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Differential equations for the local Green function in the tight-binding model on a regular lattice†

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Abstract. For the tight-binding model of electron motion in a perfect crystal we propose a method for obtaining an ordinary differential equation satisfied by the local Green function. Such an equation probably exists for every case.

1. Introduction

A variety of methods has been used in the past to calculate Green functions and the related density of states in the tight-binding model for electron motion in a perfect crystal (Morita and Horiguchi 1971, Haydock *et al* 1972, Gaspard and Cyrot-Lackmann 1973). Many of these are based on the summation of a divergent high-energy expansion (Haydock 1980). In a few cases (Joyce 1971, 1973) it has been shown that the matrix elements of the Green function satisfy an ordinary differential equation with polynomial coefficients, with energy E as an independent variable. The purpose of this paper is to suggest that the Green function matrix elements probably always satisfy an equation of this form, and to indicate how the equation may be found. We give results for a number of examples. The method originally leads to a set of coupled first-order equations, and in some cases we have not performed the reduction to a single higher-order equation. The set is just as useful and informative.

It should be possible to apply standard numerical techniques to the differential equation(s) to obtain accurate solutions, including results for those values of E near singularities such as band edges or Van Hove singularities, which are often difficult to handle with other approaches. The derivation of the equation(s) involves substantial amounts of algebra in the more complicated cases. This algebra could be carried out using one of the symbolic computation systems now available.

2. Integral representation for Green function matrix elements

We suppose that the crystal is based on a lattice of dimension ν, with lattice points given by $A\boldsymbol{n}$, where $\boldsymbol{n} = (n_1, n_2, \ldots, n_\nu)$ has integer components and A is a $\nu \times \nu$ matrix. The Schrödinger equation used in the most general form of the tight-binding model

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(e.g. as derived from the LCAO method (Jones 1975, Economou 1979)) for the motion of an electron through the crystal may be written as

$$H\Psi = EN\Psi \tag{2.1}$$

where Ψ has components $\Psi_{\boldsymbol{n}}$, $\boldsymbol{n} \in Z^{\nu}$, each of which is a η-dimensional column matrix to allow for structure within each unit cell. The matrix H has elements $H_{\boldsymbol{n},\boldsymbol{m}}$, $\boldsymbol{n}, \boldsymbol{m} \in Z^{\nu}$, each of which is a $\eta \times \eta$ matrix, and is such that $H_{\boldsymbol{n},\boldsymbol{m}}$ depends only on $\boldsymbol{n} - \boldsymbol{m}$. We write

$$H_{\boldsymbol{n},\boldsymbol{m}} = B(\boldsymbol{m} - \boldsymbol{n}) \tag{2.2}$$

where $B(\boldsymbol{l})$ will be zero unless $\boldsymbol{l}$ is close to $\boldsymbol{0}$. An additional property that follows from the Hermiticity and translational invariance of the underlying Hamiltonian is that $B(-\boldsymbol{l}) = B(\boldsymbol{l})^{+}$ (Jones 1975). The matrix N will have a similar structure to that of H, with $D(\boldsymbol{l})$ taking the place of $B(\boldsymbol{l})$, and will often be the unit matrix.

The local Green function associated with site $\boldsymbol{0}$ is a $\eta \times \eta$ matrix

$$G(z) = C_1 \int_{\boldsymbol{p} \in BZ} \left(\sum_{\boldsymbol{l}} (zD(\boldsymbol{l}) - B(\boldsymbol{l})) \exp(\mathrm{i}\boldsymbol{p} \cdot A\boldsymbol{l}) \right)^{-1} \mathrm{d}\boldsymbol{p} \tag{2.3}$$

where the integral is restricted to the first Brillouin zone, and C_1 is a constant. If we set $\boldsymbol{p} = (A^{\mathrm{T}})^{-1}\boldsymbol{h}$, then (2.3) becomes

$$G(z) = C_2 \int_0^{2\pi} \mathrm{d}h_1 \ldots \int_0^{2\pi} \mathrm{d}h_{\nu} \left(\sum_{\boldsymbol{l}} (zD(\boldsymbol{l}) - B(\boldsymbol{l})) \exp(\mathrm{i}\boldsymbol{h} \cdot \boldsymbol{l}) \right)^{-1} \tag{2.4}$$

with C_2 another constant.

