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A new method in the many-body problem: II

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Abstract. The earlier proposed method for exact determination of the energy spectra of Hamiltonians H and the quantities $\mathrm{Sp}\{f(H+W)-f(H)\}$, where W is a finite-dimensional perturbation, is extended to treat a still larger class of Hamiltonians. In particular, some two- and three-dimensional problems became amenable to this approach. In addition, the expressions for the density and local densities of states are deduced. As an example, an impurity problem is considered in a simple cubic lattice with short-range and in a linear chain with long-range interactions.

1. Introduction

In the recent work [1], we proposed a method for determination of the energy spectra of Hamiltonians H and the quantities $\mathrm{Sp}\{f(H+W)-f(H)\}$ (W is finite-dimensional, $f(x)$ is a 'general enough' function) in the case when H and $H+W$ may be represented in the form $H = T_n(L)+V$, where $T_n(x)$ is a polynomial of degree n, L is a tridiagonal (J-)matrix with a known spectral density, V is finite-dimensional and such that $H = T_n(L) + V$ remains $(2n+1)$-diagonal. We made use of the fact that H is block-tridiagonal. Examples of applications of the method include a number of problems for linear chains.

The purpose of the present work is twofold. First, we generalize the method in the way that $T_n(x)$ is replaced by an integrable function $g(x_1,\ldots,x_d)$. This, in particular, allows us to treat two-dimensional (2D) and three-dimensional (3D) problems within the framework of the method since some of the corresponding Hamiltonians can be represented in the form $H = H_0 + V$, where V is finite-dimensional and H_0 is a function of several J-matrices. For example, the one-magnon space of Heisenberg systems with a point spin defect or the two-magnon space of systems without impurities readily decompose into the orthogonal sum of subspaces in which (i) for the 2D square lattice with nearest- and next-nearest-neighbour interactions $H = L_1 \otimes L_2 + I \otimes T_1(L_2) + V$ and (ii) for the 3D simple cubic lattice with nearest-neighbour interactions $H = L_1 \otimes I \otimes I + I \otimes L_2 \otimes I + I \otimes I \otimes L_3 + V$ where L_i are J-matrices (see section 3.1). Here corresponding $g(x_1,\ldots,x_d)$, $d = 2, 3$, are polynomials in their variables. On the other hand, $g(x) = -\mathrm{e}^x + T_n(x)$, for example, is connected with a model of a linear chain with infinite-range interactions (see section 3.3).

Second, we derive the expressions for local densities of states (or spectral functions) applicable both to the Hamiltonians considered here and in [1] (see section 2.2).

When $g(x_1,\ldots,x_d)$ is a polynomial, we, as in [1], use the fact that the matrix of the Hamiltonian can be considered to be block-tridiagonal but, unlike in [1], with the infinite dimension D of a block. The properties of block-tridiagonal matrices became an object of study by physicists and mathematicians starting at least from the early works of Nagel [2] and (in connection with the moment problem for operators) Krein [3] and still remain such

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[4] (where the authors construct solutions of a three-term matrix recurrence). Naturally, physical papers on the subject were centred on determination of the matrix elements of the resolvent of a block-tridiagonal matrix. Interesting in this respect are the works of Znojil [5] and Wang [6]. However, their exact results are limited to the case of finite-dimensional matrices and of those with the simplest asymptotics of the matrix elements. On the whole, the theory of block-tridiagonal matrices ($D > 1$ or the so-called matrix case) remains much less developed than that of a scalar case, that is $D = 1$. (One obvious reason for this is matrix non-commutativity.) In this connection, the very important feature of our method is that which can be termed as reduction of the matrix case to the scalar one for a large class of block-tridiagonal matrices.

2. The method

2.1. The spectrum and thermodynamics

Let $\{L_k\}_{k=1}^d$ be a set of self-adjoint operators L_k acting in separable Hilbert spaces $\mathcal{H}_k$ and represented in orthonormal bases $\{g_i^k\}_{i=0}^\infty$ of $\mathcal{H}_k$ by J-matrices ($L_{k,ij} = L_{k,ji}$ and $L_{k,ij} = 0$ if $|i-j| > 1$). Denote $I_1 \otimes \cdots \otimes L_k \otimes \cdots \otimes I_d$ in $\mathcal{H} \equiv \otimes_{k=1}^d \mathcal{H}_k$ by $\hat{L}_k$. Let $T(x_1, \ldots, x_d)$ be a polynomial of degree n_k in x_k with real coefficients.

