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A new method in the many-body problem

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Abstract. A new method is proposed for exact calculation of the energy levels of Hamiltonians H and the quantities $\mathrm{Sp}\{f(H+W)-f(H)\}$, where W is a finite-dimensional perturbation, in the case when H and $H+W$ may be represented by a certain wide class of $(2n+1)$-diagonal matrices. As an example, two problems for a linear chain of spins with nearest- and next-nearest neighbour interactions described by the Heisenberg Hamiltonian are considered.

1. Introduction

A number of problems which involve a linear chain of particles with interactions between several (n) 'shells' of neighbours can be formulated as follows. The matrix H of the Hamiltonian is given which has a $(2n+1)$-diagonal form ($H=(H_{jk})$, where $H_{jk}=0$ if $|j-k|>n$), and whose rows are identical ($H_{jj}=a_0$; $H_{j\,j+1}=H_{j\,j-1}=a_1$; ...; $H_{j\,j+n}=H_{j\,j-n}=a_n$) starting with an rth row (r is a finite number). The problem is to find the spectrum of H and the changes in thermodynamic functions, caused by a finite-dimensional perturbation W such that $H+W$ is still $(2n+1)$-diagonal, which can be expressed in the form $\mathrm{Sp}\{f(H+W)-f(H)\}$. In the present work, we shall solve this problem using the fact that, as is easily seen, the above described Hamiltonian can be written in the form $H=T(L)+V$, where $T(x)$ is a polynomial of degree n, L is a tridiagonal (J-)matrix with identical rows, and V is finite-dimensional. In this case L is associated with the Chebyshev polynomials. We shall see, however, that these problems can be tackled whenever L is associated with polynomials having a known weight function. The latter fact enlarges the class of Hamiltonians amenable to our treatment.

The method we develop here is a generalization of the J-matrix method proposed about 25 years ago by Peresada [1–5]. The original method allowed us to solve exactly the above mentioned problem for $n=1$† (H is then a J-matrix) and, approximately, similar problems for various Hamiltonians including those for 2- and 3-dimensional systems (since any symmetric matrix can be reduced to a set of J-matrices). In fact, the recursion method of Haydock *et al* [6, 7], which is known wider, uses the same basic ideas, but the standard reference [7] does not contain the early developments [1–5] of the technique, and some important features of the method remain little known to the community. We try to fill in this gap partially in our conclusions.

2. The method

Consider the $(2n+1)$-diagonal matrix $H=T(L)+V$ ($H_{ij}=0$ if $|i-j|>n$) of a self-adjoint operator in an orthonormal basis $\{e_i\}_{i=0}^{\infty}$ of a Hilbert space $\mathcal{H}$, where $T(x)$ is a

† Although the proof of the equation for the shift function in section 2 is new even in the case $n=1$.

polynomial of degree n, L is a J-matrix ($L = (L_{ij})$, $L_{ij} = L_{ji}$ and $L_{ij} = 0$ if $|i-j| > 1$), and V is a ($(2n+1)$-diagonal) operator such that $Ve_i = 0$ if $i \geqslant r$. We shall assume that H_{ij}, L_{ij}, and the coefficients of $T(x)$ are real.

The secular equation for H is

$$(T(L) - \lambda I)\varphi = -V\varphi \qquad \varphi \in \mathcal{H}. \tag{1}$$

Note that H can be viewed as a block-tridiagonal matrix with blocks being $n \times n$ matrices. From the general theory of block-tridiagonal matrices [8], we know that an eigenvector of such a matrix

$$\begin{pmatrix} A_0 & B_0 & & & 0 \\ B_0^* & A_1 & B_1 & & \\ & B_1^* & A_2 & B_2 & \\ 0 & & \ddots & \ddots & \ddots \end{pmatrix} \qquad \dim A_i = \dim B_i = n \quad i = 0, 1, \ldots \tag{2}$$

can be expressed in the form $\varphi = P\,x$, where

$$P = \begin{pmatrix} P_0 \\ P_1 \\ \vdots \end{pmatrix}$$

and the $n \times n$ matrix polynomials (of the first kind) $P_i(\lambda)$ are defined as follows†:

$$P_{-1} = 0 \qquad P_0 = I \qquad \ldots \qquad P_i = -B_{i-1}^{-1}((A_{i-1} - \lambda I)P_{i-1} + B_{i-2}^* P_{i-2}) \qquad \ldots \tag{3}$$

x is an n-component vector

$$x = \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{pmatrix}.$$

(Further we shall use the superscript ($P_i^M(\lambda)$) to indicate polynomials associated with a block-tridiagonal M *different from* H.)

Thus we may rewrite (1) as

$$Px = -RVPx \qquad \text{where } R = (T(L) - \lambda I)^{-1}. \tag{4}$$

The sth component of the block-vector VP is

$$(VP)_s = V_{s\,s-1}P_{s-1} + V_{ss}P_s + V_{s\,s+1}P_{s+1}.$$

So

$$(VP)x = \sum_{s=0}^{[r/n]} \sum_{j,k=0}^{n-1} (VP)_{s,kj} x_j e_{ns+k}.$$

Taking the inner product of (4) with e_{nt+i}, we have

$$\sum_{j=0}^{n-1} P_{t,ij} x_j = -\sum_s \sum_{j,k=0}^{n-1} (VP)_{s,kj} x_j (Re_{ns+k}, e_{nt+i}). \tag{5}$$

† If some of the matrices B_i are degenerate (due to V), we may add to them regularizing matrix elements β_{jk} so that B_i^{-1} would exist and consider the limit as $\beta_{jk} \to 0$ in the results.

We now note that $\{e_i\}_{i=0}^{\infty}$ is the basis where J-matrix L is defined and consequently, according to the known property of J-matrices [9], $e_i = p_i^L(L)e_0$, where $p_i^L(\lambda)$ are the polynomials associated with L ((3) for $n = 1$).