In this paper we shall restrict attention to $g(z) = \eta^{-1} \operatorname{Tr} G(z)$, but the methods used can easily be extended to other elements of $G(z)$ and to elements of the Green function connecting different lattice sites.

If we write the inverse matrix in the integrand of (2.4) in the form adj/det, then it may be seen that $g(z)$ may be expressed as

$$g(z) = \int_0^{2\pi} \mathrm{d}h_1 \ldots \int_0^{2\pi} \mathrm{d}h_{\nu}\, N(z, \boldsymbol{h})/P(z, \boldsymbol{h}) \tag{2.5}$$

where $N(z, \boldsymbol{h})$, $P(z, \boldsymbol{h})$ are polynomials with real coefficients in the variables z and $\sin h_i$, $\cos h_i$, $i = 1, \ldots, \nu$.

3. Differential equations in the general case

To simplify the presentation we use the symbol $(\sin \boldsymbol{h})^{\boldsymbol{l}}$ to mean

$$(\sin \boldsymbol{h})^{\boldsymbol{l}} = \prod_{j=1}^{\nu} (\sin h_j)^{l_j} \tag{3.1}$$

and similarly $(\cos \boldsymbol{h})^{\boldsymbol{l}}$. Also we let $\int$ represent $\int_0^{2\pi} \mathrm{d}h_1 \ldots \int_0^{2\pi} \mathrm{d}h_{\nu}$. We define $|\boldsymbol{l}| = l_1 + l_2 + \ldots + l_{\nu}$ and let $\boldsymbol{\varepsilon}_i$ denote the ν component vector with 1 in the ith place, zero elsewhere. We write

$$P(z, \boldsymbol{h}) = \sum_{\boldsymbol{l},\boldsymbol{m}} (\cos \boldsymbol{h})^{\boldsymbol{l}} (\sin \boldsymbol{h})^{\boldsymbol{m}} q(\boldsymbol{l}, \boldsymbol{m}; z) \tag{3.2}$$

where the sum over $\boldsymbol{l}$, $\boldsymbol{m}$ includes a finite set of values, and $q(\boldsymbol{l}, \boldsymbol{m}; z)$ is a polynomial in z.

We show how to obtain coupled equations involving the quantities

$$\left.\begin{aligned} I(\boldsymbol{l}, \boldsymbol{m}; z) &= \int (\cos \boldsymbol{h})^{\boldsymbol{l}} (\sin \boldsymbol{h})^{\boldsymbol{m}} / P(z, \boldsymbol{h}) && (3.3a) \\ J(\boldsymbol{l}, \boldsymbol{m}; z) &= \int (\cos \boldsymbol{h})^{\boldsymbol{l}} (\sin \boldsymbol{h})^{\boldsymbol{m}} / P(z, \boldsymbol{h})^2 && (3.3b) \end{aligned}\right\} \boldsymbol{l}, \boldsymbol{m} \in Z_+^{\nu}.$$

It is then easy to obtain equations involving $g(z)$.

If we define

$$C(\boldsymbol{l}, \boldsymbol{m}) = \int (\cos \boldsymbol{h})^{\boldsymbol{l}} (\sin \boldsymbol{h})^{\boldsymbol{m}} \tag{3.4}$$

then inserting P/P in (3.4) leads to

$$\sum_{\boldsymbol{k},\boldsymbol{n}} q(\boldsymbol{k}, \boldsymbol{n}; z) I(\boldsymbol{l}+\boldsymbol{k}, \boldsymbol{m}+\boldsymbol{n}; z) = C(\boldsymbol{l}, \boldsymbol{m}) \qquad \boldsymbol{l}, \boldsymbol{m} \in Z_+^{\nu}. \tag{3.5}$$