Then, as is easily seen, the operator $H_0 \equiv T(\hat{L}_1, \ldots, \hat{L}_d)$ has a block-$(2n_1+1)$-diagonal structure in the basis $\{e_{i_1,\ldots,i_d} \equiv g_{i_1}^1 \otimes \cdots \otimes g_{i_d}^d\}_{i_1=0}^\infty \cdots {}_{i_d=0}^\infty$ with blocks of infinite dimension if $d > 1$. Let us call them the type-1 blocks. Now introduce another division into blocks (of type-2) which will be used below, namely, divide H_0 into the smallest possible blocks so that it becomes *block-tridiagonal*

$$\begin{pmatrix} A_0 & B_0 & & & 0 \\ B_0^* & A_1 & B_1 & & \\ & B_1^* & A_2 & B_2 & \\ & & \ddots & \ddots & \ddots \\ 0 & & & & \end{pmatrix} \tag{1}$$

(we assume that B_i are non-degenerate).

The case when $T(x_1, \ldots, x_d)$ is replaced by a more general real function is, obviously, less general in terms of the method, since the matrix then consists of only one block. We mention this case in section 2.3.

Consider the operator $H = H_0 + V$, where V is r-dimensional ($r < \infty$) with real matrix elements and such that H remains block-tridiagonal. We are going to find the spectrum of H and $\mathrm{Sp}\{f(H_0 + V) - f(H_0)\}$, where $f(x)$ belongs to some unspecified but 'general enough' class of functions. For $d = 1$ this problem was solved in [1].

Let $S(X)$ denote the spectrum of X. As is known [7], the spectrum of H_0 is given by the formula $S(H_0) = T(S(L_1), \ldots, S(L_d))$. $H = H_0 + V$ has the same continuous spectrum† as H_0 (which we denote by $CS(H_0)$), but its discrete spectrum may change due to V.

Suppose that $d > 1$. If we truncate the type-1 blocks of H $t \times t$, repeat the reasoning of [1] (making use of the fact that, as is easily seen,

$$T(\hat{L}_1, \ldots, \hat{L}_d) = \int \cdots \int T(\mu_1, \ldots, \mu_d)\, \mathrm{d}E_{\mu_1}^1 \otimes \cdots \otimes \mathrm{d}E_{\mu_d}^d$$

† Continuous spectrum here is the set of non-isolated points of growth of the resolution of the identity and eigenvalues of infinite multiplicity.

where $E^i_{\mu_i}$ is the resolution of the identity of L_i), and formally consider the limit as $t \to \infty$, we shall have the following results.

Let

$$\Delta(z) = |\delta_{ij} + W_{ij}|_0^\infty \tag{2}$$

where

$$W_{ij}(z) = \sum_{sk} (V P^H(z))_{s,kj} \left\{ \sum_m P^{H_0}_{s,km}(z)(R(z)e_{0;m}, e_{0;i}) + Q^{H_0}_{s,ki}(z) \right\}$$

index s is a block† index, i, j, k, m enumerate scalar elements within a block,

$$(V P^H)_s = V_{s\,s-1} P^H_{s-1} + V_{ss} P^H_s + V_{s\,s+1} P^H_{s+1}$$

where $P^M_s(z)$, $Q^M_s(z)$ are the matrix polynomials of the first and the second kind, respectively, associated with M [1]. They are defined by the following relations in terms of the blocks of M:

$$P^M_{-1} = 0 \qquad P^M_0 = I \qquad P^M_{i+1} = -B_i^{-1}((A_i - zI)P^M_i + B^*_{i-1}P^M_{i-1}) \qquad i = 0, 1, \ldots$$
$$Q^M_0 = 0 \qquad Q^M_1 = B_0^{-1} \qquad Q^M_{i+1} = -B_i^{-1}((A_i - zI)Q^M_i + B^*_{i-1}Q^M_{i-1}) \qquad i = 1, 2, \ldots$$
$$(R(z)e_{0;m}, e_{0;i}) = \int_{-\infty}^{\infty} \mathrm{d}\mu_1 \cdots \int_{-\infty}^{\infty} \mathrm{d}\mu_d \frac{p^1_{m_1}(\mu_1) \cdots p^d_{m_d}(\mu_d) \times p^1_{i_1}(\mu_1) \cdots p^d_{i_d}(\mu_d)}{T(\mu_1, \ldots, \mu_d) - z} \times \rho_1(\mu_1) \cdots \rho_d(\mu_d) \tag{3}$$

where

$$e_{0;k} = g^1_{k_1} \otimes \cdots \otimes g^d_{k_d} \qquad 0 \leqslant k_1 \leqslant n_1 - 1.$$

$p^k_i(\lambda)$ are the polynomials of the first kind associated with L_k; spectral densities $\rho_k(\mu) = (\mathrm{d}E^k_\mu g^k_0, g^k_0)/\mathrm{d}\mu$.