Thus

$$(Re_i, e_j) = (Rp_i^L(L)p_j^L(L)e_0, e_0) = \int_{-\infty}^{\infty} \frac{p_i^L(\mu)p_j^L(\mu)}{T(\mu) - \lambda}\rho(\mu)\,\mathrm{d}\mu \tag{6}$$

(λ is outside the spectrum of $T(L)$), where the spectral density $\rho(\mu) = (\mathrm{d}E_\mu e_0, e_0)/\mathrm{d}\mu$, and E_μ is the resolution of the identity of L. The effectiveness of the method is based on the fact that the $\rho(\mu)$'s are known for a large class of J-matrices [10] whose $p_i^L(\lambda)$ are known orthogonal polynomials (Laguerre, Jacobi, etc). The $\rho(\mu)$'s are the weight functions of corresponding polynomials.

Hereafter we shall need only one of these matrices (although most of our consideration will be general), that is

$$J_{\mathrm{Ch}} = \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & & & 0 \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & & \\ & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & \\ 0 & & \ddots & \ddots & \ddots \end{pmatrix}.$$

$p_i^{J_{\mathrm{Ch}}}(\lambda)$ are the Chebyshev polynomials of the second kind and $\rho_{\mathrm{Ch}}(\lambda) = \frac{8}{\pi}\sqrt{\lambda(1-\lambda)}$ if $\lambda \in [0, 1]$ and 0 otherwise. Thus, provided that the roots of $T(\mu) - \lambda = 0$ are found, the integrals in (6) can be analytically calculated.

The matrix H described in section 1 may be represented in the form $T(L) + V$, where

$$L = \begin{pmatrix} a & b & & & 0 \\ b & a & b & & \\ & b & a & b & \\ 0 & & \ddots & \ddots & \ddots \end{pmatrix} = pJ_{\mathrm{Ch}} + qI \qquad p = 4b \quad q = a - 2b \tag{7}$$

and, consequently, the spectral density of L is

$$\rho(\lambda) = \frac{1}{p}\rho_{\mathrm{Ch}}\left(\frac{\lambda - q}{p}\right) \tag{8}$$

a, b, and coefficients of $T(L)$ are defined in terms of the matrix elements of H.

The spectrum of L is known: it is continuous and fills the interval $[a-2b, a+2b]$. Hence the spectrum of $T(L)$ is also known and continuous, and since V is finite-dimensional, its addition to $T(L)$ may lead only to the formation of points of the discrete spectrum (always leaving the continuous one invariant). But at such points, equations (5) for all t, i must hold. Let us fix $t = 0$. Then for $i = 0, 1, \ldots, n-1$ we shall have a system of linear equations in the variables $x_0, x_1, \ldots, x_{n-1}$. So the condition for finding the discrete eigenvalues of H is

$$\det(P_0 + W) = |\delta_{ij} + W_{ij}(\lambda)|_0^{n-1} = 0 \tag{9}$$

where

$$W_{ij} = \sum_s \sum_{k=0}^{n-1} (VP)_{s,kj}(Re_{ns+k}, e_i). \tag{10}$$

We have just shown the necessity of this condition. However, it is also sufficient. Indeed, let λ be a solution of (9). Then the system (5) for $t = 0$, $i = 0, \ldots, n-1$ holds true for λ

and some $\{x_i\}_{i=0}^{n-1}$. To prove that λ is an eigenvalue of H, it suffices to show that the same λ, $\{x_i\}_{i=0}^{n-1}$ satisfy systems (5) for $t = 1, 2, \ldots$.

Let us set both sides of (5) for $t = -1$ to be zero and apply induction: assume that (5) $i = 0, \ldots, n-1$ holds for $t-2$, $t-1$ and prove that it holds for t.

Having multiplied the recurrence

$$(T(L) - \lambda I)e_{n(t-1)+m} = \sum_j (B_{t-2,jm} e_{n(t-2)+j} + (A_{t-1} - \lambda I)_{jm} e_{n(t-1)+j} + B^*_{t-1,jm} e_{nt+j}) \tag{11}$$

(where $T(L)$ is taken in the form (2)) by $B^{-1}_{t-1,im}$ and performed the summation over m, we express e_{nt+i} in terms of the other elements from the resulting relation and substitute this vector in the right-hand side of (5) to get (up to a matrix M such that $Mx = 0$)

$$-\sum_{sk} (VP)_{s,kj} (Re_{ns+k}, e_{nt+i}) = -(B^{-1}_{t-1}[(A_{t-1} - \lambda I)P_{t-1} + B^*_{t-2}P_{t-2} + (VP)_{t-1}])_{ij} \tag{12}$$

(the special form of (11) enabled us to cancel the resolvent in the last term).

Now expressing the blocks of V in terms of the blocks of $T(L)$ and H, we deduce that (12) is equal to $P_{t,ij}$ and thus conclude the proof.

