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REMARK TO THE PROBLEM OF EIGENVALUES OF SCHRÖDINGER EQUATION

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It is very important to find out quickly and with a satisfactory precision if an obtained potential, i.e. a certain function of the Schrödinger equation in the so called inverse problem of nuclear physics, leads to bound states or not.

From the mathematical point of view we have the following problem: The linear differential equation of the second order

$$u'' + \lambda^2 u = V(x)\, u \tag{1}$$

is given where $V(x)$ is the potential satisfying the relation

$$\int_0^\infty x|V(x)|\,\mathrm{d}x < \infty \tag{2}$$

and λ is a complex number.

If λ^2 is an eigenvalue, i.e. there is a nontrivial solution of the differential equation in the interval $(0, +\infty)$ fulfilling homogeneous boundary conditions at the both ends of the interval, we shall say that there is a bound state.

It is possible to prove that under the condition (2) there is a finite number of bound states.

We shall consider solutions $u_1(x, \lambda)$, $u_2(x, \lambda)$ of the given differential equatial equation (2) determined by conditions:

$$u_1(0, \lambda) = 0\,, \quad u_1'(0, \lambda) = 1 \tag{3}$$

$$\lim_{x\to\infty} e^{i\lambda x}\, u_2(x, \lambda) = 1\,. \tag{4}$$

The existence as well as their properties are discussed in [1] in detail (see [1], Chapter I). Further we shall introduce the function $S(\lambda) = u_2(0, \lambda)/u_2(0, -\lambda)$; it holds $|S(\lambda)| = 1$.

For real values of λ let us write $S(\lambda) = e^{2i\delta(\lambda)}$, then from the equation

$$u_1(x, \lambda) = \frac{1}{2i\lambda} [u_2(x, -\lambda) \overline{u_2(0, -\lambda)} - u_2(x, \lambda) \overline{u_2(0, \lambda)}]$$

(see [1], Chapter II, §3) which holds for real values λ, and from (4) the asymptotic relation

$$u_1(x, \lambda) \sim A(\lambda) \sin(\lambda x + \delta(\lambda)) \quad x \to \infty$$

follows. The function $\delta(\lambda)$ is called the asymptotic phase.

The following theorem holds (see [1]; Theorem 2 in Addition I is applied to only one equation).

Theorem. *Let be given differential equation* (1), *let us suppose that condition* (2) *holds. Then the number of eigenvalues is*

$$r = \frac{1}{\pi} [\delta(0) - \delta(\infty)] - \tfrac{1}{2} q$$

where $q = 0$ *if* $S(0) = 1$, $q = 1$ *otherwise.*

Let $V(x)$ be defined as follows:

$$(5) \qquad V(x) = \begin{cases} -V_0 & \text{for} \quad 0 \leqq x < 1 \\ 0 & \text{for} \quad 1 \leqq x < \infty \end{cases} .$$

Then it is possible to find the asymptotic phase in an analytic way. We obtain by a simple computation that

$$(6) \qquad \delta(\lambda) = \arctan \left[\frac{\lambda}{\sqrt{(\lambda^2 + V_0)}} \operatorname{tg} \sqrt{(\lambda^2 + V_0)} \right] - \lambda .$$

Let us consider in relation (6) always the branch of the function arctan so that the function $\delta(\lambda)$ be continuous, then we obtain

$$\delta(0) - \delta(\infty) = (n + \tfrac{1}{2}) \pi \quad \text{for} \quad \sqrt{(V_0)} = \frac{\pi}{2} + n\pi$$

$$\delta(0) - \delta(\infty) = (n + 1) \pi \quad \text{for} \quad \frac{\pi}{2} + n\pi < \sqrt{(V_0)} < \frac{\pi}{2} + (n + 1) \pi$$

and hence for $\pi/2 + n\pi \leqq \sqrt{(V_0)} < \pi/2 + (n + 1) \pi$ there exist $n + 1$ bound states.

In many cases however it is not possible to determine the analytical form of the solution of the given problem. We show that the same result can be reached by numerical computation.

We transform the equation (1) to the equation

$$(7) \qquad y'(x) = -\frac{V(x)}{\lambda}\sin^2(\lambda x + y)$$

which together with the initial condition

$$(8) \qquad y(0) = 0$$

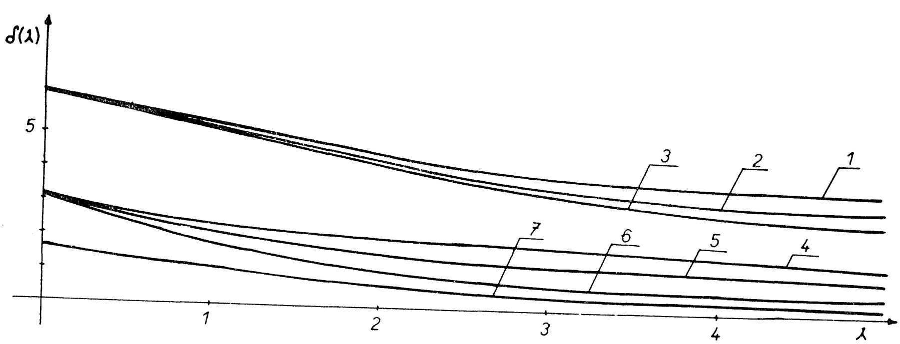
yields at infinity directly the asymptotic phase. It holds

$$\lim_{x\to\infty} y(x, \lambda) = \delta(\lambda) \quad (\text{see [2]}).$$

If the function $V(x)$ is defined by equality (5) then it is sufficient to calculate by the numerical integration of the equation (7) $y(1, \lambda)$ which in our case is $\delta(\lambda)$, and the value $1/\pi \lim_{\lambda\to 0} \delta(\lambda)$ gives the number of eigenvalues of the equation (1) when $\sqrt{(V_0)} \neq \pi/2 + n\pi$; otherwise it is $1/\pi \lim_{\lambda\to 0} \delta(\lambda) - \frac{1}{2}$. So generally the integer part of the value $1/\pi \lim_{\lambda\to 0} \delta(\lambda)$ gives the number of eigenvalues of the equation (1). On the figure the asymptotic phases for different depths of potential hole are shown so as they were obtained on the computer.

We can see that a small change of the value V_0 does not need to affect $\delta(\lambda)$ for $\lambda = 0$ which assume only discrete values.

We can also use an analogous scheme for another form of function $V(x)$ where the condition (2) is fulfilled; of course we have to integrate the equation (7) on a longer interval.



CURVE	7	6	5	4	3	2	1
Vo	$\frac{\pi^2}{4}$	$\pi^2-0.5$	π^2	$\pi^2+0.5$	$4\pi^2-0.5$	$4\pi^2$	$4\pi+0.5$

Fig. 1.

References

[1] *З. С. Агронович, В. А. Марченко:* Обратная задача теории рассеяния, Харьков, 1960.
[2] *Г. Ф. Друкарев:* ЖЗТФ, 19, 247 (1949).

Souhrn

POZNÁMKA K PROBLÉMU VLASTNÍCH ČÍSEL SCHRÖDINGEROVY ROVNICE

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V práci je ukázán efektivní způsob určení počtu vlastních čísel u Schrödingerovy rovnice.

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