Then the discrete spectrum of H (energies z) can be found from the equation

$$\Delta(z) = 0 \tag{4}$$

and

$$\mathrm{Sp}\,\{f(H) - f(H_0)\} = \int_{-\infty}^{\infty} \frac{\mathrm{d}f}{\mathrm{d}x} \xi(x)\,\mathrm{d}x + \sum_i \{f(x_{i\,\mathrm{d}}) - f(x_{i\,\mathrm{b}})\} \tag{5}$$

where

$$\xi(x) = \frac{1}{\pi} \lim_{y \downarrow 0} \arg \Delta(x + \mathrm{i}y) + \delta \tag{6}$$

(where δ is an integer) if $x \in CS(H_0)$ and $\xi(x) = 0$, otherwise. The summation in (5) is over the points $x_{i\mathrm{d}}$ of the discrete spectrum of H ($x_{i\mathrm{b}}$ is the boundary of $CS(H_0)$ from which $x_{i\mathrm{d}}$ 'split off'). We assumed in (5) that H_0 has no discrete spectrum. However, it is easy to generalize this formula [1]. To determine $\xi(x)$ uniquely, we take any continuous branch of (6) and employ (5) with, say, $f(x) = x$, that is

$$\mathrm{Sp}\,V = \int_{-\infty}^{\infty} \xi(x)\,\mathrm{d}x + \sum_i (x_{i\mathrm{d}} - x_{i\mathrm{b}})$$

to find the integer constant.

The important fact which gives sense to (2) and makes our whole programme feasible for $d > 1$ is that the first matrices in the sequence $\{P_0, P_1, \ldots\}$ are often rather sparse, and VP involves only a few of them (see, e.g., section 3.1). This, in particular, leads to the

† Henceforth we deal only with the type-2 blocks and call them simply 'blocks'.

situation when only several (say u) columns of $I + W$ differ from the corresponding ones of I. Hence, properly changing the order of enumeration of the basis vectors, we shall have

$$\Delta(z) = |\delta_{ij} + W_{ij}|_0^{u-1}.$$

The only remaining essential problem is how to find $\rho_i(\mu)$. This, however, can be done whenever $L_i = J + W$, where J is a J-matrix corresponding to a system of orthogonal polynomials with a known weight function (in other words, $\rho(\mu)$ of this matrix is known) and W is finite-dimensional (see equation (13) which gives the general expression).

2.2. The spectral functions

The density of states $\eta(\lambda)$ in the continuous spectrum $CS(H)$ of a self-adjoint operator H can be defined by the following relation:

$$\eta(\lambda) = \lim_{N\to\infty} \frac{1}{N} \sum_{i=0}^{N-1} \rho_{ii}(\lambda) \qquad \rho_{ij}(\lambda) = \frac{(\mathrm{d}E_\lambda e_j, e_i)}{\mathrm{d}\lambda} \tag{7}$$

where E_λ is the resolution of the identity of H and $\{e_i\}_{i=0}^{\infty}$ is an orthonormal basis. ρ_{ij} is the 'local' density of states (spectral function) corresponding to the vectors e_i and e_j.

If perturbation V considered in section 2.1 is caused by a defect in the lattice, then, assuming that the defects are independent and their concentration is c, we get directly from (5)

$$\eta(\lambda) = \eta_0(\lambda) - c\xi'(\lambda) \tag{8}$$

where $\eta(\lambda)$ and $\eta_0(\lambda)$ are the densities of states for a certain model of the lattice with defects and for the ideal lattice, respectively.

Sometimes it is interesting to know the spectral functions of $H_0 + V$. Further we consider the case when $H = H_0 + V = T(\hat{L}_1, \ldots, \hat{L}_d) + V$ is a block-tridiagonal matrix defined in section 2.1. If the dimensionality of its blocks is infinite ($d > 1$), we truncate them $n \times n$ and take the limit as $n \to \infty$ in the results.

Using the unnumbered equation which precedes equation (26) in [1], after simple manipulations we obtain

$$(\tilde{R}(z)e_{0;l}, e_{0;m}) \equiv \tilde{R}_{ml}(z) = \frac{1}{\Delta(z)} \sum_j \Delta_{jm}(z) \left[R_{jl}(z) - \sum_{si} (V Q^H(z))_{s,il} \left\{ \sum_k P^{H_0}_{s,ik}(z) R_{jk}(z) + Q^{H_0}_{s,ij}(z) \right\} \right] \tag{9}$$

where $\tilde{R}(z) = (H - zI)^{-1}$, $R(z) = (H_0 - zI)^{-1}$, $R_{ik}(z) = (R(z)e_{0;k}, e_{0;i})$ is given by (3) and $\Delta_{jm}(z)$ is the algebraic complement of the element $(I + W)_{jm}$.

Note that the summation over indices i, j, k in (9) is limited by $n_1 = n$ addends for $d = 1$ and often by some finite number for $d > 1$.