Let us now simplify expression (10). First we note that there is a generalization of the above-mentioned property $e_i = p_i^L(L)e_0$ of J-matrices to block-tridiagonal ones; namely, if X is a block-tridiagonal self-adjoint matrix with non-degenerate off-diagonal blocks of block dimension n in the basis $\{e_i\}_{i=0}^{\infty}$, then it is easy to show by induction that $e_{ns+k} = \sum_{m=0}^{n-1} P^X_{s,km}(\bar{X})e_m$. So we may rewrite the inner product in (10) as

$$(Re_{ns+k}, e_i) = \sum_{m=0}^{n-1} (RP^{T(L)-\lambda I}_{s,km}(T(L) - \lambda I)e_m, e_i). \tag{13}$$

Expanding equation (13) by induction in index s and substituting it in (10), we get

$$W_{ij}(\lambda) = \sum_{sk} (VP(\lambda))_{s,kj} \left\{ \sum_m P^{T(L)}_{s,km}(\lambda)(R(\lambda)e_m, e_i) + Q^{T(L)}_{s,ki}(\lambda) \right\} \tag{14}$$

$$= \sum_{s=0}^{[r/n]} \sum_{k=0}^{n-1} (VP(\lambda))_{s,kj} \left\{ \sum_{m=0}^{n-1} P^{T(L)}_{s,km}(\lambda) \int_{-\infty}^{\infty} \frac{p_m^L(\mu)p_i^L(\mu)}{T(\mu) - \lambda} \rho(\mu)\,\mathrm{d}\mu + Q^{T(L)}_{s,ki}(\lambda) \right\} \tag{15}$$

where $Q_s^{T(L)}(\lambda)$ are the matrix polynomials of the second kind associated with $T(L)$. They are defined by the same recurrence as $P_s^{T(L)}(\lambda)$ for $s = 2, 3, \ldots$, but with the different starting conditions, namely $Q_0^{T(L)} = 0$, $Q_1^{T(L)} = B_0^{-1}$.

So (9), (15) are a necessary and sufficient condition for λ to be a point of the discrete spectrum of H. The corresponding eigenvectors are Px, where x is a solution of (5) $t = 0$, $i = 0, \ldots, n-1$ with λ.

It is worth noting that in deriving (9), (14) we have not used any special properties of $T(L)$ other than its block-tridiagonal structure. Thus the condition (9), (14) may be employed to find the discrete spectrum of any $H = H_0 + V$, where H and H_0 are self-adjoint and block-tridiagonal with non-degenerate off-diagonal blocks; $H_{0ij} = H_{0ji}$; and V is finite-dimensional.

As was shown by Lifshitz [11, 12], the change in thermodynamic functions due to an impurity described by a finite-dimensional operator V can often be represented as follows

$$\mathrm{Sp}\{f(H) - f(H_0)\} = \int_{-\infty}^{\infty} \frac{\mathrm{d}f}{\mathrm{d}x} \xi(x)\,\mathrm{d}x + \sum_i \{f(x_{i\,\mathrm{d}}) - f(x_{i\,\mathrm{b}})\} \tag{16}$$

(we assume for simplicity that H_0 has only continuous spectrum $C(H_0)$; the trace with arbitrary H_0 can be reduced to a sum of such traces (cf subsection 3.1.2)), where $H = H_0 + V$; $\xi(x)$ is a so-called shift function defined in a certain manner on $C(H_0)$, $\xi(x) \equiv 0$ if $x \notin C(H_0)$; the summation is over the points x_{id} of the discrete spectrum of H (x_{ib} is the boundary nearest to x_{id} of $C(H_0)$).

We are interested in the case when H and H_0 are block-tridiagonal with non-degenerate off-diagonal blocks. Such a structure of H and H_0 will now enable us to find a much simpler equation for $\xi(x)$ than the original one proposed by Lifshitz [11].

Consider the equation

$$(H - zI)f = g \qquad \operatorname{Im} z > 0 \quad \operatorname{Re} z \in C(H_0) \tag{17}$$

where $H = H_0 + V$ (the dimension of a block is n) and $Ve_i = 0$ if $i \geqslant r$.

Let us introduce the following notation for vectors:

$$h_s = \begin{pmatrix} h_{s,0} \\ h_{s,1} \\ \vdots \\ h_{s,n-1} \end{pmatrix} \qquad h_{s,k} = (h, e_{ns+k}).$$

Then (17) is a recurrence relation for f_s, from which we obtain

$$f_s = P_s f_0 + Y_s g \qquad Y_0 = 0 \tag{18}$$

$$Y_s g = \sum_{k=1}^{s} P_{s-k}^{k} \tilde{B}_{k-1}^{-1} g_{k-1} \qquad s \neq 0 \tag{19}$$

where $\tilde{B}_i$ are the blocks of H in the form (2); $P_i^k(z)$ is the ith matrix polynomial associated with H from which the first k block-rows and k block-columns are removed ($P_i \equiv P_i^0$).

Applying the resolvent $R = (H_0 - zI)^{-1}$ to both sides of (17) gives

$$f + \sum_{k=0}^{r-1} (f, e_k) RVe_k = Rg. \tag{20}$$

Successively taking the inner products of e_i, $i = 0, \dots, n-1$ with both sides of (20), we have

$$f_0 + \sum_s K_{0s} f_s = (Rg)_0 \tag{21}$$

where K_{ts} is a block of matrix K (with matrix elements $K_{ij} = (RVe_j, e_i)$) divided into blocks $n \times n$.

By substituting (18) in (21),

$$\left(I + \sum_s K_{0s} P_s \right) f_0 = (Rg)_0 - \sum_s K_{0s} Y_s g. \tag{22}$$

Introduce the determinant (henceforth we assume that $H_{0ij} = \overline{H_{0ji}} = H_{0ji}$)

$$\begin{aligned} \Delta(z) &= \det\left(I + \sum_s K_{0s} P_s \right) \\ &= \left| \delta_{ij} + \sum_s \sum_{k=0}^{n-1} (RVe_{ns+k}, e_i) P_{s,kj} \right|_0^{n-1} \\ &= \left| \delta_{ij} + \sum_{sk} (VP)_{s,kj} \left\{ \sum_m P_{s,km}^{H_0} (Re_m, e_i) + Q_{s,ki}^{H_0} \right\} \right|_0^{n-1} \end{aligned} \tag{23}$$

and the algebraic complement Δ_{jk} of the element $\left(I + \sum_s K_{0s} P_s\right)_{jk}$. (We shall soon see that $\xi(x)$ is expressed in terms of $\Delta(z)$).

