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Spectral Density of a Periodic Jacobi Matrix

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Abstract. The spectral density of a periodic Jacobi matrix is calculated.

Define a tridiagonal (Jacobi or J-) matrix J of a self-adjoint operator in an orthonormal basis $\{e_i\}_{i=0}^{\infty}$ of a Hilbert space as follows (see, e.g., [1]):

$$\begin{pmatrix} a_0 & b_0 & & & 0 \\ b_0 & a_1 & b_1 & & \\ & b_1 & a_2 & b_2 & \\ 0 & & \ddots & \ddots & \ddots \end{pmatrix} \tag{1}$$

$$a_i, b_i \in \mathbf{R}, \qquad b_i \neq 0, \qquad i = 0, 1, \ldots$$

(the matrix elements that are not shown are zero). The spectral density of J is formally defined as $\rho^J(x) = (\mathrm{d}\Omega_x e_0, e_0)/\mathrm{d}x$, where Ω_x is the resolution of the identity of J. ($J = \int x \mathrm{d}\Omega_x$.) Further we will also need the polynomials of the first and the second kind $p_i^J(x)$ and $q_i^J(x)$ respectively, associated with the matrix J:

$$\begin{aligned} &p_{-1}^J = 0;\ p_0^J = 1;\ p_{i+1}^J = -b_i^{-1}((a_i - x)p_i^J + b_{i-1}p_{i-1}^J),\ i = 0, 1, \ldots \\ &q_0^J = 0;\ q_1^J = b_0^{-1};\ q_{i+1}^J = -b_i^{-1}((a_i - x)q_i^J + b_{i-1}q_{i-1}^J),\ i = 1, 2, \ldots \end{aligned} \tag{2}$$

Note that $\rho^J(x)$ is the weight function with respect to which the polynomials $p_i^J(x)$ are orthonormal. Indeed, using the easily verifiable identity $p_i^J(J)e_0 = e_i$, $i = 0, 1, \ldots$, we have

$$\delta_{ij} = (e_i, e_j) = (p_i^J(J)p_j^J(J)e_0, e_0) = \int_{-\infty}^{\infty} p_i^J(x)p_j^J(x)\rho^J(x)\mathrm{d}x, \qquad (3)$$

As is clear from [2,3], a number of physical problems for simple crystal lattices (such as, for example, calculation of the influence of point defects on the energy spectrum of elementary excitations and low temperature thermodynamics) can be solved by utilizing the properties of J-matrices with identical rows (that is $a_i = a$, $b_i = b$, $i = 0, 1, \ldots$). In the same sense a linear chain with nearest-neighbor interactions and several atoms in the elementary cell corresponds to a periodic J-matrix. (A J-matrix L_t of the form (1) is called periodic with a period t if $a_i = a_{i+tm}$, $b_i = b_{i+tm}$, $i, m = 0, 1, \ldots$.)

A simple example is provided by a linear chain of two different alternating spins s and σ, which is described by the Heisenberg Hamiltonian with nearest-neighbor interactions and has a point spin defect χ in it. Let the defect spin be situated in the zero node; spins s, in the odd; and spins σ, in the even nodes of the chain. Let "$|0\rangle$" be the normalized state of total spin alignment defined by the formulas $\chi_0^z|0\rangle = \chi|0\rangle$, $s_i^z|0\rangle = s|0\rangle$ and $\sigma_{i+1}^z|0\rangle = \sigma|0\rangle$, $i = \pm1, \pm3, \ldots$. In the basis $e_0 = \chi_0^-|0\rangle/\sqrt{2\chi}$, $e_i = (s_i^-|0\rangle + s_{-i}^-|0\rangle)/2\sqrt{s}$, $e_{i+1} = (\sigma_{i+1}^-|0\rangle + \sigma_{-i-1}^-|0\rangle)/2\sqrt{\sigma}$, $i = 1, 3, \ldots$ the matrix of the Hamiltonian has the form $H = L_2 + V$, where V is 2×2-matrix, and L_2 is a periodic J-matrix with the period 2. A similar representation of the operator H is in the basis $g_i = (s_i^-|0\rangle - s_{-i}^-|0\rangle)/2\sqrt{s}$, $g_{i+1} = (\sigma_{i+1}^-|0\rangle - \sigma_{-i-1}^-|0\rangle)/2\sqrt{\sigma}$, $i = 1, 3, \ldots$, that complements $\{e_i\}_{i=0}^{\infty}$ to the basis of the one-magnon space. The method of [2] allows us to find the spectrum of the Hamiltonian in this space and the changes in low temperature thermodynamics provided the spectral density of L_2 is known.