In a similar manner from the definition (3.3a) of $I(\boldsymbol{l}, \boldsymbol{m}; z)$, we obtain

$$\sum_{\boldsymbol{k},\boldsymbol{n}} q(\boldsymbol{k}, \boldsymbol{n}; z) J(\boldsymbol{l}+\boldsymbol{k}, \boldsymbol{m}+\boldsymbol{n}; z) = I(\boldsymbol{l}, \boldsymbol{m}; z) \qquad \boldsymbol{l}, \boldsymbol{m} \in Z_+^{\nu}. \tag{3.6}$$

Another type of relation comes from differentiating the expression (3.3a) for $I(\boldsymbol{l}, \boldsymbol{m}; z)$ with respect to z, and we find (with $'$ meaning d/dz)

$$I(\boldsymbol{l}, \boldsymbol{m}; z)' = -\sum_{\boldsymbol{k},\boldsymbol{n}} q(\boldsymbol{k}, \boldsymbol{n}; z)' J(\boldsymbol{l}+\boldsymbol{k}, \boldsymbol{m}+\boldsymbol{n}; z) \qquad \boldsymbol{l}, \boldsymbol{m} \in Z_+^{\nu}. \tag{3.7}$$

Relations of yet another form may be obtained by integrating (3.3a) by parts. If $l_i > 0$ we integrate the factor $\cos h_i$ and differentiate the remaining factor of the integrand with respect to the variable h_i to give

$$\begin{aligned} I(\boldsymbol{l}, \boldsymbol{m}; z) = \int \sin h_i \Big[& [(l_i - 1)(\cos \boldsymbol{h})^{\boldsymbol{l}-2\boldsymbol{\varepsilon}_i} (\sin \boldsymbol{h})^{\boldsymbol{m}+\boldsymbol{\varepsilon}_i} \\ & - m_i (\cos \boldsymbol{h})^{\boldsymbol{l}} (\sin \boldsymbol{h})^{\boldsymbol{m}-\boldsymbol{\varepsilon}_i}] / P(z, \boldsymbol{h}) \\ & + \left(\frac{\partial}{\partial h_i} P(z, \boldsymbol{h}) \right) (\cos \boldsymbol{h})^{\boldsymbol{l}-\boldsymbol{\varepsilon}_i} (\sin \boldsymbol{h})^{\boldsymbol{m}} / P(z, \boldsymbol{h})^2 \Big] \\ = {} & (l_i - 1) I(\boldsymbol{l}-2\boldsymbol{\varepsilon}_i, \boldsymbol{m}+2\boldsymbol{\varepsilon}_i; z) - m_i I(\boldsymbol{l}, \boldsymbol{m}; z) \\ & - \sum_{\boldsymbol{k},\boldsymbol{n}} q(\boldsymbol{k}, \boldsymbol{n}; z) (k_i J(\boldsymbol{l}+\boldsymbol{k}-2\boldsymbol{\varepsilon}_i, \boldsymbol{m}+\boldsymbol{n}+2\boldsymbol{\varepsilon}_i; z) \\ & - n_i J(\boldsymbol{l}+\boldsymbol{k}, \boldsymbol{m}+\boldsymbol{n}; z)) \qquad \boldsymbol{l}, \boldsymbol{m} \in Z_+^{\nu}, l_i > 0, i = 1, \ldots, \nu. \end{aligned} \tag{3.8}$$

Similarly, integrating the factor $\sin h_i$ we obtain

$$\begin{aligned} I(\boldsymbol{l}, \boldsymbol{m}; z) = {} & (m_i - 1) I(\boldsymbol{l}+2\boldsymbol{\varepsilon}_i, \boldsymbol{m}-2\boldsymbol{\varepsilon}_i; z) - l_i I(\boldsymbol{l}, \boldsymbol{m}; z) \\ & - \sum_{\boldsymbol{k},\boldsymbol{n}} q(\boldsymbol{k}, \boldsymbol{n}; z) (k_i J(\boldsymbol{l}+\boldsymbol{k}, \boldsymbol{m}+\boldsymbol{n}; z) - n_i J(\boldsymbol{l}+\boldsymbol{k}+2\boldsymbol{\varepsilon}_i, \boldsymbol{m}+\boldsymbol{n}-2\boldsymbol{\varepsilon}_i; z)) \\ & \boldsymbol{l}, \boldsymbol{m} \in Z_+^{\nu} \qquad m_i > 0, i = 1, \ldots, \nu. \end{aligned} \tag{3.9}$$