Note that when $H_0 = T(L)$

$$\Delta(z) = |\delta_{ij} + W_{ij}(z)|_0^{n-1} \tag{24}$$

where $W_{ij}(z)$ is defined in (15). We see that (24) is the same as the determinant in (9), only now z is essentially complex.

From (22)

$$f_{0,k} = \frac{1}{\Delta} \sum_{j=0}^{n-1} \Delta_{jk} \left(g, \left[R - \sum_s K_{0s} Y_s \right]^* e_j \right). \tag{25}$$

In fact, here we have introduced a new operator $\widetilde{K_{0s} Y_s} g = \sum_{i=0}^{n-1} (K_{0s} Y_s g)_i e_i$ for which we, naturally, retained the same symbol $K_{0s} Y_s$. (Moreover we shall also need the similarly defined operator Y_s.) Using (18) and then (25), we rewrite (20) in the form ($f = \tilde{R} g$)

$$\begin{aligned}(\tilde{R} - R) g &= -\sum_{si} f_{s,i} R V e_{ns+i} \\ &= -\frac{1}{\Delta} \sum_{sikj} \Delta_{jk} P_{s,ik} \left(g, \left[R - \sum_t K_{0t} Y_t \right]^* e_j \right) R V e_{ns+i} - \sum_{si} (g, Y_s^* e_i) R V e_{ns+i}.\end{aligned}$$

Consequently

$$\begin{aligned}\mathrm{Sp}(\tilde{R} - R) = -\frac{1}{\Delta} \Bigg\{ &\sum_{sikj} \Delta_{jk} P_{s,ik} \left(R V e_{ns+i}, \left[R - \sum_t K_{0t} Y_t \right]^* e_j \right) \\ &+ \Delta \sum_{si} (R V e_{ns+i}, Y_s^* e_i) \Bigg\}.\end{aligned} \tag{26}$$

As we show in the appendix, the numerator in this equation is equal to $\Delta'(z)$. Thus

$$\mathrm{Sp}(\tilde{R} - R) = -\Delta'(z)/\Delta(z). \tag{27}$$

A similar equation, $\mathrm{Sp}(\tilde{R} - R) = -\Delta_k'(z)/\Delta_k(z)$, was obtained by Krein [13] for an arbitrary (not necessarily block-tridiagonal) form of H. Here

$$\Delta_k = |\delta_{ij} + (R V e_j, e_i)|_0^{r-1}.$$

We see that $\Delta(z) = c \Delta_k(z)$, where c is a constant factor. To find this factor, we shall compare the asymptotic behaviour of $\Delta(z)$ and $\Delta_k(z)$ as $\mathrm{Im}\, z \to +\infty$. Obviously

$$\Delta_k(z) = 1 + \mathrm{O}(1/\mathrm{Im}\, z) \qquad \mathrm{Im}\, z \to +\infty \tag{28}$$

As to $\Delta(z)$, we first see by induction that

$$\begin{aligned}F(z) &\equiv (R(z) P_{t,mj}^{H-zI} (H_0 - zI) e_i, e_{ns+k}) \\ &= P_{t,mj}(z) (R(z) e_i, e_{ns+k}) + (\tilde{B}_{t-1}^{-1} \tilde{B}_{t-2}^{-1} \cdots \tilde{B}_0^{-1})_{mj} (B_0 B_1 \cdots B_{t-2})_{ik} \delta_{s\, t-1} \\ &\qquad s = t-1, t, t+1\end{aligned} \tag{29}$$

where $\tilde{B}_i$, B_i are the off-diagonal blocks of H and H_0, respectively. On the other hand, $F(z) = \sum_{q=0}^{t} \sum_{l=0}^{n-1} \gamma_{ql} (R(z) e_{nq+l}, e_{ns+k})$, $\gamma_{ql} =$ constant. Expressing $P_{t,mj}(Re_i, e_{ns+k})$

from (29) and substituting it in the matrix element $\delta_{ij} + \sum_{sk}(VP)_{s,kj}(Re_{ns+k}, e_i)$ of (23), we get

$$\Delta(z) = \det M + O(1/\operatorname{Im} z) \qquad \operatorname{Im} z \to +\infty$$
$$M_{ij} = \delta_{ij} - \sum_s (B_0 B_1 \cdots B_{s-1} V_{s\,s+1} \tilde{B}_s^{-1} \tilde{B}_{s-1}^{-1} \cdots \tilde{B}_0^{-1})_{ij}.$$

Thus $c = \det M$.

Our equation (23) for Δ is simpler than Krein's one for Δ_k, because n is often less than r and in approximate applications of the method, much less (see section 4). When $n = 1$, we simply have

$$\Delta(z) = 1 + \sum_{k=0}^{r-1} (Vp)_k \left\{ p_k^{H_0}(Re_0, e_0) + q_k^{H_0} \right\}. \tag{30}$$

Taking into account (28), let us define $\ln \Delta_k(z)$ in the upper half-plane so that it be a holomorphic function there and $\ln \Delta_k(z) = O(1/\operatorname{Im} z)$, $\operatorname{Im} z \to +\infty$. Then, as was shown by Krein [13], almost everywhere on the real axis (we have substituted $c^{-1}\Delta(z)$ for Krein's original $\Delta_k(z)$)

$$\xi(x) = \frac{1}{\pi} \lim_{y \downarrow 0} \operatorname{Im} \ln\{c^{-1}\Delta(x + iy)\} = \frac{1}{\pi} \lim_{y \downarrow 0} \arg \Delta(x + iy) + \delta \tag{31}$$

where δ is an integer. Practically, to find $\xi(x)$, we simply take any continuous branch of $\frac{1}{\pi} \lim_{y \downarrow 0} \arg \Delta(x + iy)$ and add to it an integer constant so as to satisfy (16) with some simple testing function, e.g. for $f(x) = x$

$$\operatorname{Sp} V = \int_{-\infty}^{\infty} \xi(x)\,dx + \sum_i (x_{i\mathrm{d}} - x_{i\mathrm{b}}). \tag{32}$$

