SURFACES WITH AN INTERNAL STRUCTURE

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Zero-range potentials with internal structure allow to construct quantum-mechanical models of various physical phenomena. In this lecture, we discuss a particular class of operators of this type, which can be used for description of surface phenomena in solid-state phisics.

The concept of zero-range potentials with internal structure proposed in [1] opens way to construction of new exactly solvable quantum mechanical models. In the present paper this method is used to discuss the surface effects. The boundary-contact problem without internal structure was investigated rigorously earlier by B.P.Belinsky [2]. In distinction to the work of Karwowsky [3] who considered the simplest model of a translationally invariant surface, our method allows to treat the translationally invariant surfaces as well as periodic structures. Our approach is similar to the method of Ref. [4], where a similar mathematical construction was applied to the description of energy-dependent two-body problems in few-body physics.

The scattering on a surface, described in Sec.I is quite similar to the two-particle scattering. The spectrum of the corresponding operator is purely continuous. It consists of two branches : the branch of the scattered waves and the waveguide branch, which represents an analogue to bound states. The eigenfunctions corresponding to the first branch describe various processes of transmission and reflection of the plane waves. We consider here only the simplest case of a planar surface, but all the results can be generalised for an arbitrary shaped surface. Such a generalisation, however, does not yield an exactly solvable model.

The presence of a potential barrier (considered in Sec. 3) splits the scattering branch of the continuous spectrum into two parts.The surface waves described in Sec.2 can propagate with a velocity which differs from the velocity of the "external" waves. At the same time the waveguide branch of the spectrum changes. The space anisotropy of the surface modifies the waveguide functions in a typical way. Sec.4 is devoted to description of a model of a zero-range defect localised near the surface with an internal structure. In the last Section we discuss a surface with a periodical structure.

1. Formulation of the problem

Let Γ denote a plane in R^3,

$$\Gamma = \left\{ x=(x,y,z) \in R^3,\ z=0 \right\}$$

Let $A_0 = -\Delta$ be the self-adjoint Laplace operator in $L^2(R^3)$ with the standart domain $D(A_0)=W_2^2(R^3)$. We restrict this operator to $C_0^\infty(R^3\setminus\Gamma)$,

$$A_{00} = A_0 \restriction C_0^\infty(R^3\setminus\Gamma)$$

where $C_0^\infty(\Omega)$ denotes the set of all infinitely differentiable functions with a compact support contained in Ω. This symmetric operator has infinite deficiency indices. The boundary form of the adjoint operator A_{00} restricted to the linear set of smooth functions can be written in terms of the limits of functions and their derivatives taken from the different sides of the plane Γ :

$$u_0^{\pm}(x,y) = u_0(x,y,\pm 0)$$

$$\frac{\partial u_0^{\pm}}{\partial n}(x,y) = \frac{\partial u_0^{\pm}}{\partial n}(x,y,\pm 0)$$

Then the boundary form can be expressed as follows :

$$\left\langle A_{00}^* u_0, v_0 \right\rangle - \left\langle u_0, A_{00}^* v_0 \right\rangle = \iint dx\, dy \left\{ \left[\frac{\partial u_0}{\partial n}\right] \overline{\langle v_0 \rangle} + \left\langle \frac{\partial u_0}{\partial n} \right\rangle \overline{[v_0]} - \right.$$

$$\left. - [u_0] \overline{\left\langle \frac{\partial v_0}{\partial n} \right\rangle} - \langle u_0 \rangle \overline{\left[\frac{\partial v_0}{\partial n}\right]} \right. \equiv [u_0, v_0]^{\partial} \qquad (I.I)$$

where :

$$[u_0] = u_0^+ - u_0^- \qquad \left[\frac{\partial u_0}{\partial n}\right] = \frac{\partial u_0^+}{\partial n} - \frac{\partial u_0^-}{\partial n}$$

$$\langle u_0 \rangle = (u_0^+ + u_0^-)/2 \qquad \left\langle \frac{\partial u_0}{\partial n} \right\rangle = \frac{1}{2}\left(\frac{\partial u_0^+}{\partial n} + \frac{\partial u_0^-}{\partial n}\right)$$

In order to add an internal structure we choose self-adjoint operators A_i, $i = 1,2$ acting in Hilbert spaces H_i. In accordance with the standart procedure [1], we restrict these operators to symmetric operators with deficiency indices (1,1). An arbitrary element from the domain of the adjoint operator A_{i0}^* can be represented in the following form :

$$u_i = u_i^+ w_+^i + u_i^- w_-^i + \tilde{u}_i$$

where $\tilde{u}_i \in D(A_{i0})$ and $w_\pm^i$ are basis elements in the deficiency subspaces [1] . The boundary form of the adjoint operator can be described in terms of the "boundary" values u_i^+, u_i^- :

$$\langle A_{i0}^* u_i, v_i \rangle - \langle u_i, A_{i0}^* v_i \rangle = u_i^- \overline{v_i^+} - u_i^+ \overline{v_i^-} \equiv [u_i, v_i] \qquad (1.2)$$

