $f_l(p)$ is a partial scattering amplitude. The condition at the infinity therefore contains "incoming" and "outgoing" waves.

Alternatively, resonance (Gamow-Siegert) states are defined as solutions of Schrödinger equation with boundary conditions "regular wave function" at the origin and "outgoing wave function" at the infinity [3, 4]. Such conditions may be satisfied only at some complex values of parameter p ($E = \hbar^2 p^2/2m$) because the boundary value problem in this case is not Hermitian. Solutions of the problem may be found by various methods [5, 6]. For instance one can use the regular wave function ($\Psi = \Phi$) for which boundary conditions are formulated at the origin only: $\Phi_l(p,r)|_{r\to 0} \cong \hat{j}_l(pr)$.

For the regular wave function an integral Volterra equation can be formulated, its solution under certain conditions on the potential $U(r)$ exists at all p [1]. When such solutions (either analytical or numerical) are found one can investigate at what p the regular solution has the desired behavior, i.e. "outgoing wave" (or "incoming wave") at the infinity. An alternative way is to use Jost solutions ($\Psi = \chi^{\pm}$), which satisfy the following boundary conditions at the infinity (only):

$$\chi_l(p,r)|_{r\to\infty} \cong \hat{h}_l^{\pm}(pr) = \exp\left[\pm i(pr - \ell\pi/2)\right]. \quad (3)$$

For these solutions integral equations of the Volterra type also can be formulated. The purpose of this paper is to show how this equations can be used for finding resonance states, being actually decaying states

It should be noted that for the Riccati-Bessel $\hat{j}_l(x)$, Riccati-Neuman $\hat{n}_l(x)$ and Riccati-Hankel $\hat{h}_l^{\pm}(x)$ functions we follow the definitions used by Taylor [1].

$$\hat{j}_l(x) = \sqrt{\frac{\pi x}{2}} J_{l+\frac{1}{2}}(x); \qquad \hat{n}_l(x) = (-1)^l \sqrt{\frac{\pi x}{2}} J_{-l-\frac{1}{2}}(x); \qquad \hat{h}_l^{\pm}(x) = \hat{n}_l(x) \pm i\hat{j}_l(x). \quad (4)$$

Integral Volterra equations for the solutions Φ and $\chi^{\pm}$ have the forms

$$\Phi_l(p,r) = \hat{j}_l(pr) + \int_0^r g_l(p;r,r') U(r') \Phi_l(p,r') dr', \quad (5)$$

$$\chi_l^{\pm}(p,r) = \hat{h}_l^{\pm}(pr) - \int_r^{\infty} g_l(p;r,r') U(r') \chi_l^{\pm}(p,r') dr'. \quad (6)$$

The partial Green function $g_l(p;r,r')$ for both equations is the same and may be written in either of the two kinds

$$g_l(p;r,r') = \frac{1}{p}\left[\hat{j}_l(pr)\hat{n}_l(pr') - \hat{n}_l(pr)\hat{j}_l(pr')\right], \tag{7}$$

$$g_l(p;r,r') = \frac{i}{2p}\left[\hat{h}_l^-(pr)\hat{h}_l^+(pr') - \hat{h}_l^+(pr)\hat{h}_l^-(pr')\right]. \tag{8}$$

Using the latter expression one can obtain the asymptotic behavior of $\Phi_l(p,r)$ at the infinity

$$\Phi_l(p,r)|_{r\to\infty} = \frac{i}{2}\hat{h}_l^-(pr)\mathcal{F}_l^+(p) - \frac{i}{2}\hat{h}_l^+(pr)\mathcal{F}_l^-(p), \tag{9}$$

from which is obvious that under the condition $\mathcal{F}_l^+(p) = 0$, $\left(\mathcal{F}_l^-(p) = 0\right)$ the regular solution also satisfies the "outgoing wave" ("incoming wave") condition

$$\Phi_l(p,r)|_{r\to\infty} \cong \mp\frac{i}{2}\hat{h}_l^\pm(pr)\mathcal{F}_l^\mp(p). \tag{10}$$

On the other hand one can see that the behavior of the Jost solutions *at the origin* is

$$\chi_l^\pm(p,r)\big|_{r\to 0} = \hat{n}_l(pr)X_l^\pm(p) + \hat{j}_l(pr)Y_l^\pm(p). \tag{11}$$