Thus the spectral functions belonging to the first block are

$$\rho_{ml}(x) = \frac{1}{\pi} \operatorname{Im} \lim_{y\downarrow 0} \tilde{R}_{ml}(x + \mathrm{i}y) \qquad 0 \leqslant m, l \leqslant n-1. \tag{10}$$

Hence it is easy to deduce the general expression

$$\rho_{s;i,t;j}(x) = \frac{(\mathrm{d}E_x e_{t;j}, e_{s;i})}{\mathrm{d}x} = \sum_{m,l} P^H_{s,im}(x) P^H_{t,jl}(x) \rho_{ml}(x) \tag{11}$$

where we have used the property $\sum_{m=0}^{n-1} P^H_{s,im}(H) e_{0;m} = e_{s;i}$ [1] for the ith basis vector of the sth block.

If H is tridiagonal ($d = 1$, $n = 1$), equation (10) can be considerably simplified. Indeed, let $\rho_{00} \equiv \rho$ and polynomials p_i, q_i correspond to H_0 ($H_{0\,ii} = a_i$, $H_{0\,ii+1} = H_{0\,i+1i} = b_i$) whereas $\tilde{\rho}_{00} \equiv \tilde{\rho}$, $\tilde{p}_i, \tilde{q}_i$ to $H = H_0 + V$ ($H_{ii} = \tilde{a}_i$, $H_{ii+1} = H_{i+1i} = \tilde{b}_i$). Assume that $Ve_i = 0$, $i \geqslant r$.

Then (9) and (10) reduce to

$$\tilde{\rho}(x) = \frac{1 + G_1(x) - G_2(x)}{\lim_{y \downarrow 0} |\Delta(x + \mathrm{i}y)|^2} \rho(x) \tag{12}$$

where

$$G_1(x) = \sum_s \{(V\tilde{p})_s q_s - (V\tilde{q})_s p_s\}$$

$$G_2(x) = \sum_{sk} (V\tilde{q})_s (V\tilde{p})_k \{p_s q_k - p_k q_s\}.$$

Let us now define the system of polynomials $q_i^{(k)}(x)$, $i = 0, 1, \ldots$, where k is a non-negative integer, associated with a J-matrix M as one satisfying the same recurrence as $p_i^M(x)$, $q_i^M(x)$ with the initial conditions $q_i^{(k)} = 0$, $i = -1, 0, 1, \ldots, k-1$, $q_k^{(k)} = (M_{-1\,0} M_{01} M_{12} \cdots M_{k-1\,k})^{-1}$, ($M_{-1\,0} \equiv 1$). Obviously, $p_i^M = q_i^{(0)}$, $q_i^M = q_i^{(1)}$.

Using the fact that, as is easy to verify, $q_i^{(k)} = (x - M_{kk}) q_i^{(k+1)} - M_{k\,k+1}^2 q_i^{(k+2)}$, $i > k$, we get $G_1^{(k)} - G_2^{(k)} = G_1^{(k+1)} - G_2^{(k+1)}$, $k = 0, 1, \ldots, r-2$. Here $G_i^{(k)}$, $i = 1, 2$ correspond to $H_0 + V$ and H_0 from which the first k rows and columns are removed. Since $G_1^{(r-1)} = G_2^{(r-1)} = 0$, we see that $G_1 = G_2$.

Thus (12) becomes

$$\tilde{\rho}(x) = \rho(x)/R(x)$$

$$R(x) = \left\{1 + \sum_k (V\tilde{p})_k (p_k S + q_k)\right\}^2 + \left\{\sum_k (V\tilde{p})_k p_k\right\}^2 \rho^2 \pi^2 \tag{13}$$

where $S(x) = \text{v.p.} \int_{-\infty}^{\infty} \rho(\mu)/(\mu - x)\, \mathrm{d}\mu$.

In the particular case when H_0 corresponds to the Chebyshev polynomials of the second kind [1], we have

$$\rho(x) = \begin{cases} \dfrac{8}{\pi}\sqrt{x(1-x)} & x \in [0, 1] \\ 0 & x \notin [0, 1] \end{cases}$$

$$S(x) = 4(1 - 2x)$$

and so $R(x)$ becomes a polynomial in x. This fact allows us to simplify (13) even further. Let us represent $R(x)$ in the form $R(x) = \sum_{k=0}^{m} c_k \tilde{p}_k(x)$ where m is the degree of $R(x)$ (note that $\tilde{p}_k(x)$ is of exactly degree k). Then employing the well known orthogonality condition [8] $\int_{-\infty}^{\infty} \tilde{p}_i(x) \tilde{p}_j(x) \tilde{\rho}(x)\, \mathrm{d}x = \delta_{ij}$, we get from (13) $c_k = \int_{-\infty}^{\infty} \rho(x) \tilde{p}_k(x)\, \mathrm{d}x$. Moreover, since the rows of H_0 are identical (H_0 corresponds to the Chebyshev polynomials), we have $\tilde{p}_k = \tilde{p}_r p_{k-r} - \tilde{p}_{r-1} p_{k-r-1}$ $\forall k > r$, which means (by the orthogonality condition for the polynomials associated with H_0) that $c_k = 0$, $\forall k > 2r$. Since

$$\tilde{p}_r = \frac{b_0 \cdots b_{r-2}}{\tilde{b}_0 \cdots \tilde{b}_{r-2}} p_r + \sum_{i=0}^{r-1} \alpha_i p_i \qquad \tilde{p}_{r-1} = \frac{b_0 \cdots b_{r-2}}{\tilde{b}_0 \cdots \tilde{b}_{r-2}} p_{r-1} + \sum_{i=0}^{r-2} \beta_i p_i$$

it also follows from the orthogonality condition that $c_{2r} = 0$.