It is only necessary to consider values of $m_i < 2$, for using $(\sin h_i)^2 = 1 - (\cos h_i)^2$, we have

$$\left.\begin{aligned} I(\boldsymbol{l}, \boldsymbol{m}; z) &= I(\boldsymbol{l}, \boldsymbol{m}-2\boldsymbol{\varepsilon}_i; z) - I(\boldsymbol{l}+2\boldsymbol{\varepsilon}_i, \boldsymbol{m}-2\boldsymbol{\varepsilon}_i; z) \\ J(\boldsymbol{l}, \boldsymbol{m}; z) &= J(\boldsymbol{l}, \boldsymbol{m}-2\boldsymbol{\varepsilon}_i; z) - J(\boldsymbol{l}+2\boldsymbol{\varepsilon}_i, \boldsymbol{m}-2\boldsymbol{\varepsilon}_i; z) \end{aligned}\right\} m_i \geqslant 2. \tag{3.10}$$

Now suppose we consider all the equations (3.5)-(3.10) corresponding to $|\boldsymbol{l}| \leqslant L$, $|\boldsymbol{m}| \leqslant L$ for some positive integer L. If L is large enough there will be more of these equations than there are unknown $I(\boldsymbol{l}, \boldsymbol{m}; z)$, $J(\boldsymbol{l}, \boldsymbol{m}; z)$. We conjecture that there exists a value of L such that a subset of these equations may be found which contains as many independent equations as unknowns, and that, from these unknowns, all others may be determined. We have no proof of this conjecture in the general case. The remainder of the paper consists of showing it to be true in a number of examples. The methods we use can be applied to any other case of interest in the search for the equations of the conjecture.

4. Examples

The general ideas set out in § 3 will now be illustrated by examples.

4.1. Triangular lattice

For this two-dimensional lattice we take

$$A = \begin{bmatrix} 1 & -\frac{1}{2} \\ 0 & \sqrt{3}/2 \end{bmatrix}. \tag{4.1}$$

We take $\eta = 1$ and assume only nearest-neighbour interactions, so that

$$\begin{aligned} &D(\mathbf{0}) = 1 \qquad D(\boldsymbol{l}) = 0 \qquad \boldsymbol{l} \neq \mathbf{0} \\ &B(\boldsymbol{l}) = 1 \qquad \boldsymbol{l} = (1,0), (1,1), (0,1), (-1,0), (-1,-1), (0,-1) \\ &B(\boldsymbol{l}) = 0 \qquad \text{otherwise.} \end{aligned} \tag{4.2}$$

If we use (2.3) rather than (2.4) no sine functions appear and we have

$$g(z) = (2\pi)^{-2} \int_0^{2\pi} \mathrm{d}\theta_1 \int_0^{2\pi} \mathrm{d}\theta_2 (z - T(\boldsymbol{\theta}))^{-1} \tag{4.3}$$

where

$$T(\boldsymbol{\theta}) = 4 \cos\theta_1 (\cos\theta_1 + \cos\theta_2) - 2 \tag{4.4}$$

and we have set

$$\theta_1 = p_1/2 \qquad \theta_2 = \sqrt{3} p_2/2. \tag{4.5}$$

The integral (4.3) is of the form (2.5). We can obtain coupled equations for $I(\boldsymbol{l}; z)$ given by

$$I(\boldsymbol{l}; z) = I(\boldsymbol{l}, \mathbf{0}; z) = \int (\cos\theta)^{l} (z - T(\boldsymbol{\theta}))^{-1}. \tag{4.6}$$