Therefore, if the condition $X_l^\pm(p) = 0$ holds, then near the origin $\chi_l^\pm(p,r) = \hat{j}_l(pr)Y_l^\pm(p)$. Thus, in such a case $\chi^+(p,r)$ satisfies both conditions demanded for a resonant state. It means that Jost solution χ^+ and regular solution Φ for such p must be multiplies of each other. Thus, if $X_l^\pm(p) = 0$ then $\mathcal{F}_l^\pm(p) = 0$ (and vice versa) as well as

$$\chi_l^\pm(p,r) = \Phi_l(p,r)Y_l^\pm(p) \quad \text{and} \quad \Phi_l(p,r) = \mp\frac{i}{2}\chi_l^\pm(p,r)\mathcal{F}_l^\mp(p). \tag{12}$$

The functions $\chi_l^\pm(p,r)$ may *for all* r be represented in the form

$$\chi_l^\pm(p,r) = \hat{n}_l(pr)X_l^\pm(p,r) + \hat{j}_l(pr)Y_l^\pm(p,r), \tag{13}$$

with the "coefficients" $X_l^\pm(p,r)$ and $Y_l^\pm(p,r)$ being expressed in terms of $\chi_l^\pm(p,r)$:

$$X_l^\pm(p,r) = 1 + \frac{1}{p}\int_r^\infty \hat{j}_l(pr')U(r')\chi_l^\pm(p,r')dr';$$
$$Y_l^\pm(p,r) = \pm i - \frac{1}{p}\int_r^\infty \hat{n}_l(pr')U(r')\chi_l^\pm(p,r')dr'. \tag{14}$$

It is obvious that if $X_l^\pm(p,0) = 0$, then $Y_l^\pm(p,0) = Y_l^\pm(p)$. Using for the Green function expression (8) one can easily find an alternative representation of Jost solutions:

$$\chi_l^\pm(p,r) = \hat{h}_l^+(pr)\mathcal{F}_{1l}^\pm(p,r) - \hat{h}_l^-(pr)\mathcal{F}_{2l}^\pm(p,r). \tag{15}$$

Here the functions $\mathcal{F}_{1,2}^\pm(p,r)$ are expressed in terms of $\chi^\pm(p,r)$ as

$$\mathcal{F}_{1l}^\pm(p,r) = \mathcal{F}_{1l}^\pm + \frac{i}{2p}\int_r^\infty \hat{h}_l^-(pr')U(r')\chi_l^\pm(p,r')dr';$$
$$\mathcal{F}_{2l}^\pm(p,r) = \mathcal{F}_{2l}^\pm + \frac{i}{2p}\int_r^\infty \hat{h}_l^+(pr')U(r')\chi_l^\pm(p,r')dr', \tag{16}$$

where the constants are

$$\mathcal{F}_1^+ = 1; \qquad \mathcal{F}_1^- = 0; \qquad \mathcal{F}_2^+ = 0; \qquad \mathcal{F}_2^- = -1. \tag{17}$$

The functions $X^\pm$,$Y^\pm$ and $\mathcal{F}_{1,2}^\pm$ are connected through

$$X_l^\pm(p,r) = \mathcal{F}_{1l}^\pm(p,r) - \mathcal{F}_{2l}^\pm(p,r); \qquad Y_l^\pm(p,r) = i\left[\mathcal{F}_{1l}^\pm(p,r) + \mathcal{F}_{2l}^\pm(p,r)\right]. \tag{18}$$

Therefore the condition $X_l^\pm(p,0) = 0$ may be represented in the following form:

$$\mathcal{F}_{1l}^\pm(p,0) - \mathcal{F}_{2l}^\pm(p,0) = 0. \tag{19}$$

From (16) and (17) it follows that in terms of Jost solutions this condition means

$$X_l^\pm(p,0) = 1 + \frac{i}{2p}\int_0^\infty \hat{h}_l^-(pr')U(r')\chi_l^\pm(p,r')dr' - \frac{i}{2p}\int_0^\infty \hat{h}_l^+(pr')U(r')\chi_l^\pm(p,r')dr' = 0. \tag{20}$$

Taking into account the behavior of the Riccati-Hankel functions and Jost solutions at the infinity one can conclude that if the potential $U(r)$ does not decrease sufficiently rapidly at $r \to \infty$, then the integrals in (20) converge only in a part of the complex p-plane. Moreover the integrals diverge just in that part of the plane which is the most interesting from the viewpoint of finding resonances. For this purpose we have to continue functions $X_l^\pm(p,0)$ analytically to the other part of the complex p-plane.