Now we can construct symmetric operators with infinite deficiency indices. We start with self-adjoint operators defined in the Hilbert spaces $L^2(R^2, H_i)$ as follows :

$$(\mathcal{A}_i u)(x,y) = -\left(\frac{\partial^2 u_i}{\partial x^2} + \frac{\partial^2 u_i}{\partial x^2}\right)(x,y) + (A_i u_i)(x,y)$$

$$D(\mathcal{A}_i) = W_2^2(R^2, D(A_i))$$

We restrict these operators to the linear set of smooth functions $C^\infty(R^2, D(A_{i0}))$. The boundary form of the adjoint operator restricted to the set of smooth functions can be written as :

$$\langle \mathcal{A}_{i0}^* u_i, v_i \rangle - \langle u_i, \mathcal{A}_{i0}^* v_i \rangle = \iint dx\, dy\, (u_i^- \overline{v_i^+} - u_i^+ \overline{v_i^-}) \equiv [u_i, v_i]^\partial \qquad (1.3)$$

We shall consider the symmetric operator $\mathcal{L}_0$ acting in the Hilbert space

$$L_2(R^3) \oplus L_2(R^2, H_1) \oplus L_2(R^2, H_2)$$

whose elements are denoted by $U=(u_0,u_1,u_2)$ as follow

$$\mathcal{L}_0 = \mathcal{A}_{00} \oplus \mathcal{A}_{10} \oplus \mathcal{A}_{20}$$

This operator has infinite deficiency. The boundary form of its adjoint on the set of smooth functions represents a sum of boundary forms of the operators $\mathcal{A}_{00}, \mathcal{A}_{10}, \mathcal{A}_{20}$:

$$\langle \mathcal{L}_0^* U, V \rangle - \langle U, \mathcal{L}_0^* V \rangle = \sum_{\alpha=0}^{2} [u_\alpha, v_\alpha]^\partial$$

This form vanishes on the domain $D_0^{\alpha\beta}$ which is determined by the boundary conditions :

$$\left[\frac{\partial u_0}{\partial n}\right] = \alpha u_1^- \qquad [u_0] = \beta u_2^+ \tag{1.4}$$
$$u_1^+ = \bar{\alpha} \langle u_0 \rangle \qquad u_2^- = \bar{\beta} \left\langle \frac{\partial u_0}{\partial n} \right\rangle$$

Thus the restriction of the adjoint operator $\mathcal{L}_0^*$ to the domain $D_0^{\alpha\beta}$ is a below semibounded symmetric operator. We can therefore construct Friedrichs extention $\mathcal{L}^{\alpha\beta}$ of the symmetric operator $\mathcal{L}_0$. One can show that $\mathcal{L}^{\alpha\beta}$ does not coincide with the original operator so this Friedrichs extension is not trivial. The spectrum of this operator is purely continuous. There exist two branches of the continuous spectrum : the scattering branch and the waveguide branch. The external component of the scattered waves can be decomposed into plain waves of three types :

incoming waves $\exp i(k,x)$
reflected waves $R \exp i(\tau k,x)$
transmitted waves $S \exp i(k,x)$
(see Fig.1)
where :

$$\tau(k_x,k_y,k_z) = (k_x,k_y,-k_z)$$

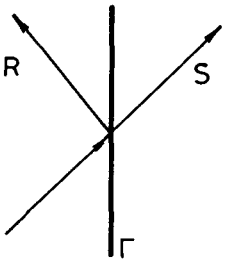

Fig. 1

The external component satisfies the following equation :

$$-\Delta u_0 = k^2 u_0$$

The boundary values for the external component are :

$$\langle u_0 \rangle = \frac{1}{2} (1 + S + R) \exp i(k_x x + k_y y)$$

$$[u_0] = (S - 1 - R) \exp i(k_x x + k_y y)$$

$$\left\langle \frac{\partial u_0}{\partial n} \right\rangle = \frac{ik_z}{2} (1 + S - R) \exp i(k_x x + k_y y)$$

$$\left[\frac{\partial u_0}{\partial n} \right] = ik_z (S - 1 + R) \exp i(k_x x + k_y y) \qquad (1.5)$$

