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SPECTRUM PERTURBATIONS, THE KNESER-TYPE CONSTANTS AND THE EFFECTIVE MASSES OF ZONES-TYPE POTENTIALS

F.S. Rofe-Beketov

I. Introduction. It is well known [I], that the spectrum $\sigma(L_o)$ of the one-dimensional Schrödinger equation with a real-valued periodic potential (i.e. otherwise of the Hill equation) in $\mathcal{L}^2(-\infty,\infty)$

$$L_o u \equiv -u'' + q(x)u = \lambda u, \qquad q \in \mathcal{L}^I_{loc} \tag{I}$$

is purely continuous: $\sigma(L_o) = \sigma_{ess}(L_o)$, bounded from below and consists of a sequence of closed intervals $[\lambda_{2\nu}, \lambda_{2\nu+1}]$, $\nu = 0, I, 2 \ldots$, which are closures of stability zones (or the so-called allowed zones in the quantum theory of solids). These intervals are separated by spectral lacunas

$$(-\infty, \lambda_o),\ (\lambda_I, \lambda_2),\ \ldots\ (\lambda_{2\nu-I}, \lambda_{2\nu}), \ldots \tag{2}$$

(open instability zones or forbidden zones). The lacuna ends are eigenvalues of the periodic or antiperiodic (semiperiodic) boundary problems for Eq. (I) in an interval which is equal to the period.

If the potential q(x) is uniformly almost periodic function (a.p. after H. Bohr [2]), then the equality $\sigma(L_o) = \sigma_{ess}(L_o)$ holds [3], i.e. the whole spectrum is essential, isolated eigenvalues are absent, however the spectrum structure may, in general case, become much more complicated than spectrum of the Hill equation. The necessary and sufficient conditions, under which the zones-type spectrum $\sigma(L_o)$ corresponds to the periodic potential q(x) belonging to the prescribed Sobolev class $W^m_{2,loc}$ [4], are given by the Marchenko-Ostrovskiy theorem [5] (see also [6]).

The perturbed equation

$$L_I y \equiv -y'' + \left[q(x) + p(x)\right] y = \lambda y \qquad (3)$$

with the real-valued perturbation $p \in \mathcal{L}^I_{loc}$, small at infinity in the integral sense:

$$\lim_{|x| \to \infty} \int_x^{x+I} |p(t)| \, dt = 0 \qquad (4)$$

has, by the Birman theorem [7] (see also [8]), the same essential spectrum as the initial equation (I) has: $\sigma_{ess}(L_I) = \sigma_{ess}(L_o) = \sigma(L_o)$, but at every of the spectral lacunas (2) of the operator L_o there may arise, from the perturbation finite or infinite numbers of discrete levels (isolated eigenvalues) which can converge only to the endpoints of lacunas.

2. Perturbations of periodic potential. The first finiteness test for the number of discrete levels of the perturbed periodic equation (3) refers to the levels in the semiinfinite lacuna $(-\infty, \lambda_o)$; this test was found by M.Sh. Birman [7] (see also [8]) and requires

$$\lim_{|x| \to \infty} |x| \left\{ \int_{-\infty}^{-|x|} + \int_{|x|}^{\infty} |p(t)| \, dt \right\} = 0 \quad . \qquad (5)$$

The first finiteness test for the number of eigenvalues of the perturbed Hill equation (3) in each finite lacuna (2) was established in [9] and is given by sufficient condition

$$\int_{-\infty}^{\infty} (I + |x|) \, |p(x)| \, dx < \infty \, . \qquad (6)$$

Besides, each sufficiently remote spectral lacuna, under condition (6), contains not more than two discrete levels [9].

Eigenvalues on the continuous spectrum of the perturbed Hill equation (3) do not arise under condition (6)[9], while under condition $p(x) \in \mathcal{L}^I(-\infty, \infty)$ they do not arise either with the possible exception at the endpoints of lacunas [I0].

If, in addition to (6), the following is valid

$$\int_{-\infty}^{\infty} p(x) \, dx \neq 0, \qquad (7)$$

then at each of sufficiently remote lacunas (2) there arise exactly one eigenvalue of the perturbed problem (3). (This was found in [II], cf. also [I2], [I3]; existence of eigenvalues at remote lacunas under more rigid conditions was established in [I4]).

Under condition (4) preserving the limiting spectrum, for each lacuna there are such numbers K_n, $(-I)^n K_n > 0$, that if $p(x) \leqslant -(K_{2n} + \mathcal{E})\, x^{-2}$ for $x \to +\infty$ or $x \to -\infty$, then near the endpoint λ_{2n} in the prescribed lacuna there arises an infinite number of eigenvalues of the perturbed Hill equation (3), and similarly, when $p(x) \geqslant (|K_{2n-I}| + \mathcal{E})\, x^{-2}$ near the endpoint λ_{2n-I}, as was shown in Ref. [I5] presented at the 2-nd All-Union Summer Mathematical School at Baku in I975 (see also Refs. [I0], [I6]).

