# Spectrum of a Schrödinger operator on a lattice with broken bonds

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The exact solution for the density of states of a Schrödinger operator on a $d$-dimensional lattice with broken bonds between two neighboring planes is found to be expressible in terms of the density of states of the operator on a $d$- and $(d-1)$-dimensional perfect lattice. The influence of the introduction of some infinitesimal amount of off-diagonal disorder is thereby revealed.

Solving problems on lattices, is a natural approach in crystal physics and offers a convenient discretization in the continuum. But even in the simple case of the Schrödinger operator, when dealing with multidimensional disordered systems, there is an obvious lack of analytical solutions, Lloyd's model,[1] with diagonal disorder only, being the only exactly soluble model in three dimensions. Much information is offered by the determination of the density of states, and numerical studies of this function have been undertaken recently in the off-diagonal disorder case.[2–4] But as an analytical solution of such fully disordered $d$-dimensional systems seems presently out of reach, it seems sensible to treat analytically a simpler case, namely, an HSC (hyper simple cubic) lattice with broken bonds between two neighboring planes in order to enlighten the off-diagonal disorder onset and to offer a new basis for further studies of more disordered systems. The system under consideration offers wide applications, such as tight-binding electron band, harmonic elastic vibrations, discretized waves propagation equations, etc.

In the one-dimensional case, the system considered in this Brief Report is described by the Hamiltonian operator equivalent to a $N\times N$ real symmetric matrix, where $N$ is the number of lattice sites. By shifting the origin of the energy to eliminate the constant diagonal matrix elements, the off-diagonal matrix elements are left, and are assumed to be nonzero for nearest neighbors, except for one broken bond between sites 0 and 1. A periodic boundary condition is imposed: so that the matrix is defined as follows:

$$\underline{H}_1=(\underline{I}-\underline{D}_0)\underline{m}_1+\underline{m}_{-1}(\underline{I}-\underline{D}_0)\ , \tag{1}$$

where the entries of the $N\times N$ cyclic matrix $\underline{m}_p, p\geq 0$, are given by $(\underline{m}_p)_{0\alpha}=\delta_{\alpha,p}$, other rows being obtained by cyclic permutation and $\underline{m}_{-p}$ is the transpose and inverse of $\underline{m}_p$; they satisfy the following identities:

$$\underline{m}_0=\underline{m}_N=\underline{I}_N\ , \tag{2}$$

$$\underline{m}_p\underline{m}_q=\underline{m}_q\underline{m}_p=\underline{m}_{p+q}\ , \tag{3}$$

$$(\underline{m}_p)^q=\underline{m}_{pq}\ . \tag{4}$$

The diagonal $N\times N$ matrix $\underline{D}_p$ $(p\geq 0)$ is defined by $(\underline{D}_p)_{\alpha\beta}=\delta_{\alpha\beta}\delta_{\alpha p}$ with $0\leq\alpha\leq N-1$; also $(\underline{D}_{-p})_{\alpha\beta}=\delta_{\alpha\beta}\delta_{\alpha,N-p}$, from which it follows that $\underline{D}_p^2=\underline{D}_p$ and $\underline{D}_p\underline{D}_q=0$ $(p\neq q)$. The matrices $\underline{m}_p$ and $\underline{D}_p$ do not commute but obey the rule

$$\underline{D}_p\underline{m}_q=\underline{m}_q\underline{D}_{p+q} \text{ or } \underline{m}_q\underline{D}_p=\underline{D}_{p-q}\underline{m}_q\ . \tag{5}$$

Those matrices can also be used to represent the Hamiltonian, on a simple hypercubical lattice with one broken bond (between sites 0 and 1) in each one-dimensional row directed along the first space coordinate, in the form of a sum of direct products of $d$ $N\times N$ matrices:

$$\underline{H}_d=\underline{I}\otimes\underline{I}\otimes\cdots\otimes\underline{H}_1+\underline{I}\otimes\cdots\otimes(\underline{m}_1+\underline{m}_{-1})\otimes\underline{I}$$
$$+\underline{I}\otimes\cdots\otimes(\underline{m}_1+\underline{m}_{-1})\otimes\underline{I}\otimes\underline{I}+\cdots+(\underline{m}_1+\underline{m}_{-1})\otimes\underline{I}\cdots\otimes\underline{I}\ . \tag{6}$$