The internal components are assumed to be of the following form :

$$u_i(x,y) = f(x,y)\, u_i$$

where $f \in W^2_{2,loc}(R^2)$, $u_i \in H_i$. Let $f(x,y)$ be given by

$$f(x,y) = \exp i(k_x x + k_y y)$$

We obtain the following equations for elements of the internal spaces H_i :

$$A_{i0} u_i = (K^2 - k_x^2 - k_y^2)\, u_i = k_z^2\, u_i$$

It follows [1] that

$$\frac{u_i^-}{u_i^+} = D_i(k_z^2)$$

where D_i are Schwarz integrals of the internal operators A_i on the deficiency elements Θ_i :

$$D_i(\quad) = \left\langle \frac{I + \lambda A_i}{A_i - \lambda} \Theta_i, \Theta_i \right\rangle$$

Substituting $u_0^{\pm}$, $u_i^{\pm}$ into the boundary conditions (1.4), we can calculate the transmission and reflection amplitudes :

$$S = \frac{\left(\frac{|\alpha|^2}{2D_1} - \frac{2}{|\beta|^2 D_2}\right) ik_z}{\left(ik_z - \frac{|\alpha|^2}{2D_1}\right)\left(ik_z - \frac{2}{|\beta|^2 D_2}\right)}$$

$$R = \frac{(ik_z)^2 - \frac{|\alpha|^2}{2D_1} \quad \frac{2}{|\beta|^2 D_2}}{(ik_z - \frac{|\alpha|^2}{2D_1})\ (ik_z - \frac{2}{|\beta|^2 D_2})} \tag{1.6}$$

They fulfil the identity :

$$|R|^2 + |S|^2 = 1$$

The internal components u_1, u_2 of U can be easily calculated in terms of the deficiency elements θ_i.

Let us investigate now behaviour of the scattering matrics in the case of a weak coupling between the internal and external channels, $\alpha \to 0$ and $\beta \to 0$. The transmission amplitude S vanishes if

$$\frac{|\alpha|^2}{2D_1} - \frac{2}{|\beta|^2 D_2} = 0$$

The zero lines of this equation in the (k,t) - plane coincide (approximately) with the zero lines of the function D_1/D_2 . The reflection amplitude R vanishes if

$$D_1 D_2 = \frac{|\alpha|^2}{|\beta|^2} \frac{1}{(ik_z)^2}$$

The eigenfunction of this type form the $[0,\infty)$ branch of the continuous spectrum.

The external component of waveguide functions can be found in the following way : we put

$$u_0(x,y,z) = \begin{cases} B^+ \exp(-\varkappa z) & \exp i(k_x x + k_y y),\ z>0\ ,\ \varkappa > 0 \\ B^- \exp(\varkappa z) & \exp i(k_x x + k_y y),\ z<0\ ,\ \varkappa > 0 \end{cases} \tag{1.8}$$

So the boundary values are

$$\left[\frac{\partial u_0}{\partial n}\right] = -\varkappa\ (B^+ + B^-)\ \exp i(K_x x + k_y y)$$

$$\left\langle \frac{\partial u_0}{\partial n} \right\rangle = \frac{\varkappa}{2} (B^- - B^+) \exp i(k_x x + k_y y)$$

$$\left[u_0 \right] = (B^+ - B^-) \exp i(k_x x + k_y y)$$

$$\left\langle u_0 \right\rangle = \frac{1}{2} (B^+ + B^-) \exp i(k_x x + k_y y)$$

The conditions (1.4) now yield

$$\left[\frac{\partial u_0}{\partial n} \right] = \frac{|\alpha|^2}{D_1(-\varkappa^2)} \left\langle u_0 \right\rangle$$

$$\left[u_0 \right] = |\beta|^2 D_2(-\varkappa^2) \left\langle \frac{\partial u_0}{\partial n} \right\rangle \tag{1.9}$$

The constants B^+, B^- satisfy the following homogeneous linear system of equations

$$(\varkappa + \frac{|\alpha|^2}{2 D_1}) B^+ + (\varkappa + \frac{|\alpha|^2}{2 D_1}) B^- = 0$$

$$(1 + \varkappa \frac{|\beta|^2 D_2}{2}) B^+ - (1 + \varkappa \frac{|\beta|^2 D_2}{2}) B^- = 0 \tag{1.10}$$

which has a nontrivial solution only in the following cases

$$\varkappa + \frac{|\alpha|^2}{2 D_1} = 0$$

$$1 + \varkappa \frac{|\beta|^2 D_2}{2} = 0 \tag{1.11}$$

The solution of the first equation in (1.11) gives symmetric waveguide functions while the solution of the second equation gives the antisymmetric ones. In the weak-coupling case the solutions of the equations (1.11) are near to the zero lines of D_1 and D_2^{-1}, respectively. The waveguide eigenfunctions correspond to the following branches of the continuous spectrum :

$$[-\varkappa_i^2, \infty) \quad ,$$

where $\varkappa_i$ are arbitrary real solutions of one of the equations (1.11).