Under conditions $C_I |x|^{-\alpha} < |p(x)| < C_2 |x|^{-\alpha}$, $0 < \alpha < I$, $p(x) \nearrow 0$ for $|x| \to \infty$ monotonically on $\mathbb{R}_{\pm}$, [I7] established the formula of asymptotic distribution of eigenvalues of the perturbed Hill equation (3) in lacunas (2) near its endpoints. We shall cite it. Let $N(\mu, \lambda)$ denote the number of the operator's L_I (3) eigenvalues being situated in the interval (μ, λ). Then, when $\lambda_{2\nu-1} < \lambda \nearrow \lambda_{2\nu}$

$$N(\lambda_{2\nu-I}, \lambda) \sim (\pi\omega)^{-I} |F'(\lambda_{2\nu})|^{I/2} \int\limits_{p(x) < \lambda - \lambda_{2\nu}} (\lambda - \lambda_{2\nu} - p(x))^{I/2} dx \quad (8)$$

Here ω is the period of the potential $q(x) = q(x + \omega)$, $F(\lambda)$ the trace of the monodromy matrix or otherwise the Lyapunov function or the Hill discriminant, i.e.

$$F(\lambda) = \theta(\omega, \lambda) + \varphi'(\omega, \lambda), \quad (9)$$

where $\theta(x, \lambda)$, $\varphi(x, \lambda)$ are solutions of (I) with initial conditions

$$\theta(0,\lambda) = \varphi'(0,\lambda) = 1, \quad \theta'(0,\lambda) = \varphi(0,\lambda) = 0. \quad (I0)$$

When $q(x) \equiv 0$, the asymptotics (8) turns into the classical asymptotic formula of distribution of eigenvalues preceding the essential spectrum [I], [I8-2I]. There are also books [22-25] which treat important topics associated with distribution of eigenfrequencies for problems of a different type.

Discrete levels of perturbed periodic systems of any order with all coefficients perturbed were studied in Ref. [26].

3. Perturbations of the almost periodic potential. Let us consider now the one-dimensional Schrödinger equation (I) and its perturbation (3), assuming the potential $q(x)$ to be either periodic or the a.p. function. Below we shall present the principal results of Ref. [27] containing exact conditions for the perturbations $p(x)$

providing either finiteness or alternatively infiniteness of the number of the discrete levels introduced into a given lacuna in the vicinity of a prescribed endpoint of it. These results appear to be novel not only for a.p., but also for periodic $q(x)$. They are based on the transformation [15] (see also Refs [10] and [16], Section 4) of the perturbed Schrödinger equation into another Schrödinger equation with a locally summable potential, such that the problem of finiteness/infiniteness of the eigenvalue number in the spectral lacuna of the first of these equations is reduced into a similar problem for a semi-infinite spectral lacuna of the second equation. To this last equation and equations

$$y'' + \frac{1 \pm \mathcal{E}}{4x^2}\, y = 0$$

we apply the Taam-Hille-Wintner integral comparison theorem [28, 29]. To realize such way of investigation, we consider the structure of the fundamental system of solutions to an a.p. equation at the endpoint of its spectral lacuna.

<u>Lemma 1.</u> If $q(x)$ is an a.p. function and Eq. (1) has, for certain $\lambda \in \mathbb{R}$, a nontrivial a.p. real-valued solution $u = e(x,\lambda)$, then the linearly independent solution $u = \mathcal{E}(x,\lambda)$ has the form

$$\mathcal{E}(x,\lambda) = \left[A_\lambda + o(1)\right] x e(x,\lambda) + O(1), \quad (|x| \to \infty),$$

where, if $W\{e, \mathcal{E}\} \equiv e\mathcal{E}' - e'\mathcal{E} = 1$

$$A_\lambda = M_x\{F_k(x,\lambda\,|\,e)\} \equiv \lim_{b-a\to\infty} \frac{1}{b-a}\int_a^b F_k\,dx \qquad (11)$$

and where it is put that

$$F_k(x,\lambda\,|\,u) = (q + 1 - \lambda^{1-k})(\lambda^k u^2 - u'^2)(\lambda^k u^2 + u'^2)^{-2}, \qquad (12)$$

$k = 0, 1$ (When $\lambda > 0$, A_λ does not depend on the choice between F_0 or F_1, but when $\lambda \leq 0$ one has to take only F_0).