When $H_0 = T(L)$, we use (24) for $\Delta(z)$. In the limit as $y \to 0$ from above, the relevant integrals

$$\lim_{y \downarrow 0} \int_{-\infty}^{\infty} \frac{p_i^L(\mu) p_j^L(\mu)}{T(\mu) - (x + iy)} \rho(\mu)\,d\mu$$
$$= \text{v.p.} \int_{-\infty}^{\infty} \frac{p_i^L(\mu) p_j^L(\mu)}{T(\mu) - x} \rho(\mu)\,d\mu + i\pi \sum_l p_i^L(\tilde{x}_l) p_j^L(\tilde{x}_l) \rho(\tilde{x}_l) \left| \frac{d\tilde{x}}{dx}(T(\tilde{x}_l)) \right|$$
$$x = T(\tilde{x}_l). \tag{33}$$

When $H_0 = L$, we obtain, using (30),

$$\xi(x) = \frac{1}{\pi} \tan^{-1} \frac{\pi \sum_k (Vp(x))_k p_k^L(x) \rho(x)}{1 + \sum_k (Vp(x))_k \left(p_k^L(x)\, \text{v.p.} \int_{-\infty}^{\infty} \frac{\rho(\mu)\,d\mu}{\mu - x} + q_k^L(x) \right)}. \tag{34}$$

Thus, equations (16), (31), (32), (24), (15), (33) complete our solution of the problem of finding changes in thermodynamic functions.

3. Examples

Here we have chosen as examples the problems whose solutions, in appropriate limiting cases, are either already known or can be obtained independently using the scalar variant ($n = 1$) of our theory. Note that although we have chosen spin systems, problems for linear chains of mechanically oscillating particles also suggest themselves immediately.

3.1. Linear chain with impurity

Consider a linear system of spins s with a point spin defect σ described by the Heisenberg Hamiltonian involving interactions between nearest and next-nearest neighbours

$$H = -\sum_{\nu=1}^{2}\left[J_\nu \sum_{i\,(i,i+\nu\neq 0)} (s_i s_{i+\nu} - s^2) + J_{\sigma\nu}(\sigma s_\nu + s_{-\nu}\sigma - 2s\sigma)\right] \tag{35}$$

An additive constant is chosen so that $H|0\rangle = 0$ where $|0\rangle$ is the state of total spin alignment ($s_i^+|0\rangle = 0$, $i = \pm1, \pm2, \ldots$; $\sigma^+|0\rangle = 0$). We are going to find the change in the thermodynamics due to the impurity in the approximation of non-interacting magnons and discrete energy levels in the one-magnon space $\mathcal{H}$ of the system, that is in the space spanned by the vectors $h_0 = \sigma^-|0\rangle/\sqrt{2\sigma}$, $h_i = s_i^-|0\rangle/\sqrt{2s}$, $i = \pm1, \pm2, \ldots$.

First we note that the system is invariant under the reflection with respect to the site of the impurity spin. Hence, $\mathcal{H}$ splits into the two subspaces invariant under H: $\mathcal{H}_s$ spanned by $e_0^s = h_0$, $e_i^s = (h_i + h_{-i})/\sqrt{2}$ and $\mathcal{H}_a$ spanned by $e_i^a = (h_i - h_{-i})/\sqrt{2}$. Accordingly, $H = H_s \oplus H_a$. Acting with H on vectors $e_i^s(e_i^a)$ and using the commutation relations, we obtain a matrix in this basis which can be written as follows:

$$H_{s(a)} = \mp L^2 + V_{s(a)} + (2s(J_1 + J_2) \pm \alpha)I \tag{36}$$

where L has the form (7) with

$$a = \frac{\beta}{2\sqrt{\gamma}} \qquad b = \sqrt{\gamma} \qquad \beta = \pm sJ_1 \qquad \gamma = |sJ_2| \qquad \alpha = a^2 + 2b^2 \tag{37}$$

(in the double sign ($\pm$ or $\mp$) the upper corresponds to $J_2 > 0$; the lower, to $J_2 < 0$),

$$V_s = \begin{pmatrix} \mp\gamma + v_{s1} & \beta' & \gamma' \\ \beta' & v_{s2} & 0 \\ \gamma' & 0 & v_{s3} \end{pmatrix} \qquad \beta' = \pm\beta - J_{\sigma1}\sqrt{2s\sigma} \qquad \gamma' = \pm\gamma - J_{\sigma2}\sqrt{2s\sigma}$$

$$v_{s1} = 2s(J_{\sigma1} + J_{\sigma2} - J_1 - J_2) \qquad v_{s2} = \sigma J_{\sigma1} - s(J_1 + J_2) \qquad v_{s3} = \sigma J_{\sigma2} - sJ_2$$

$$V_a = \begin{pmatrix} \mp\gamma + v_{a1} & 0 \\ 0 & v_{a2} \end{pmatrix} \qquad v_{a1} = s(J_2 - J_1) + \sigma J_{\sigma1} \qquad v_{a2} = \sigma J_{\sigma2} - sJ_2.$$

So we can use the general theory for $T(L) + V = \mp L^2 + V_{s(a)}$, the multiple-of-unity operator being easily accountable for in the results.