Chebysheff polynomials (of the second kind) $C_p$ of cyclic matrices proved to be useful in dealing with perfect periodic lattices[5] by virtue of the identity

$$C_p(\underline{m}_1+\underline{m}_{-1})=\underline{m}_p+\underline{m}_{-p}\ . \tag{7}$$

Similarly, to prove here that the trace of the matrices $C_p(\underline{H}_1)$ have a constant value will enable us to calculate the power moments of the density of states. First, considering the nature of the matrices in (1), it is evident that the trace of any odd power of $\underline{H}_1$ is zero, so that

$$\mathrm{Tr}C_q(\underline{H}_1)=0\quad(q\text{ odd}) \tag{8}$$

and clearly

$$\mathrm{Tr}C_0(\underline{H}_1)=2N\ . \tag{9}$$

Using Eqs. (2)–(5), we find for the first even order polynomials

$$C_2(\underline{H}_1)=-(\underline{D}_1+\underline{D}_0)-(\underline{D}_0+\underline{D}_{-1})\underline{m}_2-\underline{m}_{-2}(\underline{D}_0+\underline{D}_{-1})+\underline{m}_2+\underline{m}_{-2}\ ,$$

$$C_4(\underline{H}_1)=-(\underline{D}_2+\underline{D}_{-1})-(\underline{D}_1+\underline{D}_{-2})\underline{m}_2-\underline{m}_{-2}(\underline{D}_1+\underline{D}_{-2})$$
$$-(\underline{D}_0+\underline{D}_{-1}+\underline{D}_{-2}+\underline{D}_{-3})\underline{m}_4-\underline{m}_{-4}(\underline{D}_0+\underline{D}_{-1}+\underline{D}_{-2}+\underline{D}_{-3})+\underline{m}_4+\underline{m}_{-4}\ ,$$

 

so that we guess that the general term of the sequence is

$$C_{2p}(\underline{H}_1) = -(\underline{D}_p + \underline{D}_{-p+1}) - (\underline{D}_{p-1} + \underline{D}_{-p})\underline{m}_2 - \underline{m}_{-2}(\underline{D}_{p-1} + \underline{D}_{-p}) - \cdots \quad (p > 1) \; , \tag{10}$$

where in anticipation of the next step, we have considered the cyclic matrix components up to second order only. The derivation by recurrence that the diagonal part of (10) is correct is obtained by using the recursion formula

$$C_{2p+2}(\underline{H}_1) = C_2(\underline{H}_1)C_{2p}(\underline{H}_1) - C_{2p-2}(\underline{H}_1) \; , \tag{11}$$

which is satisfied by Chebysheff polynomials. We note that cyclic matrices of order $> 2$ cannot contribute to the diagonal term of

$$\begin{aligned} C_2(\underline{H}_1)C_{2p}(\underline{H}_1) &= [-(\underline{D}_1 + \underline{D}_0) - (\underline{D}_0 + \underline{D}_{-1})\underline{m}_2 - \underline{m}_{-2}(\underline{D}_0 + \underline{D}_{-1}) + \underline{m}_2 + \underline{m}_{-2}] \\ &\quad \times [-(\underline{D}_p + \underline{D}_{-p+1}) - (\underline{D}_{p-1} + \underline{D}_{-p})\underline{m}_2 - \underline{m}_{-2}(\underline{D}_{p-1} + \underline{D}_{-p}) - \cdots] \; , \\ &= -(\underline{m}_2 + \underline{m}_{-2})[(\underline{D}_{p-1} + \underline{D}_{-p})\underline{m}_2 + \underline{m}_{-2}(\underline{D}_{p-1} + \underline{D}_{-p}) - \cdots] \; , \\ &= -(\underline{D}_{p-1} + \underline{D}_{-p}) - \underline{m}_{-2}(\underline{D}_{p-1} + \underline{D}_{-p})\underline{m}_2 - \cdots \; , \\ &= -(\underline{D}_{p+1} + \underline{D}_{-p+2} + \underline{D}_{p-1} + \underline{D}_{-p}) - \cdots \; , \end{aligned} \tag{12}$$

so that obtaining $C_{2p-2}(\underline{H}_1)$ from (10), Eq. (11) yields

$$C_{2p+2}(\underline{H}_1) = -(\underline{D}_{p+1} + \underline{D}_{-p}) - \cdots \; . \tag{13}$$