In order to do this let us consider the case of analytic potentials. For such potentials we may change the real variable r into the complex variable z and rewrite (1)

$$\left\{\frac{d^2}{dz^2} - \frac{\ell(\ell+1)}{z^2} + p^2 - U(z)\right\}\chi_l^\pm(p,z) = 0. \tag{21}$$

Let us now discuss the solutions of this equation on the ray $z = re^{i\theta}$, $r \in [0,\infty)$ [6–8]. Using the same arguments as before for the solutions $\chi_l^\pm(p,r)$, which on this ray must be written as $\chi_l^\pm(p,z)$ one can obtain the integral Volterra equation

$$\chi_l^\pm(p,z) = \hat{h}_l^\pm(pz) - \int_z^\infty g_l(p;z,z')U(z')\chi_l^\pm(p,z')dz'. \tag{22}$$

From this equation the representation

$$\chi_l^\pm(p,z) = \hat{h}_l^+(pz)\mathcal{F}_{1l}^\pm(p,z) - \hat{h}_l^-(pz)\mathcal{F}_{2l}^\pm(p,z) \tag{23}$$

follows immediately, and the functions $\mathcal{F}_{12}^\pm$ are expressed in terms of the Jost solutions:

$$\mathcal{F}_{1l}^\pm(p,z) = \mathcal{F}_{1l}^\pm + \frac{i}{2p}\int_z^\infty \hat{h}_l^-(pz')U(z')\chi_l^\pm(p,z')dz';$$
$$\mathcal{F}_{2l}^\pm(p,z) = \mathcal{F}_{2l}^\pm + \frac{i}{2p}\int_z^\infty \hat{h}_l^+(pz')U(z')\chi_l^\pm(p,z')dz'. \tag{24}$$

Having an intension to investigate equation (22) numerically we rewrite it as

$$\chi_l^\pm(p,re^{i\theta}) = \hat{h}_l^\pm(pre^{i\theta}) -$$
$$\frac{i}{2p}\int_r^\infty \left[\hat{h}_l^-(pre^{i\theta})\hat{h}_l^+(pr'e^{i\theta}) - \hat{h}_l^+(pre^{i\theta})\hat{h}_l^-(pr're^{i\theta})\right]U(re^{i\theta})\chi_l^\pm(p,r'e^{i\theta})e^{i\theta}dr' \tag{25}$$

Introducing for convenience the denotations

$$\chi_l^{(\theta)\pm}(p,r) = \chi_l^{\pm}(p, re^{i\theta}); \quad \tilde{p} = pe^{i\theta}; \qquad U^{(\theta)}(r) = U(re^{i\theta})e^{i\theta}, \tag{26}$$

one may represent the functions $\chi_l^{(\theta)\pm}(p,r)$ in the following form:

$$\chi_l^{(\theta)\pm}(p,r) = \hat{h}_l^{+}(\tilde{p}r)\mathcal{F}_{1l}^{(\theta)\pm}(p,r) - \hat{h}_l^{-}(\tilde{p}r)\mathcal{F}_{2l}^{(\theta)\pm}(p,r), \tag{27}$$

which is analogous to (15) and the functions $\mathcal{F}_{2l}^{\pm}$ can be expressed in terms of $\chi_l^{(\theta)\pm}(p,r)$ as

$$\begin{aligned} \mathcal{F}_{1l}^{(\theta)\pm}(p,r) &= \mathcal{F}_{1l}^{\pm} + \frac{i}{2p}\int_r^{\infty} \hat{h}_l^{-}(\tilde{p}r')U^{(\theta)}(r')\chi_l^{(\theta)\pm}(p,r')dr'; \\ \mathcal{F}_{2l}^{(\theta)\pm}(p,r) &= \mathcal{F}_{2l}^{\pm} + \frac{i}{2p}\int_r^{\infty} \hat{h}_l^{+}(\tilde{p}r')U^{(\theta)}(r')\chi_l^{(\theta)\pm}(p,r')dr', \end{aligned} \tag{28}$$

similar to (16). But the region of validity of these formulas (which depends on angle θ) in the complex p-plane is different from that of (16).