If we set

$$T(\boldsymbol{\theta}) = \sum_{\boldsymbol{l}} t(\boldsymbol{l}) (\cos\boldsymbol{\theta})^{\boldsymbol{l}} \tag{4.7}$$

where $t(\mathbf{0}) = -2$, $t(2,0) = 4$, $t(1,1) = 4$ and $t(\boldsymbol{l}) = 0$ otherwise, then (3.5) may be written as

$$zI(\boldsymbol{l}; z) = \sum_{\boldsymbol{k}} t(\boldsymbol{k}) I(\boldsymbol{l} + \boldsymbol{k}; z) + C(\boldsymbol{l}) \qquad \boldsymbol{l} \in Z_+^2 \tag{4.8}$$

where

$$C(\boldsymbol{l}) = C(\boldsymbol{l}, \boldsymbol{0}).$$

In this case $J(\boldsymbol{l}, \boldsymbol{m}; z) = -I(\boldsymbol{l}, \boldsymbol{m}; z)'$ and $I(\boldsymbol{l}, 2\boldsymbol{\varepsilon}_i; z) = I(\boldsymbol{l}, \boldsymbol{0}; z) - I(\boldsymbol{l}+2\boldsymbol{\varepsilon}_i, \boldsymbol{0}; z)$, so that the equations obtained by integrating (4.6) by parts, the special cases of (3.8), may be written

$$I(\boldsymbol{l}; z) = (l_i - 1)(I(\boldsymbol{l}-2\boldsymbol{\varepsilon}_i; z) - I(\boldsymbol{l}; z)) + \sum_{\boldsymbol{k}} t(\boldsymbol{k}) k_i (I(\boldsymbol{k}+\boldsymbol{l}; z)' - I(\boldsymbol{k}+\boldsymbol{l}-2\boldsymbol{\varepsilon}_i; z)') \qquad \boldsymbol{l} \in Z_+^2,\ l_i > 0,\ i = 1, \ldots, \nu. \tag{4.9}$$

We take (4.8) for $\boldsymbol{l} = (0,0), (2,0), (1,1), (0,2)$ and (4.9) for $\boldsymbol{l} = (2,0), (0,2)$ and $(1,1)$ with $i = 1, 2$, which gives eight equations for the eight unknowns $I(\boldsymbol{k}; z)$ corresponding to $\boldsymbol{k} = (0,0), (2,0), (0,2), (1,1), (4,0), (3,1), (2,2), (1,3)$. In terms of

$$\phi(z) = \begin{bmatrix} I(0,0;z) \\ I(2,0;z) \\ I(1,1;z) \\ I(0,2;z) \end{bmatrix} \quad \text{and} \quad \psi(z) = \begin{bmatrix} I(4,0;z) \\ I(3,1;z) \\ I(2,2;z) \\ I(1,3;z) \end{bmatrix} \tag{4.10}$$

the equations may be written

$$z\phi = W\phi + X\psi + \gamma \tag{4.11}$$

$$Y\phi' + Z\psi' + S\phi = 0 \tag{4.12}$$

$$W = \begin{bmatrix} -2 & 4 & 4 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & -2 \end{bmatrix} \quad X = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 4 & 4 & 0 & 0 \\ 0 & 4 & 4 & 0 \\ 0 & 0 & 4 & 4 \end{bmatrix} \quad \gamma = \pi^2 \begin{bmatrix} 4 \\ 2 \\ 0 \\ 2 \end{bmatrix}$$

$$Y = \begin{bmatrix} 0 & -8 & -4 & 0 \\ 0 & 0 & -4 & 0 \\ 0 & 0 & -8 & -4 \\ 0 & -4 & 0 & 0 \end{bmatrix} \quad Z = \begin{bmatrix} 8 & 4 & 0 & 0 \\ 0 & 0 & 0 & 4 \\ 0 & 8 & 4 & 0 \\ 0 & 0 & 4 & 0 \end{bmatrix} \quad S = \begin{bmatrix} 1 & -2 & 0 & 0 \\ 1 & 0 & 0 & -2 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix}. \tag{4.13}$$