If $\lambda = \lambda_0 = \inf \sigma(L_0)$, then

$$A_{\lambda_0} = M_x\{e^{-2}(x,\lambda_0)\}.$$

Lemma 1 follows from the generalization of the Liouville-Ostrogradskiy formula

$$u_2(x,\lambda) = u_1(x,\lambda)\int u_1^{-2}(x,\lambda)\,dx.$$

This generalization is applicable to oscillating solutions and require no shewing together for the values of $u_2(x, \lambda)$ at zeroes of $u_I(x, \lambda)$. It is given by the following

Lemma 2. Let u_I, u_2 be the solutions of Eq. (I) with any $q(x) \in \in \mathcal{L}^I_{loc}$ ($q(x)$ is not supposed to be a.p.) and let Wronskian $W\{u_I, u_2\} = I$. Then

$$u_2(x,\lambda) = u_I(x,\lambda) \int F_k(x,\lambda | u_I)dx - u_I'(x,\lambda)(\lambda^k u_I^2 + u_I'^2)^{-I}; (k=0,I)$$

where $F_k(x, \lambda | u)$ is specified by Eq. (I2). True is also the formula with $|u|^2 + |u'|^2$ in the denominator, which represents a modifica - tion of the above one, applicable also to the non-real-valued case:

$$u_2 = u_I \int \frac{(\bar{q}+I)\,\bar{u}_I^2 - (q+I)\,\bar{u}_I'^2}{(|u_I|^2 + |u_I'|^2)^2}\,dx - \frac{\bar{u}_I'}{|u_I|^2 + |u_I'|^2}.$$

Theorem I. Let $q(x)$ be an a.p. function (or periodic of $\mathcal{L}^1_{loc}$) $p(x)$ satisfy Eq. (4), $(\lambda_{2\nu-I}, \lambda_{2\nu})$ be a certain lacuna in σ_{ess} of L_o. Then, if Eq. (I) has an a.p. solution $u = e(x, \lambda_j)$ for $j = 2\nu - I$ or for $j = 2\nu$, then between λ_j and $(\lambda_{2\nu-I} + \lambda_{2\nu})/2$ there is an infinite number of eigenvalues of equation $L_I\, y = \lambda y$ (3), if for certain $N > 0$, $\mathcal{E} > 0$

$$(-I)^{j+I}\, p(x) \geqslant \left[|K_j| + \mathcal{E}\right] \cdot x^{-2}, \quad x > N \quad \text{or} \quad x < -N,$$

and not more than a finite number of eigenvalues, if

$$(-I)^{j+I}\, p(x) \leqslant \left[|K_j| - \mathcal{E}\right] x^{-2}, \quad |x| > N$$

where

$$K_j = (4A_{\lambda_j} \cdot M_x\{e^2(x, \lambda_j)\})^{-I}; \quad (-I)^j K_j > 0. \qquad (I3)$$

The requirement of existence of the a.p. solution $e(x, \lambda_j)$ is always fulfilled in the case of periodic $q(x)$, but for a.p. $q(x)$, this is not always.

Lemma 3. If the spectrum of L_o (I) with a.p. $q(x)$ has a zones-type structure (band structure):

$$\sigma(L_o) = \bigcup_{\nu=0}^{\infty} [\lambda_{2\nu}, \lambda_{2\nu+1}]$$

where

$$-\infty < \lambda_0 < \lambda_1 < \dots < \lambda_{2\nu-1} < \lambda_{2\nu} < \dots$$

and

$$\exists\, C>0, \alpha>0 : \lambda_{n+2} - \lambda_n > Cn^{\alpha}, \quad n=0, I, \dots$$

and moreover

$$\exists\, \beta > 1 : \sum_{\nu=1}^{\infty} \lambda_{2\nu}^{\beta} (\lambda_{2\nu} - \lambda_{2\nu-1}) < \infty,$$

then if $\lambda = \lambda_n$, Eq. (I) has a nontrivial a.p. solution ($n=0, I, 2, \dots$)

Note that almost periodicity of potentials of the said type and some of their important properties were established by B.M. Levitan [30-32]. Almost periodicity of $q(x)$ alone, without additional conditions is insufficient for existence of a.p. solutions $e(x, \lambda_j)$ at lacuna endpoint (Ref. [3] supplies an appropriate counterexample). In the case of the finite gaps a.p. potential $q(x)$, the statement of Lemma 3 may be derived from explicit formulas for solutions of the Schrödinger equation in terms of the Riemann θ-functions, that were found by A.R. Its and V.B. Matveev [33] who used the relationship discovered by N.I. Akhiezer [34] in I96I between the Jacobi inverse problem and finite gaps Schrödinger operators. A delicate point however is here verification of the condition that the denominator in these formulas cannot approach zero infinitely close which would guarantee boundedness of the corresponding solution on the axis.