We conclude that

$$\mathrm{Tr} C_q(\underline{H}_1) = -2 \quad (q \text{ even}) \; . \tag{14}$$

Now using the properties of the direct product of matrices, we have for large $N\,(N \gg p)$

$$\mathrm{Tr}(\underline{H}_d)^p = \sum_{p_1 + \cdots + p_d = p} \frac{p!}{p_1! \cdots p_d!} (\mathrm{Tr}\underline{H}_1^{p_1})[\mathrm{Tr}(\underline{m}_1 + \underline{m}_{-1})^{p_2}] \cdots [\mathrm{Tr}(\underline{m}_1 + \underline{m}_{-1})^{p_d}] \; , \tag{15}$$

which can be evaluated by expansion in the set of orthogonal Chebysheff polynomials, and making use of (7) as

$$\begin{aligned} \mathrm{Tr}(\underline{m}_1 + \underline{m}_{-1})^p &= \sum_{q=0}^{p} \langle x^p, C_q(x) \rangle \mathrm{Tr}(\underline{m}_q + \underline{m}_{-q}) \; , \\ &= 2N \langle x^p, C_0(x) \rangle \; , \end{aligned} \tag{16}$$

where the inner product is

$$\langle f(x), C_q(x) \rangle = [2\pi(1+\delta_q)]^{-1} \int_{-1}^{1} (1-x^2)^{-1/2} f(2x) C_q(2x)\, dx \; . \tag{17}$$

Similarly, we have from (9) and (14)

$$\mathrm{Tr}(\underline{H}_1)^p = 2N \langle x^p, C_0(x) \rangle - 2 \sum_{q=2}^{p} \langle x^p, C_q(x) \rangle \quad (p \text{ even}) \; . \tag{18}$$

Making use of the identity

$$2^{p-1} = \sum_{q=0}^{p} \langle x^p, C_q(x) \rangle \; , \tag{19}$$

we have

$$\mathrm{Tr}(\underline{H}_1)^p = (2n+2)\langle x^p, C_0(x) \rangle - 2^p \quad (p \text{ even}) \; ,$$

$$\mathrm{Tr}(\underline{H}_1)^p = (2N+2)\langle x^p, C_0(x) \rangle = 0 \quad (p \text{ odd}) \; ,$$

so that (15) can be rewritten as follows:

$$\begin{aligned} \mathrm{Tr}(\underline{H}_d)^p &= \sum_{p_1 + \cdots + p_d = p} \frac{p!}{p_1! \cdots p_d!} \Bigg( (2N+2)(2N)^{d-1} \langle x_1^{p_1} \cdots x_d^{p_d},\, C_0(x_1) \cdots C_0(x_d) \rangle \\ &\quad - \frac{(2N)^{d-1}}{2} (2^{p_1} + (-2)^{p_1}) \langle x_2^{p_2} \cdots x_d^{p_d},\, C_0(x_2) \cdots C_0(x_d) \rangle \Bigg) \; , \\ &= (2N+2)(2N)^{d-1} \left\langle \left[ \sum_{i=1}^{d} x_i \right]^p, \prod_{i=1}^{d} C_0(x_i) \right\rangle - \frac{(2N)^{d-1}}{2} \left\langle \left[ 2 + \sum_{i=2}^{d} x_i \right]^p + \left[ -2 + \sum_{i=2}^{d} x_i \right]^p, \prod_{i=2}^{d} C_0(x_i) \right\rangle \; . \end{aligned} \tag{20}$$