A screen with an internal structure allows us to construct a resonance transmission of plane waves across the surface. The external components S_{oo} of the scattering matrix depends on the normal component of the momentum k_z. In this way we can obtain waveguide eigenfunctions in this surface model.

2. Velocity of waves in the internal space

In this section we are going to describe a model of the surface with a special internal channel. The velocity of internal waves is, in general, different from the velocity of the external ones. Let $\mathcal{A}_i$ be the unperturbed internal operator :

$$\mathcal{A}_i = - c_i^2 \Delta_{xy} + A_i$$

The constants $c_i \in R_+$ are velocities of the internal waves. One can construct a self-adjoint operator following the procedure outlined in the previous section.

The spectrum of such an operator is also purely continuous and all eigenfunctions can be calculated in the same way as in the Sec.1. The waveguide functions depends on the quasi-momentum $t=(t_x,t_y)$ and the same is true for the energy λ. One can easily obtain the dispersion equations :

$$- (\lambda - t^2) + \frac{|\alpha|^2}{2\, D_1(\lambda - c_1^2\, t^2)} = 0 \tag{2.1}$$

$$-1 + (\lambda - t^2) \frac{|\beta|^2\, D_2(\lambda - c_1^2\, t^2)}{2} = 0 \tag{2.2}$$

Let us investigate the solution of these equations in the case of weak coupling between the external and internal channels. There are two different cases to be distinguished

1) $c_i > 1$
2) $c_i < 1$

In the first case all energy bands are finite while in the second case they are infinite. We shall prove this result graphically using Fig.2 . Zero lines of the Schwarz integral $D_1(-c_1^2 t^2)$ are parabolas $\lambda - c_1^2\, t^2 = \text{const}$ denoted by the dotted lines. In the

case $c_1 > 1$, the parabolas of this family intersect the parabola $\lambda = t^2$ or lie inside it (Fig.2a). If $c_1 < 1$ then the parabolas lie in the exterior of the parabola $\lambda = t^2$ or intersect it (Fig.2b).

Solutions to the equations (2.1), (2.2) are situated near the zero lines of the Schwarz integrals in the region $\lambda < t^2$. They are denoted by full lines on the figures. The projection of the solutions on the energy axis yield the spectral bands of the corresponding operator.

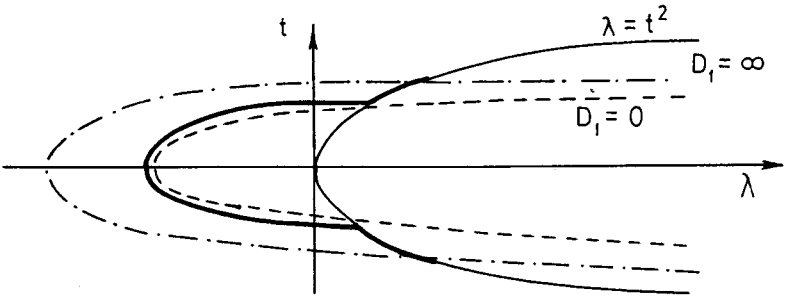

Fig.2a

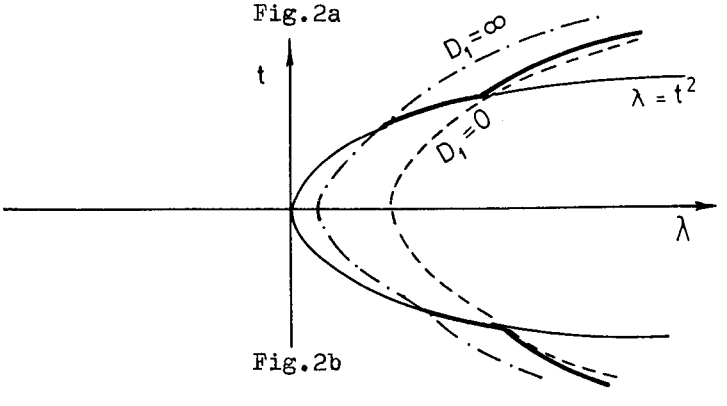

Fig.2b

The simplest generalisation of this model is connected with the space anisotropy of the surface. Suppose that the unperturbed internal operator $\mathcal{A}_i$ is of the form :

$$\mathcal{A}_i = - c_{ix}^2 \frac{\partial^2}{\partial x^2} - c_{iy}^2 \frac{\partial^2}{\partial x^2} + A_i$$