Note that the problem of a Bloch electron in an external magnetic field also reduces to a study of periodic tridiagonal matrices (see, e.g., [4–10]).

Let us find the spectral density $\rho(x)$ of a t-periodic J-matrix L_t, after which all the theory of [2,3] will be amenable to L_t.

For this purpose, introduce a block-tridiagonal matrix E_t of the form

$$\begin{pmatrix} 0 & I & & & 0 \\ I & 0 & I & & \\ & I & 0 & I & \\ 0 & & \ddots & \ddots & \ddots \end{pmatrix}, \tag{4}$$

where I is the $t \times t$ unity matrix.

The following equation holds:

$$S_t(L_t) = E_t + V, \tag{5}$$

where $S_t(x) = p_t^{L_t}(x) - b_{t-1}q_{t-1}^{L_t}(x)$, and $V_{ik} = 0$ when $i, k \geq t-1$ (the indices of matrix elements are $i, k = 0, 1, \ldots$). The polynomial $S_t(x)$ is known (see, e.g., [11]) and called the discriminant of the discrete Hill's equation $(L\phi)_n = \varepsilon\phi_n$. Here L is a t-periodic tridiagonal matrix infinite in both directions defined in an orthonormal basis $\{e_i\}_{i=-\infty}^{\infty}$ of a Hilbert space and has the following matrix elements

$$(Le_i, e_{i+k}) = \delta_{-1k}b_{i-1} + \delta_{0k}a_i + \delta_{1k}b_i,$$
$$a_i = a_{i+tm}, \qquad b_i = b_{i+tm} \neq 0, \qquad i = 0, 1, \ldots, t-1 \qquad m = 0, \pm 1, \pm 2, \ldots$$

The equation (5) can be deduced from the results of [12,13], but it is much simpler to give its direct proof:

Let us associate with L the two systems of polynomials $p_i(x)$, $q_i(x)$, defined by the equations $p_{-1} = 0$, $p_0 = 1$, $q_{-1} = 1$, $q_0 = 0$ and the recurrence relation $y_{i+1} = \{(x - a_i)y_i - b_{i-1}y_{i-1})/b_i$, $i = 0, 1, \ldots$ (here either $y_i = p_i$, $i = 0, 1, \ldots$ or $y_i = q_i$, $i = 0, 1, \ldots$).

Define the matrix E by the relations $E_{i\,i+j} = E_{i\,i-j} = \delta_{jt}$, $i, j = 0, \pm 1, \pm 2, \ldots$

Lemma

$$p_t(L) + q_{t-1}(L) = E \tag{6}$$

Proof. Using the recurrence relations for the polynomials $p_i(x)$, $q_i(x)$ and the obvious identity $Le_i = b_{i-1}e_{i-1} + a_ie_i + b_ie_{i+1}$, we obtain by induction that

$$p_k(L)e_0 = e_k - q_k(L)e_{-1}, \qquad k = 0, 1, \ldots \tag{7}$$

Consequently,

$$p_t(L)e_0 + q_{t-1}(L)e_0 = e_t + \varphi, \tag{8}$$
$$\varphi = -q_t(L)e_{-1} + q_{t-1}(L)e_0. \tag{9}$$

Substituting in (9) instead of $q_t(L)$ its expression in terms of L, $q_{t-1}(L)$, $q_{t-2}(L)$ from the recurrence relation, and then operating with L on the vector e_{-1}, we get

$$\varphi = \frac{b_{t-2}}{b_{t-1}}(-q_{t-1}(L)e_{-2} + q_{t-2}(L)e_{-1}). \tag{10}$$