We are now in a position to calculate the Fourier transform of the density of states, i.e., the moments generating function[6]

$$\hat{n}_d(t) = \sum_{p=0}^{\infty} \frac{(-it)^p}{p!} \mathrm{Tr}(\underline{H}_d)^p \; , \tag{21}$$

which, from (20), reads

$$\hat{n}_d(t) = (2N+2)(2N)^{d-1}\left\langle \exp\left[-it\sum_{k=1}^{d} x_k\right], \prod_{k=1}^{d} C_0(x_k)\right\rangle$$
$$-\frac{(2N)^{d-1}}{2}\left\langle \exp\left[-it\left(2+\sum_{k=2}^{d} x_k\right)\right] + \exp\left[-it\left(-2+\sum_{k=2}^{d} x_k\right)\right], \prod_{k=2}^{d} C_0(x_k)\right\rangle , \quad (22)$$

taking the inverse Fourier transform and dividing by $N^d$ yields the density of states in the form

$$n_d(E) = (1+N^{-1})2^d\left\langle \delta\left[E-\sum_{i=1}^{d} x_i\right], \prod_{i=1}^{d} C_0(x_i)\right\rangle$$
$$-\frac{N^{-1}}{2}2^{d-1}\left\langle \delta\left[E-2-\sum_{i=2}^{d} x_i\right] + \delta\left[E+2-\sum_{i=2}^{d} x_i\right], \prod_{i=2}^{d} C_0(x_i)\right\rangle , \quad (23)$$

using generalization of the inner product (17) to $d$ dimensions we have

$$n_d(E) = (1+N^{-1})\pi^{-d}\int_{-1}^{1}\delta\left[E-2\sum_{i=1}^{d} x_i\right]\prod_{i=1}^{d}(1-x_i^2)^{-1/2}dx_i$$
$$-\frac{N^{-1}\pi^{-d+1}}{2}\int_{-1}^{1}\left[\delta\left[E-2-2\sum_{i=1}^{d-1} x_i\right] + \delta\left[E+2-2\sum_{i=1}^{d-1} x_i\right]\right]\prod_{i=1}^{d-1}(1-x_i^2)^{-1/2}dx_i . \quad (24)$$

Noting that this formula involves classical expressions[5,7] of the density of states for a perfect lattice; now we can formulate the fundamental *theorem*. Let $\nu_d(E)$ be the density of states for the Schrödinger operator

$$\underline{H}_d^0 = (\underline{m}_1+\underline{m}_{-1}) \otimes \underline{I} \otimes \cdots \otimes \underline{I} + \underline{I} \otimes (\underline{m}_1+\underline{m}_{-1}) \otimes \underline{I} \otimes \cdots \otimes \underline{I} + \cdots + \underline{I} \otimes \cdots \otimes (\underline{m}_1+\underline{m}_{-1}) , \quad (25)$$

defined on a perfect SHC lattice with $N^d$ sites; then the density of states for the Schrödinger operator (6), defined on the same lattice with one broken bond between sites 0 and 1 of each row, is given in the limit $N \to \infty$ by

$$n_d(E) = \nu_d(E) + N^{-1}\{\nu_d(E) - \tfrac{1}{2}[\nu_{d-1}(E-2) + \nu_{d-1}(E+2)]\} . \quad (26)$$

From this formula, the total number of states is easily checked to be equal to $N^d$; and we notice that $-2d \leq E \leq 2d$, which is the bandwidth of the perfect crystal. In fact, the broken bonds do not give rise to new eigenvalues out of the band; but the main effect of the introduction of this infinitesimal amount of off-diagonal disorder is to reduce the Van Hove singularities: the singularities at the band edges $E=\pm 2$, in $\nu_1(E)$, are destroyed by Dirac functions $\nu_0(E\pm 2)=\delta(E\pm 2)$; the logarithmic singularity of $\nu_2(E)$ is reduced by the singularities of $\nu_1(E\pm 2)$ at $E=0$; . . . .

Finally, very simple and illuminating conclusions can be drawn from this theorem, which reveal several features of the spectrum in imperfect lattices.

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[1]P. Lloyd, J. Phys. C **2**, 1717 (1969).

[2]G. Theodorou and M. H. Cohen, Phys. Rev. B **13**, 4597 (1976).

[3]A. C. Fertis, A. N. Andriotis, and E. N. Economou, Phys. Rev. B **24**, 5806 (1981).

[4]K. Niizeki, Prog. Theor. Phys. **62**, 1 (1979).

[5]Ph. Audit, J. Phys. (Paris) **42**, 903 (1981).

[6]F. Cyrot-Lackmann, J. Phys. Chem. Solids **29**, 1235 (1968).

[7]R. J. Jelitto, J. Phys. Chem. Solids **30**, 609 (1969).