In the case $c_{ix}=c_{iy}$, the diagrams on Fig.2 become three-dimensional. Solutions to the corresponding equations lie near the zero surfaces of the functions $D_1(\lambda - c_{1x}^2 t_x^2 - c_{1y}^2 t_y^2)$ and

$$D_2^{-1}(\lambda - c_{2x}^2 t_x^2 - c_{2y}^2 t_y^2)$$

The picture is symmetric with respect to the energy axis. The waveguide functions can propagate nearly in a **particular** direction in one of the following cases :

$$c_{ix} \gg c_{iy} \qquad \text{or} \qquad c_{ix} \ll c_{iy}$$

The corresponding energy bands are infinite if in some direction the velocity of the internal wave is less than the velocity of the external one .

3. Surfaces with a potential barrier

Suppose now that the external unperturbed operator is of the form $\mathcal{A}_0 = -\Delta + q(z)$, where

$$q(z) = \begin{cases} 0, & z > 0 \\ -A, & z < 0 \end{cases}$$

For some $A > 0$ we can construct the internal structure in the same way as in Sec.1. The model is now nonsymmetric with respect to the plane Γ . Consequently the scattering matrices are different in the positive and negative z-axis directions, (S^+,R^+) and (S^-,R^-) respectively.

The external component of the scattered waves have the same form, as in the previous cases but the momenta of the incoming and transmitted waves are different. If we have an incoming wave of a momentum $k' = (k'_x, k'_y, k'_z)$, $k'_z > 0$ the reflected wave has the momentum $\tau k'$ and the transmitted one $k = (k'_x, k'_y, k'^2_z - A)$. If $k'_z - A < 0$, then the transmitted wave is damped. The standard procedure gives us the following results :

$$S^+ = \frac{2\, ik'_z \left(\frac{|\alpha|^2}{2\, D_1} - \frac{2}{|\beta|^2 D_2} \right)}{\left(ik_z - \frac{|\alpha|^2}{2\, D_1}\right)\left(ik'_z - \frac{2}{|\beta|^2 D_2}\right) + \left(ik'_z - \frac{|\alpha|^2}{2\, D_1}\right)\left(ik_z - \frac{2}{|\beta|^2 D_2}\right)}$$

$$R^+ = \frac{\left(ik_z - \frac{|\alpha|^2}{2\, D_1}\right)\left(ik'_z + \frac{2}{|\beta|^2 D_2}\right) + \left(ik'_z + \frac{|\alpha|^2}{2\, D_1}\right)\left(ik_z - \frac{2}{|\beta|^2 D_2}\right)}{\left(ik_z - \frac{|\alpha|^2}{2\, D_1}\right)\left(ik'_z - \frac{2}{|\beta|^2 D_2}\right) + \left(ik'_z - \frac{|\alpha|^2}{2\, D_1}\right)\left(ik_z - \frac{2}{|\beta|^2 D_2}\right)}$$

One can check directly that $R^+ = 1$ holds for $k_z' < A$; in this case the incoming wave is totally reflected by the potential barrier.

The eigenfunctions of this type form the waveguide branch $[-A,\infty)$ of the continuous spectrum.

The scattered waves corresponding to the normal component of the incoming wave $k_z < 0$ can be described in the same way :

$$S^- = \frac{2\, ik_z \left(\frac{2}{|\beta|^2 D_2} - \frac{|\alpha|^2}{2\, D_1} \right)}{\left(ik_z' + \frac{|\alpha|^2}{2\, D_1}\right)\left(ik_z + \frac{2}{|\beta|^2 D_2}\right) + \left(ik_z + \frac{|\alpha|^2}{2\, D_1}\right)\left(ik_z' + \frac{2}{|\beta|^2 D_2}\right)}$$

$$R^- = \frac{\left(ik_z' + \frac{|\alpha|^2}{2\, D_1}\right)\left(ik_z - \frac{2}{|\beta|^2 D_2}\right) + \left(ik_z - \frac{|\alpha|^2}{2\, D_1}\right)\left(ik_z' + \frac{2}{|\beta|^2 D_2}\right)}{\left(ik_z' + \frac{|\alpha|^2}{2\, D_1}\right)\left(ik_z + \frac{2}{|\beta|^2 D_2}\right) + \left(ik_z + \frac{|\alpha|^2}{2\, D_1}\right)\left(ik_z' + \frac{2}{|\beta|^2 D_2}\right)}$$

These eigenfunctions form the branch $[0,\infty)$ of the continuous spectrum.