In order to evaluate the determinant (9) using (15), we express $\mp L^2$, $V_{s(a)}$ as block-tridiagonal matrices with blocks 2×2 and then calculate VP to get

$$(V_sP_s)_0 = \begin{pmatrix} \gamma'\frac{\lambda\pm\alpha-v_{s1}}{\gamma'\mp\gamma} + v_{s1} \mp \gamma & \beta' - \gamma'\frac{\beta'\mp\beta}{\gamma'\mp\gamma} \\ \beta' & v_{s2} \end{pmatrix}$$

$$(V_sP_s)_1 = \begin{pmatrix} v_{s3}\frac{\lambda\pm\alpha-v_{s1}}{\gamma'\mp\gamma} + \gamma' & -v_{s3}\frac{\beta'\mp\beta}{\gamma'\mp\gamma} \\ 0 & 0 \end{pmatrix} \qquad (V_sP_s)_i = 0 \quad i = 2, 3, \ldots \tag{38}$$

$$(V_aP_a)_0 = \begin{pmatrix} v_{a1} \mp \gamma & 0 \\ 0 & v_{a2} \end{pmatrix} \qquad (V_aP_a)_i = 0 \quad i = 1, 2, \ldots .$$

Thus we need $P_t^{\mp L^2}(\lambda)$, $Q_t^{\mp L^2}(\lambda)$ only for $t = 0, 1$.

The integrals

$$\int_{-\infty}^{\infty} \frac{p_i^{\mp L}(\mu)p_j^{\mp L}(\mu)}{\mp\mu^2 - \lambda}\rho(\mu)\,d\mu \qquad (i, j) = \{(0,0); (1,0); (1,1)\} \tag{39}$$

($\rho(\mu)$ is given by (8)) reduce to the following:

$$\frac{1}{\pi}\int_0^1 \frac{x^m}{x-\tau}\sqrt{x(1-x)}\,dx = \sum_{i=1}^{m} \tau^{i-1}\frac{(2(m-i)+2)!}{2^{2(m-i)+3}(m-i+1)!(m-i+2)!}$$
$$+\tau^m\left(\tfrac{1}{2}-\tau+\omega\tau\sqrt{\frac{\tau-1}{\tau}}\right) \qquad \omega=\begin{cases}0 & \text{if } \tau\in[0,1]\\ 1 & \text{if } \tau\notin[0,1].\end{cases} \tag{40}$$

If $\tau \in [0, 1]$, the integrals are taken in the principal value sense. As τ is not necessarily real, note that the branch of the square root in (40) is the following: for $z = re^{i\varphi}$ where $\varphi \in (-\pi, \pi]$, $\sqrt{z} = \sqrt{r}e^{i\varphi/2}$.

From this point onwards, we have to proceed with the calculation of the discrete spectrum and the shift function separately.

3.1.1. Discrete energy levels. Substituting (38), the matrix elements of $P_t^{\mp L^2}(\lambda)$, $Q_t^{\mp L^2}(\lambda)$, $t = 0, 1$ and the integrals with $\omega = 1$ in (9), (15), we get an algebraic equation with square roots whose solutions are discrete energy levels. It is too cumbersome, however, to write it out explicitly.

Now let us consider the limit as $J_2, J_{\sigma 2} \to 0$. By taking the limit under the integral sign in (39) and using the fact that in this limit H becomes a J-matrix and (that is why) $x_0 = 1$; $x_1 = (\lambda \pm \alpha - v_{s(a)1})/(\beta' \mp \beta)$, we obtain from the first row of (5) ($n = 2, t = 0, i = 0$) the final conditions

$$\left.\begin{aligned} &\text{s:} \quad \left(\frac{z-1}{z}\right)^{\frac{1}{2}} = 1-\frac{\kappa}{2(\kappa-1)z+\theta}\\ &\text{a:} \quad \left(\frac{z-1}{z}\right)^{\frac{1}{2}} = 1-\frac{\kappa}{2(\kappa-1)z}\end{aligned}\right\} \qquad \theta=\frac{J_{\sigma 1}}{J_1} \quad \kappa=\theta\frac{\sigma}{s} \tag{41}$$

and the eigenvalues of H to be $\varepsilon = 4sJ_1z$.

When $\sigma = s = \frac{1}{2}$, these conditions reduce to those found by Oguchi and Ono [14].

3.1.2. The shift function. The change in various thermodynamic functions (per atom) due to the impurities in the approximation of non-interacting magnons can be written as follows:

$$\Delta F = \chi\,\mathrm{Sp}\{f(H) - f(H_0)\} \tag{42}$$

where χ is the concentration of the impurity spins which we consider independent; H_0 is H with $s = \sigma$ and also $J_{\sigma i} = J_i$, $i = 1, 2$.

To apply (16) here, we write

$$\Delta F = \sum_{t=s,a} \chi[\mathrm{Sp}\{f(H_t) - f(T(L))\} - \mathrm{Sp}\{f(H_{0t}) - f(T(L))\}]$$

where $T(L) = \mp L^2 + (2s(J_1 + J_2) \pm \alpha)I$.

So the final shift function is composed of the four addends, each of which is evaluated first by applying (33)

$$\lim_{y\downarrow 0}\int_{-\infty}^{\infty}\frac{p_i^{\mp L}(\mu)p_j^{\mp L}(\mu)}{\mp\mu^2-(x+iy)}\rho(\mu)\,d\mu$$
$$= \mathrm{v.p.}\int_{-\infty}^{\infty}\frac{p_i^{\mp L}(\mu)p_j^{\mp L}(\mu)}{\mp\mu^2 - x}\rho(\mu)\,d\mu \mp i\pi p_i^{\mp L}(\sqrt{\mp x})p_j^{\mp L}(\sqrt{\mp x})\frac{\rho(\sqrt{\mp x})}{2\sqrt{\mp x}}$$
$$\mp x \in C(L^2) \tag{43}$$

second, by substituting (43) in (15) in which the limit as $y \to 0$ is already taken, and third, by calculating the argument of (24) divided by π. Finally, (32) is employed to decide upon an additive integer constant in the resulting sum as prescribed in section 2.