Thus

$$\tilde{\rho}(x) = \frac{\rho_{\mathrm{Ch}}(x)}{\sum_{k=0}^{2r-1} c_k \tilde{p}_k(x)} \qquad c_k = \int_{-\infty}^{\infty} \rho_{\mathrm{Ch}}(x) \tilde{p}_k(x)\, \mathrm{d}x. \tag{14}$$

As we mentioned in [1], this expression was originally used in [9]. Note that we do not even have to calculate the integrals in (14): $c_k = d_0$ in the expansion $\tilde{p}_k(x) = \sum_{i=0}^{k} d_i\, p_i(x)$ which is constructed directly.

2.3. Comparison with the Green function method

The standard Green function method formulated for a Hamiltonian $H = H_0 + V$ where V is r-dimensional, yields the following conditions [10, 11].

For the discrete eigenvalues ε of H,

$$|I + R(\varepsilon)V|_0^{r-1} = 0 \tag{15}$$

for the density of states in a lattice with impurities,

$$\begin{aligned}\eta(x) &= \eta_0(x) - \frac{c}{\pi}\frac{\mathrm{d}}{\mathrm{d}x}\lim_{y\downarrow 0}\operatorname{Im}\ln|I + R(x+\mathrm{i}y)V|_0^{r-1} \\ &= \eta_0(x) - \frac{c}{\pi}\frac{\mathrm{d}}{\mathrm{d}x}\lim_{y\downarrow 0}\arg|I + R(x+\mathrm{i}y)V|_0^{r-1}\end{aligned} \tag{16}$$

where $R(z) = (H_0 - zI)^{-1}$ and its matrix elements (Green functions) are computed by the formula

$$(Re_j, e_i) \equiv R_{ij} = \sum_k \frac{c_k^{i*} c_k^j}{\varepsilon_k - z}$$
$$e_i = \sum_k c_k^i \varphi_k \qquad H_0\varphi_k = \varepsilon_k\varphi_k \qquad (\varphi_i, \varphi_j) = \delta_{ij}.$$

In fact, the equation for R_{ij} is written for the $N \times N$ truncated H, and we still have to take the limit as $N \to \infty$.

The disadvantage of this method when applied to H of section 2.1 is that it is too general; the differences of our approach stem from the utilization of the special properties of H and H_0. (a) The block-tridiagonal structure of H and H_0 entails the fact that, first, the dimensionality of $\Delta(z)$ (2) can actually be less than that of the determinants in (15) and (16) and, second, the integrals (3) belong only to the first block. This fact is especially valuable if the dimensionality of the blocks is finite (e.g. in the case of linear systems [1]). (b) $H_0 = T(\hat{L}_1, \ldots, \hat{L}_d)$ leads to our using the spectral densities $\rho_i(\lambda)$ in the integrals (3) whereas in the Green function method we have to know the full solution to the spectral problem for H_0 ($\varepsilon_k, \varphi_k, N \to \infty$).

When B_i in (1) have a complicated structure so that B_i^{-1} and, hence, P_i are difficult to compute, we may use $|I + R(z)V|_0^{r-1}$ instead of $\Delta(z)$ (we saw in [1] that these determinants coincide up to a constant real factor) in our formulae thus forgoing possible advantages of point (a). (This is also the case when $H_0 = g(\hat{L}_1, \ldots, \hat{L}_d)$ where g is a more general function than a polynomial as, e.g., in section 3.3.) Point (b), however, may still be applied to simplify the formulae for R_{ij}. Similarly, we may deal with the case when V violates the block-tridiagonal structure of H_0. On the other hand, point (a) is obviously valid for any block-tridiagonal H and H_0 with non-degenerate off-diagonal blocks.

3. Examples

3.1.

Consider a simple but non-trivial example: a simple cubic lattice of spins s with a point spin defect σ governed by the Heisenberg Hamiltonian with nearest-neighbour interactions

$$H = -\frac{J}{2}\sum_{r,\delta(r,r+\delta\neq 0)}(\boldsymbol{s}_r\boldsymbol{s}_{r+\delta} - s^2) - J_\sigma\sum_{\delta}(\boldsymbol{\sigma}\boldsymbol{s}_\delta - s\sigma). \tag{17}$$

The one-magnon space $\mathcal{H}$ of the system is spanned by $e_0 = \sigma^-|0\rangle/\sqrt{2\sigma}$, $e_r = s_r^-|0\rangle/\sqrt{2s}$, $\boldsymbol{r} \neq 0$, where $\boldsymbol{r}$ runs over all lattice sites; $|0\rangle$ is the state of total spin alignment ($s_r^+|0\rangle = 0, \sigma^+|0\rangle = 0$). $H|0\rangle = 0$.