Corollary I. When $q(x) \equiv 0$, we have $\lambda_0 = 0$, $K_0 = I/4$ and Theorem I transforms into the spectral formulation of the classical Kneser theorem, which is usually formulated in terms of oscillation of solutions (see, e.g., Ref. [35]).

In view of the said fact, we call K_j Kneser-type constants.

Example. For the single gap Lamé equation

$$- u'' + 2k^2 \cdot \mathrm{sn}^2\, x \cdot u = \lambda u,$$

where $0<k<I$, we have $\lambda_0 = k^2$, $\lambda_I = I$, $\lambda_2 = I + k^2$ and the associated Kneser-type constants are rationally expressible through full elliptic I-st and 2-nd kind integrals K and E:

$$0 < K_0 = \frac{I}{4} k'^2 K^2 E^{-2} < \frac{I}{4}, \quad k'^2 = I - k^2,$$

$$K_I = -\frac{I}{4} k^2 k'^2 K^2 (E - k'^2 K)^2, \quad K_2 = \frac{I}{4} k^2 K^2 (E - K)^2.$$

Remark. Always $0 < K_0 \leqslant \frac{I}{4}$, where the equality may only be valid when $q(x) = \text{const}$, as may be easily seen from Eqs. (I3) and (II) for $\lambda = \lambda_o$.

Corollary 2. If $|p(x)| \leq Cx^{-2}$, $(C>0, |x|>N)$, then each of sufficiently remote spectral lacunas of problem (I) contains not more than a finite number of eigenvalues of perturbed problem (3). (Note here that $K_n \to 0$ when $n \to \infty$).

4. Effective masses. In the case of the periodic potential, an important role in physical problems for Eq. (I) is played by the concept of the effective mass $\mathscr{H}_n$:

$$\mathscr{H}_n \stackrel{\text{def}}{=\!=} \left[(d^2\lambda / d\xi^2) \Big|_{\lambda=\lambda_n} \right]^{-I},$$

where ξ is the quasi-impulse [36-38]. This definition of the effective mass may be extended as it is to the case of the zones-type a.p. potentials.

Theorem 2. In the case of any periodic or a.p. potential $q(x)$ of the zones-type mentioned in Lemma 3,

$$K_n = (8\mathscr{H}_n)^{-I}, \quad n = 0, I, 2, \ldots \tag{I4}$$

Note that in the periodic case, expressions for the effective masses $\mathscr{H}_n$ were obtained in Refs [36, 37], in terms of solutions of the Hill equation (I) and in Ref. [39] as an infinite product containing $\lambda_o, \lambda_I, \lambda_2, \ldots$ and roots of $F'(\lambda) = 0$, where $F(\lambda)$ is the Lyapunov function (9) both without any relation to perturbation estimates or Kneser-type constants. As was shown by B.M. Levitan [30, 3I] for infinite bands a.p. potentials, the conditions

$$\int_{\lambda_{2\nu-1}}^{\lambda_{2\nu}} \left[f^{-I/2}(z) \prod_{k=I}^{\infty} \frac{\eta_k - z}{\lambda_{2k}} \right] dz = 0, \quad \nu = I, 2, \ldots$$

where

$$f(z) = z \prod_{k=1}^{\infty} \left(I - \frac{z}{\lambda_k}\right)$$

uniquely specify the numbers $\eta_k \in (\lambda_{2k-I}, \lambda_{2k})$. (For the sake of simplicity, we assumed here $\lambda_o = 0$).

Theorem 3. For the effective masses $\mathscr{H}_n$, in the case of a.p. $q(x)$ of the zones-type mentioned in Lemma 3, the following representation is valid:

$$\varkappa_n = \frac{1}{2}\left\{ \frac{\lambda - \lambda_n}{\lambda - \lambda_0} \prod_{j=1}^{\infty} \frac{(\lambda - \eta_j)^2}{(\lambda - \lambda_{2j-1})(\lambda - \lambda_{2j})} \right\} \Bigg|_{\lambda = \lambda_n}, \quad n = 0, 1, 2, \ldots$$

and by virtue of Eq. (14), hence follows also a representation of Kneser-type constants K_n as an infinite product.

Corollary 3. In the case of the band a.p. potential under consideration,

$$\sum_{n=0}^{\infty} \varkappa_n = \frac{1}{2}, \quad \text{and} \quad \sum_{n=0}^{\infty} K_n^{-1} = 4.$$

(The former of the equalities, for the periodic case, was obtained by N.E. Firsova [39]).

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Institute for Low Temperature
Physics & Engineering
UkrSSR Academy of Sciences
47, Lenin Avenue, Kharkov, 310164, USSR