In the limit as J_2, $J_{\sigma 2} \to 0$, the shift function takes the form

$$\xi(z) = \begin{cases} \dfrac{1}{\pi}\tan^{-1}\left\{\left(\dfrac{z}{1-z}\right)^{\frac{1}{2}}\left[1 - \dfrac{4z(\kappa-1)^2 + 2\theta(\kappa-1) - \kappa^2}{8z^2(\kappa-1)^2 - 4z(\kappa-\theta)(\kappa-1) - \kappa\theta}\right]\right\} \\ \qquad z \in [0,1] \\ 0 \qquad z \notin [0,1] \end{cases} \tag{44}$$

where $\varepsilon = 4sJ_1 z$; κ, θ are defined in (41).

This equation *per se* (as well as (41)) is, of course, found much more easily if we set $J_2 = J_{\sigma 2} = 0$ at the very beginning thus reducing H to a J-matrix and proceed according to the scalar variant ($n = 1$) of the theory. Formula (44) follows then from (34).

Substituting (44) in (16), we find changes caused by the impurities in any desired thermodynamic quantity (setting $\chi = 1$).

As the density of states $\eta(x)$ is defined from the relation $F = \int f(x)\eta(x)\,dx$, it readily *follows from (42), (16) that* $\eta(x) = \eta_0(x) - \chi\xi'(x)$, *where* $\eta(x)$, $\eta_0(x)$ *are the densities of* one-magnon states (in the continuous spectrum) in the chain with impurities and the ideal chain, respectively.

3.2. *Two-magnon bound states*

Consider a linear chain of spins described by the Hamiltonian (35) but without the impurity. We are now interested in the two-magnon space $\mathcal{G}$ of this system. $\mathcal{G}$ is spanned by the vectors $D(i, i-j) = s_i^- s_j^- |0\rangle/2s$, $i \neq j$; $D(i,0) = s_i^- s_i^- |0\rangle/(2\sqrt{s(2s-1)})$.

In each subspace $\mathcal{G}_k$ spanned by $\varphi(k,p) = \lim_{N\to\infty}\sum_m e^{ikm} D(m,p) e^{ikp/2}/\sqrt{N}$, $p = 0, 1, \ldots$, where the summation is over all sites m of the chain containing N sites, there may exist levels of the discrete spectrum known as the energies of bound states of two-spin waves. These energies for the system considered here were found by Ono *et al* [15] in the case $s = \frac{1}{2}$†.

The matrix of H in the basis of vectors $\varphi(k,p)$, $p = 0, 1, \ldots$ can be represented in a form similar to (36), (37)

$$H = \mp L^2 + V + (4s(J_1 + J_2) \pm \alpha)I$$

where L has the form (7) with

$$a = \frac{\beta}{2\sqrt{\gamma}} \qquad b = \sqrt{\gamma} \qquad \beta = \pm 2J_1 s\cos\tfrac{k}{2} \qquad \gamma = |2J_2 s\cos k| \qquad \alpha = a^2 + 2b^2$$

$$V = \begin{pmatrix} \mp\gamma & \beta' & \gamma' \\ \beta' & -J_1 \mp \gamma & 0 \\ \gamma' & 0 & -J_2 \end{pmatrix} \qquad \begin{cases} \beta' = \pm\beta - 2J_1\sqrt{s(2s-1)}\cos\frac{k}{2} \\ \gamma' = \pm\gamma - 2J_2\sqrt{s(2s-1)}\cos k. \end{cases}$$

In the signs ($\pm$,$\mp$) the upper one is taken when

(1) $\qquad k \in [0, \frac{\pi}{2}]$ and $J_2 > 0$

(2) $\qquad k \in [\frac{\pi}{2}, \pi]$ and $J_2 < 0$

† However, we used the approximate methods of [17] for comparison with our exact results.

and the lower when

(1) $k \in [0, \frac{\pi}{2}]$ and $J_2 < 0$

(2) $k \in [\frac{\pi}{2}, \pi]$ and $J_2 > 0$.

Repeating the reasoning of subsection 3.1, we obtain the condition for the energies of bound states. In the limiting case $J_2 \to 0$, this condition becomes equivalent to that found by Wortis [16], see also [17, 18].

4. Conclusions

Let us stress the following points.

(1) As we saw in section 2, there is a clear connection between the formulated problems for $H = T(L) + V$ and the well-developed theory of orthogonal polynomials, which, in particular, allows us to treat a wide class of operators H that way.

(2) The method gives approximate solutions for an even larger class of Hamiltonians. The point is that if a $(2n + 1)$-diagonal representation of a Hamiltonian is not analytically available, we can easily obtain it numerically. Let us start the discussion with the scalar variant ($n = 1$) of the method. As is known [7, 19, 20], given a symmetric matrix H and a starting vector φ , we can reduce H in the subspace spanned by $\varphi, H\varphi, H^2\varphi, \ldots$, to the tridiagonal (i.e. J-matrix) form by means of the Lanczos algorithm. (The resulting J-matrix J turnes out then to be defined in the basis obtained by orthogonalization of the sequence $\varphi, H\varphi, H^2\varphi, \ldots$). Practically, of course, we can find only a finite number, say r, of the elements of the J-matrix. Already at this step, we can obtain approximations to the discrete energy levels and the quantities $(f(H)\varphi, \varphi)$ by utilizing the properties of polynomials $p_i^J(\lambda)$ and the quadrature equation [9], respectively. However, if the asymptotic behaviour of the elements of J (J_{ik} as $i, k \to \infty$) can be found, then it becomes possible to employ a more powerful theory. A review of the first developments in this (recursion) method and its applications (except for [1–5]) is given in [7]. Further progress, with emphasis on the asymptotic behaviour of J_{ik}, is partly reflected in [21]. Other examples of the uses of the technique include, in particular, [22, 23]. Note, by the way, that it is possible to broaden the range of applications of the method by considering recurrence relations and J-matrices in a Hilbert space of *operators* and making use of the Liouville equation [24–27].