If $\frac{|\alpha|^2}{2\, D_1} - \frac{2}{|\beta|^2 D_2} = 0$ then the transmission amplitudes $S^{\pm}$ are equal to zero. while the moduli of the corresponding reflection amplitudes are equal to one.

The waveguide functions can be constructed in the standard form

$$u_0(x,y,z) = \begin{cases} B^+ \exp(-\varkappa z) \exp i(k_x x + k_y y) \ , & z > 0 \\ B^- \exp(+\varkappa' z) \exp i(k_x x + k_y y) \ , & z < 0 \end{cases} \qquad \varkappa, \varkappa' > 0 \qquad \varkappa' = \sqrt{\varkappa^2 - A}$$

One can easily obtain the following dispersion equations :

$$\frac{|\beta|^2 D_2}{2} = - \frac{\varkappa + \varkappa' + 2\, \frac{|\alpha|^2}{2\, D_1}}{2\varkappa\varkappa' + (\varkappa + \varkappa')\, \frac{|\alpha|^2}{2\, D_1}}$$

$$-\frac{|\alpha|^2}{2\,D_1} = \frac{\varkappa+\varkappa'+2\varkappa\varkappa'\frac{|\beta|^2 D_2}{2}}{2+(\varkappa+\varkappa')\frac{|\beta|^2 D_2}{2}}$$

Thus the potential barrier splits the scattering branch of the spectrum into two parts $[-A,\infty)$ and $[0,\infty)$ and changing at the same time the waveguide branch.

4. A zero-range defect near the surface

Let us restrict the self-adjoint operator $\mathcal{L}^{\alpha\beta}$ of the section 1 to the linear set of smooth functions vanishing in a neighbourhood of a point $(0,0,-z_0)$, $z_0>0$. The obtained symmetric operator $\mathcal{L}^{\alpha\beta}_{z_0}$ has the deficiency indices (1,1). The external component of an element from the domain of the adjoint operator $(\mathcal{L}^{\alpha\beta}_{z_0})^*$ has the following asymptotic behaviour in a neighbourhood of the point z_0 :

$$u_0(x,y,z) \sim \frac{u_0^+}{4\pi R_1} + u_0^- + o(R_1)$$

where $R_1=(x,y,z+z_0)$. The boundary form of the adjoint operator can be written in the standard way

$$\left\langle \mathcal{L}^{\alpha\beta *}_{z_0} U,\ V \right\rangle - \left\langle U, \mathcal{L}^{\alpha\beta *}_{z_0} V \right\rangle = u_0^- \overline{v_0^+} - u_0^+ \overline{v_0^-} = [U,V]^{ex} \qquad (4.1)$$

The deficiency element $G(k)$ corresponding to the spectral parameter $k=\sqrt{\lambda}$, $\operatorname{Im} k>0$, has the external component of the following type:

$$G_0 = \begin{cases} \dfrac{\exp ikR_1}{4\pi R_1} + \tilde{G}_0 , & z<0 \\ \tilde{G}_0 , & z>0 \end{cases}$$

where $\tilde{G}_0$ is the result of scattering of the spherical wave $\dfrac{\exp ikR_1}{4\pi R_1}$ on the surface with the internal structure. The unknown function G_0 can be calculated with the help of the following expansion (see[5])

$$\frac{\exp ikR_1}{4\pi R_1} = \frac{ik}{8\pi^2}\int_0^{\pi/2-i\infty} d\theta \int_0^{2\pi} d\varphi\ \exp i(k_x x+k_y y+k_z(z+z_0))\sin\theta,\quad z\geqslant z_0$$

where $k_x = k \sin\theta \cos\varphi$ $\qquad k_z = k \cos\theta$

$k_y = k \sin\theta \cos\varphi$

Plane waves coming to the surface stimulate reflected and transmitted waves. The formulas (1.6) are valid in the case of damped waves too, because all the functions involved are analytic in the upper semiplane. For $\widetilde{G}_0$ we get the following expressions :
the reflected wave

$$\widetilde{G}_0 = \frac{ik}{8\pi^2} \int d\theta \int d\varphi \ \exp i(k_x x + k_y y - k_z(z-z_0))\ R(k\cos\theta)\sin\theta$$

the scattered wave

$$\widetilde{G}_0 = \frac{ik}{8\pi^2} \int d\theta \int d\varphi \ \exp i(k_x x + k_y y + k_z(z+z_0))\ S(k\cos\theta)\sin\theta$$

where S and R are the transmission and reflection amplitudes introduced in Sec.1. Symmetry of the model allows us to transform these expressions to

$$\widetilde{G}_0 = \frac{ik}{8\pi} \int_{-\pi/2+i\infty}^{\pi/2-i\infty} H_0^{(1)}(kR'\sin\theta)\ \exp(-ik(z-z_0)\cos\theta) R(k\cos\theta)\sin\theta\, d\theta$$

and $\qquad R' = |(x,y,z-z_0)|$

$$G_0 = \frac{ik}{8\pi} \int H_0^{(1)}(kR_1\sin\theta)\ \exp(ik(z+z_0)\cos\theta)\ S(k\cos\theta)\sin\theta\, d\theta$$