We shall look for the discrete energy levels of H in $\mathcal{H}$ and for the changes in thermodynamic functions (in the approximation of non-interacting magnons) caused by the impurity. This problem was considered in [10–12] by the Green function technique. The approximate solution can also be found by the J-matrix method ($d = 1, n = 1$): the argument is similar to that of [13]. Obviously, physically interesting results correspond to $J > 0$.

Acting with H on the basis vectors enumerated successively along adjacent chains in a fixed plain and then over adjacent planes, we get a block-tridiagonal matrix with blocks corresponding to planes. The diagonal blocks have an analogous subblock-tridiagonal structure with subblocks corresponding to chains. All these tridiagonal matrices are infinite, however, in *both* directions. Let us now introduce Cartesian coordinates with the centre at the site $\boldsymbol{r} = 0$ so that H be invariant under the reflections in coordinate plains 0xy, 0xz, 0yz and change the basis using these symmetries. Accordingly, H splits into the direct sum of eight matrices, four of which are the same as in the lattice without impurities, and the other four can be written in the form

$$H = L_{xi}\otimes I\otimes I + I\otimes L_{yi}\otimes I + I\otimes I\otimes L_{zi} + V_i \qquad i = 1,\ldots,4 \tag{18}$$

where

$$L_{x1} = L_{y1} = L_{z1} = L_{y2} = L_{z2} = L_{x3} = L_{z3} = L_{x4} = L_{y4} = 4Js(I - L_{\mathrm{Ch1}})$$
$$L_{x2} = L_{y3} = L_{z4} = 4Js(I - L_{\mathrm{Ch2}})$$

$$L_{\mathrm{Ch1}} = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{2}}{4} & & & 0 \\ \frac{\sqrt{2}}{4} & \frac{1}{2} & \frac{1}{4} & & \\ & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & \\ & & \ddots & \ddots & \ddots \\ 0 & & & & \end{pmatrix} \qquad L_{\mathrm{Ch2}} = \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & & & 0 \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & & \\ & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & \\ & & \ddots & \ddots & \ddots \\ 0 & & & & \end{pmatrix}.$$

$L_{\mathrm{Ch1}}, L_{\mathrm{Ch2}}$ correspond to the Chebyshev polynomials of the first and the second kind, respectively, and their spectral densities are $\rho_{\mathrm{Ch1}}(x) = \frac{1}{\pi}[x(1-x)]^{-1/2}$, $\rho_{\mathrm{Ch2}}(x) = \frac{8}{\pi}[x(1-x)]^{1/2}$ if $x \in [0,1]$ and zero otherwise.

Hence, the spectral density of $L_i = 4Js(I - L_{\mathrm{Ch}i})$ is

$$\rho_{L_i}(x) = -\frac{1}{4Js}\rho_{\mathrm{Ch}i}\left(1 - \frac{x}{4Js}\right).$$

$$V_1 = \begin{pmatrix} 6s(J_\sigma - J) & \gamma & \gamma & \gamma \\ \gamma & \beta & & 0 \\ \gamma & & \beta & \\ \gamma & 0 & & \beta \end{pmatrix} \qquad \beta = J_\sigma\sigma - Js \qquad \gamma = Js\sqrt{2} - J_\sigma\sqrt{2s\sigma}$$

in the basis $\{e_{0,0,0}; e_{0,0,1}; e_{0,1,0}; e_{1,0,0}\}$; $V_2 = V_3 = V_4 = \beta$ in the basis $e_{0,0,0}$.

Note that in the subspace $i = 1$, $\Delta(z)$ is 3×3 but $r = 4$. Further analysis is a straightforward application of the theory of section 2. As a result we have the discrete energy levels and the shift function $\xi(\lambda)$. According to (5), this is enough to find the changes in thermodynamic functions caused by the independent impurities in the approximation of non-interacting magnons.

From the symmetry considerations, the magnon density of states $\eta_0(\lambda)$ for the lattice without impurities can be written as follows:

$$\eta_0(\lambda) = \frac{(\mathrm{d}E_\lambda e_0, e_0)}{\mathrm{d}\lambda} = \rho_{00}(\lambda) = \int_{-\infty}^{\infty} \mathrm{d}\mu \int_{-\infty}^{\infty} \mathrm{d}\nu \rho_{L_1}(\mu)\rho_{L_1}(\nu)\rho_{L_1}(\lambda - \mu - \nu).$$

The density of states of the lattice with the impurities is then given by (8); the local densities of states can be calculated using (9)–(11).