This is the first step in derivation of the expression for φ. The second step is to perform the same operation with respect to $q_{t-1}(L)$ in (10). Proceeding this way, we get at the $t-1$'th step

$$\varphi = \frac{b_0}{b_{t-1}}(-q_1(L)e_{-t} + q_0(L)e_{-t+1}) = e_{-t}. \tag{11}$$

I.e.

$$p_t(L)e_0 + q_{t-1}(L)e_0 = e_t + e_{-t}. \tag{12}$$

Now using (7), (12), and the identity $p_t(L)e_{-1} - p_{t-1}(L)e_0 = e_{-t-1}$ that can be proved similarly to the derivation of (11), we obtain (the argument L is omitted for brevity)

$$\begin{aligned}(p_t + q_{t-1})e_k = (p_t + q_{t-1})(p_k e_0 + q_k e_{-1}) =\\ p_k(e_t + e_{-t}) + q_k(p_t e_{-1} + e_{t-1} - p_{t-1}e_0) =\\ p_k e_t + q_k e_{t-1} + p_k e_{-t} + q_k(p_t e_{-1} - p_{t-1}e_0) =\\ e_{t+k} + p_k e_{-t} + q_k e_{-t-1} = e_{k+t} + e_{k-t},\end{aligned}$$

which concludes the proof of the lemma.

Identity (5) follows immediately from the lemma by multiplying the relation (6) from both sides by the operator W of the orthogonal projection onto the subspace spanned by the vectors $\{e_i\}_{i=0}^{\infty}$, and from the fact that for any positive integer k, $WL^kW = (WLW)^k + V_k$, where $V_k e_i = 0$ for $i \geq k-1$.

Since the matrix E has a $2t$-degenerate spectrum that fills the interval $[-2, 2]$, and the spectrum of L is no more than doubly degenerate, it follows from (6) that the spectrum of L consists of a set of t intervals: the image of the interval $[-2, 2]$ under the inverse of the transform $S_t(\lambda) = \nu$. (Thus, we obtained so far a well known fact (see, e.g., [11]).) Hence, the continuous spectrum of the matrix $L_t = WLW$ consists of the same set of intervals.

It follows from (5) that apart from the continuous spectrum filling the interval $[-2, 2]$, the operator $S_t(L_t)$ may have up to $t-1$ discrete eigenvalues (each one of them is counted the number of times equaling its multiplicity). These eigenvalues can be found by the method of [2]. If λ_0 is one of the eigenvalues of multiplicity m than there exists such a basis $\{\psi_i\}_{i=1}^m$ of the corresponding eigenspace that $L_t\psi_i = \varepsilon_i\psi_i$, where ε_i satisfy the equation $S_t(\varepsilon_i) = \lambda_0$. So L_t may have up to $t-1$ discrete nondegenerate eigenvalues. (Recall the known fact [1] that the spectrum of a J-matrix is simple.)

Let us call the following quantities the spectral functions of a self-adjoint operator H

$$\rho_{ij}(\lambda) = \frac{(\mathrm{d}\Omega_\lambda^H e_j, e_i)}{\mathrm{d}\lambda}, \tag{13}$$

where Ω_λ^H is the resolution of the identity of H.

It is easily seen that the spectral functions of E_t corresponding to the first t basis vectors are given by the formula

$$\rho_{(0)\,jk}(x) = \delta_{jk}\frac{1}{4}\rho_{\mathrm{ch}}(\frac{x+2}{4}), \qquad j,k = 0,1,\ldots,t-1, \tag{14}$$

where $\rho_{\mathrm{ch}}(\lambda) = \frac{8}{\pi}\sqrt{\lambda(1-\lambda)}$ if $\lambda \in [0,1]$ and $\rho_{\mathrm{ch}}(\lambda) = 0$ otherwise, is the spectral density of the J-matrix J_{ch} with the elements $a_i = 1/2$, $b_i = 1/4$, $i = 0,1,\ldots$. It is also the weight function of the Chebyshev polynomials of the second kind $p_i^{J_{\mathrm{ch}}}(\lambda)$ orthogonal on the interval $[0,1]$ (see, e.g., [14]).

The spectral functions $\tilde\rho_{ij}(x)$ of the block-tridiagonal matrix $E_t + V$ can now be calculated using, for example, the technique of [3].