The main fact we want to stress in this section is that, if the asymptotic behaviour of J_{ik} as $i, k \to \infty$ coincides with that of the elements of a J-matrix L which corresponds to a known system of orthogonal polynomials, we can apply the theory of section 2 for $n = 1$ (since then $J \approx L + V$, where V is truncated $r \times r$) [5] and also obtain results connected with the evaluation of the local density of states. There follows an example of such results already published in 1970 [2].

An analytical approximation to the distribution function $g(\varepsilon)$ of the squared harmonic oscillation frequences of a single-atom cubic lattice is written as follows: $g_{\mathrm{appr}}(x) = \rho_{\mathrm{Ch}}(x)/R(x)$, $x = \varepsilon/\varepsilon_{\max}$, where

$$R(x) = \sum_{i=0}^{2r} a_i p_i^{J/\varepsilon_{\max}} \qquad a_i = \int_0^1 p_i^{J/\varepsilon_{\max}} \rho_{\mathrm{Ch}}(x)\,\mathrm{d}x$$

and $\rho_{\mathrm{Ch}}(x)$ is defined in section 2. The starting vector φ used here is one collinear with the displacement of one of the atoms of the lattice along one of the fourfold axes.

For $n > 1$, we can apply the algorithm similar to that of Lanczos which involve n starting orthonormal vectors and reduce a matrix to the $(2n+1)$-diagonal form. The further parallel between the $n = 1$ and $n > 1$ cases is clear, but implementation is non-trivial, the major problem once again being the estimation of the asymptotic behaviour of the matrix elements. To the authors' knowledge, a systematic work on the subject has not so far been carried out.

Appendix

Here we prove that $\Delta'(z)$ is equal to (henceforth, we assume summation over repeating indices)

$$\Delta_{jk} P_{s,ik}(RVe_{ns+i}, R^* e_j) - \Delta_{jk} P_{s,ik}(RVe_{ns+i}, [K_{0t} Y_t]^* e_j) + \Delta(RVe_{ns+i}, Y_s^* e_i). \tag{A1}$$

We have

$$\begin{aligned} \Delta'(z) &= \Delta_{jk}(\delta_{jk} + (R(z)Ve_{ns+i}, e_j) P_{s,ik}(z))' \\ &= \Delta_{jk}(R^2 Ve_{ns+i}, e_j) P_{s,ik} + \Delta_{jk}(RVe_{ns+i}, e_j) P'_{s,ik}. \end{aligned} \tag{A2}$$

We see that the first terms in (A1) and (A2) are equal. Furthermore, as it is easy to show

$$P'_s = Y_s \begin{pmatrix} P_0 \\ \vdots \\ P_{s-1} \end{pmatrix}.$$

So the second term in (A2) becomes

$$Y_{s,i\,nq+l} Z_{q,lsi} \qquad Z_{q,lsi} = \Delta_{jk} P_{q,lk}(RVe_{ns+i}, e_j).$$

On the other hand, the second and the third terms in (A1) can be written as follows:

$$Y_{s,i\,nq+l} X_{q,lsi} \tag{A3}$$

$$X_{q,lsi} = -\Delta_{jk} P_{t,mk}(RVe_{ns+i}, e_j)(RVe_{nt+m}, e_{nq+l}) + \Delta(RVe_{ns+i}, e_{nq+l}). \tag{A4}$$

We shall now show that $X_q = Z_q$ and thus complete the proof. That this equality holds for $q = 0$ is seen directly from (A4): Indeed, we write the first addend in (A4) in the form $-\Delta_{jk}(P_{t,mk}(RVe_{nt+m}, e_l) + \delta_{lk} - \delta_{lk})(RVe_{ns+i}, e_j)$ and employ the well-known relation for a matrix G: $\Delta_{jk} G_{lk} = \delta_{jl} \det G$, where Δ_{jk} is the algebraic complement of G_{jk}.

Assuming $Z_{-1} = X_{-1} = 0$, we may proceed by induction. From the recurrence relation (cf equation (11)) (no summation over q!)

$$(H_0 - \bar{z}I)e_{n(q-1)+m} = (B_{q-2,jm} e_{n(q-2)+j} + (A_{q-1} - \bar{z}I)_{jm} e_{n(q-1)+j} + B^*_{q-1,jm} e_{nq+j})$$

where A_s, B_s are the blocks of H_0 written in the form (2), we express e_{nq+l} and substitute it in (A4) to get

$$\begin{aligned} X_{q,lsi} = {} & \{B^{-1}_{q-1}(zI - A_{q-1})\}_{lj} X_{q-1,jsi} - (B^{-1}_{q-1} B^*_{q-2})_{lj} X_{q-2,jsi} \\ & - B^{-1}_{q-1,lm} P_{t,gk} \Delta_{jk}(RVe_{ns+i}, e_j)(Ve_{nt+g}, e_{n(q-1)+m}). \end{aligned} \tag{A5}$$

Deriving (A5), we used the fact that $(Ve_{ns+i}, e_{n(q-1)+m}) = 0$ whenever $s > q$; and the summation over q in (A3) is from 0 to $s - 1$. It now remains for us to express the matrix elements of V in (A5) in terms of A_s, B_s, $\tilde{A}_s$, $\tilde{B}_s$ (blocks of H_0 and H); replace X_{q-1}, X_{q-2} by Z_{q-1}, Z_{q-2}; and as a result we have a relation which yields $Z_{q,lsi}$.

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