The internal components can be easily calculated in the same way. The boundary values G_0^+, G_0^- for the deficiency element are the following :

$$G_0^+ = 1\ , \quad G_0^- = \frac{ik}{4\pi}\left(1 + \int_0^{\pi/2-i\infty} \exp(ik\cos\theta\ 2z_0)\ R(k\cos\theta)\sin\theta\, d\theta\right)$$

The asymptotic behaviour at infinity can be investigated by the method of Brechovskich [5] . If we fix a direction specified by an angle θ, then

$$\widetilde{G}_0 \sim \frac{\exp ikR_1}{4\pi R_1}\ R(k\cos\theta)\ , \quad \theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$$

$$\widetilde{G}_0 \sim \frac{\exp ikR_1}{4\pi R_1}\ S(k\cos\theta)\ , \quad \theta \in \left[\frac{\pi}{2}, \frac{3}{2}\pi\right]$$

This deficiency element is the kernel for the external component of the resolvent of the self-adjoint operator described in Sec.1 .

In order to construct the zero-range potential with an internal structure, let us choose a self-adjoint operator A_3 acting in the Hilbert space H_3. We shall restrict it to a symmetric operator A_0 with deficiency indices (1,1). The boundary form can be expressed in a standard way :

$$\langle A_{30}^{*} u_3, v_3 \rangle - \langle u_3, A_{30}^{*} v_3 \rangle = u_3^- \overline{v_3^+} - u_3^+ \overline{v_3^-} \equiv [u_3, v_3]^{in} \quad (4.2)$$

Next we define the symmetric operator $N_0 = \mathcal{L}_{z_0}^{\alpha\beta} \oplus A_{30}$ acting in the Hilbert space $L_2(R^3) \oplus L_2(R^2, H_1) \oplus L_2(R^2, H_2) \oplus H_3$. Its deficiency indices are (2.2), boundary form is the sum of the boundary forms :

$$\langle N_0^{*} U, V \rangle - \langle U, N_0^{*} V \rangle = [U, V]^{ex} + [u_3, v_3]^{in}$$

We can define the sought self-adjoint operator by restricting the adjoint operator N_0^{*} to the linear set specified by the boundary conditions :

$$u_0^+ = \gamma\, u_3^+$$
$$-u_3^- = \overline{\gamma}\, u_0^-$$

The continuous spectrum of N_γ consists of eigenfunctions of two types, the scattered waves and waveguide functions. The external components of all eigenfunctions of the continuous spectrum can be expressed in the following form :

$$u_0^N(\lambda) = u_0^{\mathcal{L}}(\lambda) + \varrho\, G_0(\lambda)$$

where $u_0^{\mathcal{L}}(\lambda)$ are the eigenfunctions of the self-adjoint operator $\mathcal{L}^{\alpha\beta}$. The boundary values of such function are the following :

1) $u_0^{\mathcal{L}+} = 0 \qquad u_0^{\mathcal{L}-} = \exp -ik_z z_0 + R \exp ik_z z_0 \,,\ k_z > 0$

$\qquad\qquad\qquad\qquad\qquad\qquad u_0^{\mathcal{L}-} = S \exp -ik_z z_0 \,,\ k_z < 0$

2) $u_0^{\mathcal{L}+} = 0 \qquad u_0^{\mathcal{L}-} = B^- \exp \varkappa z_0$

Hence we can calculate the amplitude ϱ from the boundary conditions and from the standard correlation between the boundary values of the internal component

$$\frac{u_3^-}{u_3^+} = D_3(\lambda)$$

where D_3 is the Schwarz integral of the operator A_3.

The amplitude ρ is expressed as follows

$$\rho = \frac{-u_0^{\alpha -}}{|\gamma|^{-2} D_3(\lambda)\, G_0^+ + G_0^-}$$

The external components of the scattered waves has the following asymptotics at infinity

$$u_0^N(\lambda) \sim u_0^{\alpha}(\lambda) + f(\vec{k},\theta)\, \frac{\exp ikR_1}{4\ R_1}$$

where

$$f(k,\theta) = \rho\, R(k \cos\theta), \quad \theta \in \left[\frac{\pi}{2}, \frac{3}{2}\pi\right]$$

$$f(k,\theta) = S(k \cos\theta), \quad \theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$$

and the function $f(\vec{k},\theta)$ is the scattering amplitude.