The condition $\chi_l^{\pm}(p,0) = 0$ means that $\chi_l^{(\theta)\pm}(p,0) = 0$, that is

$$\mathcal{F}_{1l}^{(\theta)\pm}(p,0) - \mathcal{F}_{2l}^{(\theta)\pm}(p,0) = 0. \tag{29}$$

Taking into account that $\mathcal{F}_1^{\pm} - \mathcal{F}_2^{\pm} = 1$ the condition (29) may be written as

$$1 + \frac{i}{2p}\int_0^{\infty} \hat{h}_l^{-}(\tilde{p}r')U^{(\theta)}(r')\chi_l^{(\theta)\pm}(p,r')dr' - \frac{i}{2p}\int_0^{\infty} \hat{h}_l^{+}(\tilde{p}r')U^{(\theta)}(r')\chi_l^{(\theta)\pm}(p,r')dr' = 0. \tag{30}$$

To solve equation (25) we approximate the potential $U^{(\theta)}(r)$ with a superposition of the δ-potentials (r is real)

$$U^{(\theta)}(r) \to \sum_{k=1}^{N} U_k^{(\theta)}\delta(r - r_k); \quad r_k = r_{max} - h(k-1); \quad h = \frac{r_{max}}{N}; \quad U_k^{(\theta)} = U^{(\theta)}(r_k)h. \tag{31}$$

After such a change the integrals in (25) become sums and we obtain

$$\begin{aligned} \chi_l^{(\theta)\pm}(p,r) &= \hat{h}_l^{+}(\tilde{p}r)\left[\mathcal{F}_{1l}^{\pm} + \frac{i}{2p}\sum_{k=1}^{N}\Theta(r_k - r)\hat{h}_l^{-}(\tilde{p}r_k)U_k^{(\theta)}(r')\chi_l^{(\theta)\pm}(p,r_k)\right] - \\ &- \hat{h}_l^{-}(\tilde{p}r)\left[\mathcal{F}_{2l}^{\pm} + \frac{i}{2p}\sum_{k=1}^{N}\Theta(r_k - r)\hat{h}_l^{+}(\tilde{p}r_k)U_k^{(\theta)}(r')\chi_l^{(\theta)\pm}(p,r_k)\right], \end{aligned} \tag{32}$$

where $\Theta(r_k - r)$ is the Heaviside step function. Now we can easily find all $\chi_l^{(\theta)\pm}(p,r_j)$:

$$\begin{aligned} \chi_l^{(\theta)\pm}(p,r_j) &= \hat{h}_l^{+}(\tilde{p}r_j)\left[\mathcal{F}_{1l}^{\pm} + \frac{i}{2p}\sum_{k=1}^{j-1}\hat{h}_l^{-}(\tilde{p}r_k)U_k^{(\theta)}(r)\chi_l^{(\theta)\pm}(p,r_k)\right] - \\ &- \hat{h}_l^{-}(\tilde{p}r_j)\left[\mathcal{F}_{2l}^{\pm} + \frac{i}{2p}\sum_{k=1}^{j-1}\hat{h}_l^{+}(\tilde{p}r_k)U_k^{(\theta)}(r)\chi_l^{(\theta)\pm}(p,r_k)\right]. \end{aligned} \tag{33}$$

$\chi_l^{(\theta)\pm}(p, r_1) = \hat{h}_l^{\pm}(\tilde{p} r_1)$ we can determine all $\chi_l^{(\theta)\pm}(p, r_j)$ step by step. Having calculated all these values we can finally find the expression

$$\mathcal{F}_{1l}^{(\theta)\pm}(p,0) - \mathcal{F}_{2l}^{(\theta)\pm}(p,0) = 1 + \frac{i}{2p}\sum_{k=1}^{N} \hat{h}_l^{-}(\tilde{p} r_k) U_k^{(\theta)}(r) \chi_l^{(\theta)\pm}(p, r_k) - \frac{i}{2p}\sum_{k=1}^{N} \hat{h}_l^{+}(\tilde{p} r_k) U_k^{(\theta)}(r) \chi_l^{(\theta)\pm}(p, r_k) \quad (34)$$

For the numerical treatment we consider analytical potentials

$$U(r) = U_0 r^n e^{-r}. \quad (35)$$

On figure 1 we present the results computed using expression (34) for these potentials