As we saw in [1] considering a linear chain, the two-magnon problem for an ideal lattice allows a very similar formulation to that of the one-magnon-space problem for the same lattice with a point impurity. This fact also holds for 2D and 3D cases. Here formulae (4), (10), and (11) enable us to find two-magnon bound states and spectral functions in the continuous spectrum (Raman spectrum, in particular). By other methods these studies for the simple cubic lattice in question were carried out in [14–16] (including nearest- and next-nearest-neighbour interactions).

3.2.

We have just seen how the problem about an impurity in a homogeneous cubic lattice is connected with the Chebyshev polynomials. Conversely, any system of orthogonal polynomials with known weight functions $\rho_i(\lambda)$ (see the last paragraph of section 2.1) generate similar soluble problems (about the spectrum and $\mathrm{Sp}\{f(H+V) - f(H)\}$ when H and $H + V$ have the form as in section 2.1) for systems with different interactions between particles.

Let us, for example, consider the Jacobi polynomials. Using equations (4.3.4) and (4.5.1) in [17], we obtain the elements of the J-matrix $L^{(\alpha,\beta)}$ as the coefficients in the recurrence relation for the orthonormal polynomials as

$$L^{(\alpha,\beta)}_{ii} = \frac{\beta^2 - \alpha^2}{(2i + \alpha + \beta + 2)(2i + \alpha + \beta)} \qquad i = 0, 1, 2, \ldots$$

$$L^{(\alpha,\beta)}_{i-1\,i} = L^{(\alpha,\beta)}_{i\,i-1} = \frac{2}{2i + \alpha + \beta}\left(\frac{i(i+\alpha)(i+\beta)(i+\alpha+\beta)}{(2i+\alpha+\beta)^2 - 1}\right)^{1/2} \qquad i = 1, 2, 3, \ldots$$

$$\alpha, \beta > -1.$$

The polynomials of the first kind associated with this J-matrix are the Jacobi polynomials with the weight function (which is also the spectral density of $L^{(\alpha,\beta)}$)

$$\rho(x) = \begin{cases} \dfrac{\Gamma(\alpha+\beta+2)}{2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)}(1-x)^\alpha(1+x)^\beta & x \in [-1, 1] \\ 0 & x \notin [-1, 1] \end{cases}$$

where $\Gamma(x)$ is the Euler Gamma function.

3.3.

Consider a linear Heisenberg chain of spins s with long-range interactions. Let J_i be the exchange constant corresponding to the interaction of a spin with its i-nearest neighbours.

Physically interesting is the case when $J_i \to 0, i \to \infty$. Let us introduce a point defect with the same spin $\sigma = s$ but different exchange constants $\tilde{J}_i, i = 1, \ldots, r, \tilde{J}_i = J_i, i > r$, where r is finite. The generalization being straightforward, we shall assume $r = 1$ for simplicity. Now let us look for the same quantities in this system as in the one considered in 3.1.

The matrix of the Hamiltonian $H = H^+ \oplus H^-$ in the basis†

$$\varphi_0^+ = \sigma^-|0\rangle/\sqrt{2s} \qquad \varphi_k^\pm = (S_k^-|0\rangle \pm S_{-k}^-|0\rangle)/2\sqrt{s} \qquad k = 1, 2, \ldots \tag{19}$$

$$H^+ = H_0^+ + V^+ \qquad H_{0,ij}^+ = -(J_{|i-j|} + J_{i+j}) \qquad i, j > 0 \qquad J_0 \equiv -2\sum_{i=1}^{\infty} J_i$$

$$H_{0,00}^+ = -J_0 \qquad H_{0,i0}^+ = -\sqrt{2}J_i \qquad i > 0 \tag{20}$$

$$V^+ = (\tilde{J}_1 - J_1)\begin{pmatrix} 2 & -\sqrt{2} \\ -\sqrt{2} & 1 \end{pmatrix} \quad \text{in the basis} \quad \{\varphi_0^+, \varphi_1^+\}.$$

Similarly, $H^- = H_0^- + V^-$, $V^- = \tilde{J}_1 - J_1$ in the basis φ_1^-.

On the other hand, let us find the matrix elements of the exponent of the following tridiagonal matrix L infinite in both directions: $L_{i\,i-1} = L_{i-1\,i} = b$, $L_{ii} = 0$, $i = \ldots, -1, 0, 1, \ldots$, where b is a positive constant. Having performed a change of the basis similar to (19), we have $L = L^+ \oplus L^-$,

$$e_{ik}^{L^+} = (e^{L^+} p_i(L^+) p_k(L^+)\varphi_0, \varphi_0) = \int_{-2b}^{2b} e^x p_i(x) p_k(x)\rho(x)\mathrm{d}x$$

$$= \frac{1}{\sqrt{2}}(e_{0\,i+k}^{L^+} + (1 + (\sqrt{2} - 1)\delta_{ik})e_{0\,|i-k|}^{L^+}) \qquad i, k > 0.$$

Here we have used the fact that $p_i\, p_k = \{p_{i+k} + (1 + (\sqrt{2} - 1)\delta_{ik})\, p_{|i-k|}\}/\sqrt{2}$, $i, k > 0$. The spectral density $\rho(x) = (2b\pi\sqrt{1 - \{x/(2b)\}^2})^{-1}$.