The eigenvalues of the discrete spectrum correspond to solutions of the equation :

$$\frac{G_0^-}{G_0^+} = -\frac{D_3(\lambda)}{|\gamma|^2}$$

In the case of weak coupling, $\gamma \to 0$, the eigenvalues are situated near the negative zeroes of $D_3(\lambda)$, while all positive solutions of this equation correspond to resonances.

5. A periodic structure on the surface

There are different ways how to construct such a periodic structure within our approach. One can choose the internal operators A_i dependent on the point (x,y) of the surface in some periodic way. One can add also a periodic potential $g(x,y)$ into the definition of the operator $\mathcal{A}_i$:

$$\mathcal{A}_i = -\Delta_{xy} + A_i + g(x,y)$$

We are going to investigate here the simplest exactly solvable model. We can replace the constants α and β in the boundary conditions (1.4) by arbitrary periodic smooth functions $a(x,y)$ and $b(x,y)$. Let a, b be the following exponential functions

$$a(x,y) = \alpha \quad \exp i(p_{1x}x + p_{1y}y)$$

$$b(x,y) = \beta \quad \exp i(p_{2x}x + p_{2Y}y)$$

Let us investigate the spectrum of the waveguide functions. The external components constructed in a standard way :

$$u_0(x,y,z) = \begin{cases} B^+ \exp -\varkappa z \quad \exp i(\, t_x x + t_y y\,) \,, & z > 0 \\ B^- \exp \varkappa z \quad \exp i(\, t_x x + t_y y\,) \,, & z < 0 \end{cases}$$

From the boundary conditions we get that the constants B^+, B^- solve the standard homogeneous system :

$$\left(\varkappa + \frac{|\alpha|^2}{2\, D_1(\,\lambda - (t - p_1)^2)}\right) B^+ + \left(\varkappa + \frac{|\alpha|^2}{2\, D_1(\,\lambda - (t-p_1)^2)}\right) B^- = 0$$

$$\left(1 + \varkappa \frac{|\beta|^2 D_2(\,\lambda - (t-p_2)^2)}{2}\right) B^+ - \left(1 + \varkappa \frac{|\beta|^2 D_2(\,\lambda - (t-p_2)^2)}{2}\right) B^- = 0$$

The system has a nontrivial solution only if

$$\varkappa + \frac{|\alpha|^2}{2\, D_1(\,\lambda - (t-p_1)^2)} = 0$$

$$1 + \varkappa \frac{|\beta|^2 D_2(\,\lambda - (t-p_2)^2)}{2} = 0$$

Let us investigate the solutions of the first equation which lead to symmetric wavefunctions. The real solutions can be localised only in the region $\lambda < t^2$ (see Fig.3) because $\varkappa = \sqrt{t^2 - \lambda}$. In the case of weak coupling between the external and internal channels, the solutions lie near the zero surfaces of $D_1(\,\lambda - (t-p)^2)$ (marked by the

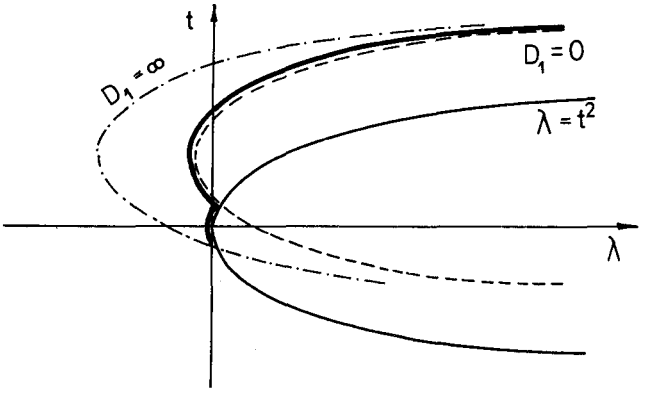

Fig.3

dashed lines), which are parabolas of the following type :

$$\lambda - (t - p)^2 = \text{const}$$

These parabolas are symmetric with respect to the axis t=p. Thus the branches of the solutions are infinite (marked by the full line), and they are not symmetric with respect to the energy axis.

If a waveguide function propagates in some direction, there is no waveguide function of the same energy propagating in the opposite direction. The same is true for the antisymmetric functions.

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