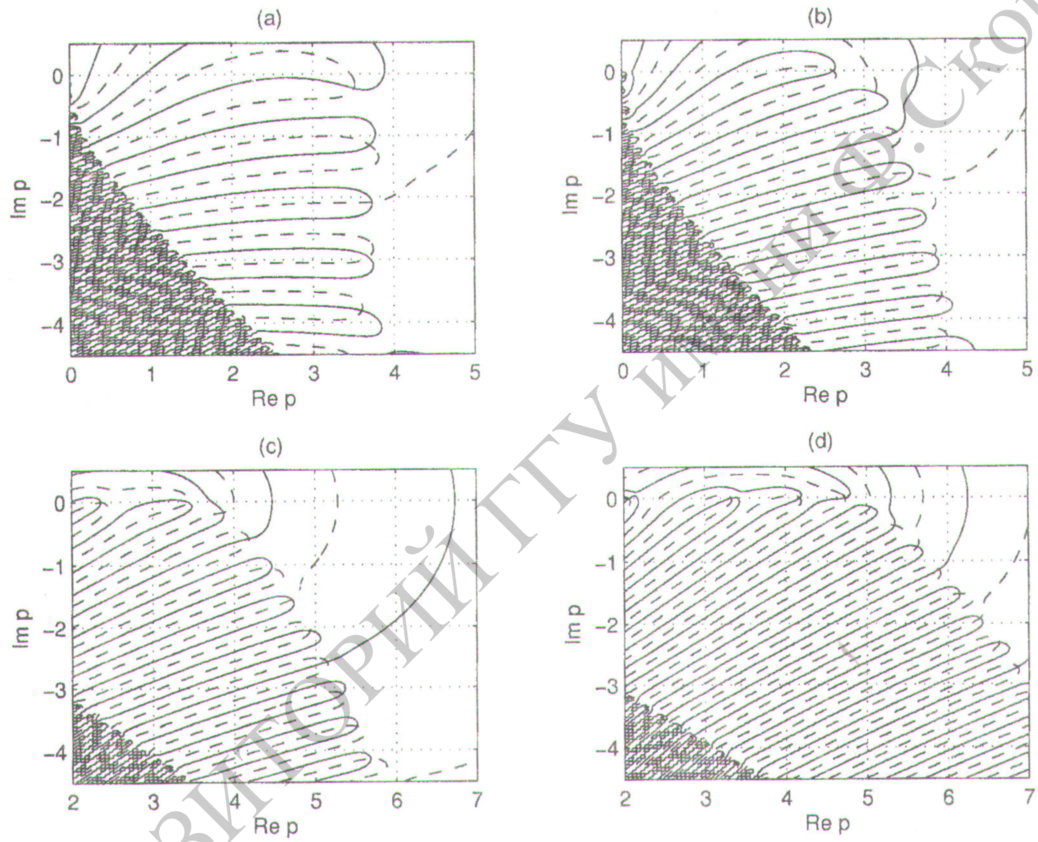

Рис. 1: The real and the imaginary parts of the expression (34) in the complex p-plane at zero level. Points of intersection correspond to resonances of the potentials (35) with parameters: a)$V_0 = 30$; $n = 1(\theta = 1)$, b)$V_0 = 15$; $n = 2(\theta = 1)$, c)$V_0 = 10$; $n = 3(\theta = 0.8)$, d)$V_0 = 5$; $n = 4(\theta = 0.7)$.

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References

1. Taylor J R 1972 *Scattering theory* (New-York, London, Sydney, Toronto, John Wiley & Sons, Inc)

2. R.G. Newton 1966 *Scattering theory of waves and particles* (New-York, San Francisco, St. Louis, Toronto, London, Sydney: McGraw-Hill Book, Inc.)

3. Gamow G 1928 *Z.Phys.* **51** 204

4. Siegert A J F 1939 *Phys. Rev.* **56** 750

5. Kukulin V I, Krasnopol'sky V M, and Horáček J 1989 *Theory of Resonances: Principles and Applications* (Academia, Praha)

6. *Lecture Notes in Physics* **325** 1989 (Ed. Brändas E. and Elander N., Springer Verlag, Heidelberg)

7. Sofianos S A, Rakityansky S A 1997 *J. Phys. A: Math. Gen.* **30** 3725

8. Rakityansky S A, Sofianos S A 1998 *J. Phys. A: Math. Gen.* **31** 5149

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