Further,

$$e_{00}^{L^+} = \frac{1}{\pi}\int_{-1}^{1} e^{2bx}\frac{\mathrm{d}x}{\sqrt{1 - x^2}} = I_0(2b).$$

$I_\mu(x)$ is a well known cylindrical function defined in terms of the Bessel function $J_\mu(x)$: $I_\mu(x) = \mathrm{e}^{-\mathrm{i}\pi\mu/2} J_\mu(ix)$.

Using the recurrence relations $p_n(x) = (x/b)p_{n-1}(x) - p_{n-2}(x)$ and $I_n(x) = 2\mathrm{d}(I_{n-1}(x) - I_{n-2}(x))/\mathrm{d}x$, $n = 2, 3, \ldots$, $p_1 = x/b$, $I_1(x) = \mathrm{d}I_0(x)/\mathrm{d}x$, we finally get

$$e_{0i}^{L^+} = \sqrt{2}I_i(2b).$$

Hence, in the original basis $e_{i\,i+k}^{L} = I_k(2b)$.

So if we put the exchange integrals $J_i = I_i(2b)$, $i = 1, 2, \ldots$ (a trivial generalization being $J_i = cI_i(2b)$, where c is a scaling factor), then

$$H_0^\pm = -e^{L^\pm} + \{I_0(2b) + 2\sum_{i=1}^{\infty} I_i(2b)\}I = -e^{L^\pm} + e^{2b}I. \tag{21}$$

As is easily seen from the power-series expansion of the Bessel functions, $J_{k+1}/J_k < b$. Thus, changing b, we can regulate the rate of interaction decay.

In equation (2)

$$W_{ij}^+(z) = -\sum_{k=0}^{1} V_{kj}^+ \int_{-2b}^{2b} \frac{p_k(\mu)p_i(\mu)}{e^\mu - e^{2b} + z}\rho(\mu)\,\mathrm{d}\mu \tag{22}$$

† For convenience, the Hamiltonian is divided by s.

and similarly for $W_{ij}^{-}(z)$. Now we have all we need to calculate the changes in thermodynamic functions, discrete energy levels, and local densities of states using (4), (5), (10), and (11).

Note finally that we can assign any predefined values to J_i, $i = 1, 2, \ldots, n$, where n is finite, and the problem will still remain exactly soluble. Indeed, in such a case we shall have the representation $H_0 = -e^L + T_n(L)$.

References

[1] Krasovsky I V and Peresada V I 1995 *J. Phys. A: Math. Gen.* **28** 1493
[2] Nagel H 1936 *Math. Ann.* **112** 247 (in German)
[3] Krein M G 1949 *Doklady AN SSSR* **69** 125 (in Russian)
[4] Ahlbrandt C D and Patula W T 1995 *J. Diff. Eq. Appl.* **1** 1
[5] Znojil M 1977 *J. Math. Phys.* **18** 717; 1984 *J. Math. Phys.* **25** 2979
[6] Wang R 1987 *J. Math. Phys.* **28** 2329, 2333
[7] Reed M and Simon B 1972 *Methods of Modern Mathematical Physics (Functional Analysis 1)* (New York: Academic) ch 8
[8] Akhiezer N I 1965 *The Classical Moment Problem* (London: Oliver and Boyd) chs 1, 4
[9] Peresada V I and Afanas'ev V N 1970 *Sov. Phys.–JETP* **31** 78; [*Zh. Eksp. Teor. Fiz.* **58** 135 (in Russian)]
[10] Izyumov Yu A and Medvedyev M V 1970 *Theory of Magnetically Ordered Crystals with Impurities* (Moscow: Nauka) (in Russian)
[11] Izyumov Yu A and Medvedyev M V 1965 *Zh. Eksp. Teor. Fiz.* **48** 574 (in Russian)
[12] Wolfram T and Callaway J 1963 *Phys. Rev.* **130** 2207
[13] Peresada V I, Afanas'ev V N and Borovickov V S 1975 *Fiz. Nizk. Temp.* **1** 461 (in Russian)
[14] Loly P D and Choudhury B J 1976 *Phys. Rev.* B **13** 4019
[15] Bahurmuz A A and Loly P D 1980 *Phys. Rev.* B **21** 1924
[16] Bahurmuz A A and Loly P D 1981 *Acta Phys. Pol.* A **60** 805
[17] Szego G 1939 *Orthogonal Polynomials* (Colloquium Publications XXIII) (Providence, RI: American Mathematical Society)