To find the spectral density of L_t, let us apply an arbitrary single-valued integrable function $f(x)$ to both sides of (5) and rewrite the result in the form

$$\int_{-\infty}^{\infty} f(\lambda)\left\{\sum_{i=0}^{t-1}\frac{\mathrm{d}\Omega_{\varepsilon_i}}{\mathrm{d}\varepsilon_i}\left|\frac{\mathrm{d}\varepsilon_i}{\mathrm{d}\lambda}\right|\right\}\mathrm{d}\lambda = \int_{-\infty}^{\infty} f(\lambda)\frac{\mathrm{d}\widetilde\Omega_\lambda}{\mathrm{d}\lambda}\mathrm{d}\lambda, \tag{15}$$

where $\lambda = S_t(\varepsilon_i)$, $i = 0,1,\ldots,t-1$, and Ω_x, $\widetilde\Omega_x$ are the resolutions of the identity of L_t and $E_t + V$, respectively.

It follows from (15) that

$$\left(\int_{-\infty}^{\infty} f(\lambda)\left\{\sum_{i=0}^{t-1}\frac{\mathrm{d}\Omega_{\varepsilon_i}}{\mathrm{d}\varepsilon_i}\left|\frac{\mathrm{d}\varepsilon_i}{\mathrm{d}\lambda}\right|\right\}\mathrm{d}\lambda\, e_0, e_j\right) = \left(\int_{-\infty}^{\infty} f(\lambda)\frac{\mathrm{d}\widetilde{\Omega}_\lambda}{\mathrm{d}\lambda}\mathrm{d}\lambda\, e_0, e_j\right), \qquad (16)$$

$j = 0, 1, \ldots, t-1$.

Introducing the notation $\rho'(\varepsilon_i) = \rho(\varepsilon_i)\left|\frac{\mathrm{d}\varepsilon}{\mathrm{d}\lambda}\Big|_{\varepsilon=\varepsilon_i}\right|$, where $\rho(\varepsilon)$ is the spectral density of L_t, and using the fact that $p_j^J(J)e_0 = e_j$, we get from the system (16)

$$\sum_{i=0}^{t-1} p_j^{L_t}(\varepsilon_i)\rho'(\varepsilon_i) = \tilde{\rho}_{0j}(\lambda), \qquad j = 0, 1, \ldots, t-1. \qquad (17)$$

Hence $\rho'(\varepsilon_i) = \frac{D_i}{D}$, where $D = |p_m^{L_t}(\varepsilon_n)|_0^{t-1}$, and D_i is $t \times t$ determinant that we obtain from D by replacing the i'th column with the column composed of the quantities $\tilde{\rho}_{0j}(\lambda)$. The expression for D can be simplified by expanding the polynomials $p_m^{L_t}(\varepsilon_n)$ by the recurrence relation successively in each row of the determinant beginning with the last row. Having repeated this operation $t-1$ times, we get

$$D = \frac{|\varepsilon_n^m|_0^{t-1}}{b_{t-2}b_{t-3}^2\cdots b_0^{t-1}} = \prod_{i=1}^{t-1}\prod_{k=0}^{i-1}\frac{\varepsilon_i - \varepsilon_k}{b_k}.$$

Thus, the spectral density of L_t in the i'th interval of the continuous spectrum is

$$\rho(\varepsilon_i) = \frac{D_i}{D}\left|\frac{\mathrm{d}S_t(\varepsilon)}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=\varepsilon_i}\right|, \qquad S_t(\varepsilon_i) \in [-2, 2], \qquad i = 0, 1, \ldots, t-1, \quad (18)$$

and the addend to the spectral density due to each point ε_k of the discrete spectrum has the form

$$\rho_k(\varepsilon) = \delta(\varepsilon - \varepsilon_k)|(\psi_k, e_0)|^2, \qquad (19)$$

where the eigenvector ψ_k is supposed to be normalized.

Relations (18) and (19) conclude the solution of the formulated problem. Note that for small t, the coefficients of polynomial $S_t(x)$ and the matrix elements of V are found easier directly by the formula (5) by comparing the matrix elements at the right and the left side of the equation.

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