Differentiating (4.11) gives

$$(z - W)\phi' - X\psi' + \phi = 0. \tag{4.14}$$

The matrix Z is not singular, so that we may solve (4.12) for ψ' and substitute in (4.14), with the result that

$$(z - U)\phi' + V\phi = 0 \tag{4.15}$$

where

$$U = W - XZ^{-1}Y = \begin{bmatrix} -2 & 4 & 4 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 2 & 2 & 2 \\ 0 & 4 & 4 & -2 \end{bmatrix}$$

$$V = 1 + XZ^{-1}S = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & -1 \end{bmatrix}. \tag{4.16}$$

Equation (4.15) constitutes four independent equations for four unknowns. Since V is of rank 2, two first-order equations for ϕ_1, $\phi_3+\phi_4$ may be obtained, from which $\phi_3+\phi_4$ may be eliminated to give a second-order equation for $\phi_1 = g(z)$,

$$(z+3)(z+2)(z-6)g^{(2)}+(3z^2-2z-24)g^{(1)}+zg=0. \tag{4.17}$$

The finite singular points of the equation occur at the zeros of the coefficient of $g^{(2)}$, namely $z=-3, -2, 6$.

4.2. Simple cubic lattice (Joyce 1973)

For the simple cubic lattice with nearest-neighbour interactions we have $\eta = 1$ and

$$A=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix} \tag{4.18}$$

$$\begin{aligned} &D(\mathbf{0})=1 \qquad D(\boldsymbol{l})=0 \qquad \boldsymbol{l}\neq 0\\ &B(\boldsymbol{l})=1 \qquad \boldsymbol{l}=(\pm1,0,0),(0,\pm1,0),(0,0,\pm1)\\ &B(\boldsymbol{l})=0 \qquad \text{otherwise.}\end{aligned} \tag{4.19}$$

With $h_i = \theta_i$, $i=1, 2, 3$, we may write

$$g(z)=(2\pi)^{-3}\int_0^{2\pi}\mathrm{d}\theta_1\int_0^{2\pi}\mathrm{d}\theta_2\int_0^{2\pi}\mathrm{d}\theta_3\,(z-T(\boldsymbol{\theta}))^{-1} \tag{4.20}$$

where

$$T(\boldsymbol{\theta})=2(\cos\theta_1+\cos\theta_2+\cos\theta_3). \tag{4.21}$$

In this case we have (4.7) with

$$t(1,0,0)=t(0,1,0)=t(0,0,1)=2 \qquad \text{and} \qquad t(\boldsymbol{l})=0 \text{ otherwise.} \tag{4.22}$$

Relations (4.8) and (4.9) apply with this choice of $t(\boldsymbol{l})$. The symmetry of $T(\boldsymbol{\theta})$ leads to $I(l_1, l_2, l_3; z) = I(\sigma(l_1, l_2, l_3); z)$ for all permutations σ of l_1, l_2, l_3, etc, and we use this below.

We take (4.8) for $\boldsymbol{l}=(0,0,0)$, $(1,0,0)$, $(1,1,0)$, $(1,1,1)$ and (4.9) for $\boldsymbol{l}=(1,0,0)$, $(1,1,0)$, $(1,1,1)$. The result may be written

$$z\phi = W\phi + X\psi \tag{4.23}$$

$$Y\phi' + Z\psi' + S\phi' = 0 \tag{4.24}$$

where

$$\phi(z)=\begin{bmatrix}I(0,0,0;z)\\I(1,0,0;z)\\I(1,1,0;z)\\I(1,1,1;z)\end{bmatrix} \qquad \text{and} \qquad \psi(z)=\begin{bmatrix}I(2,0,0;z)\\I(2,1,0;z)\\I(2,1,1;z)\end{bmatrix} \tag{4.25}$$

with

$$W=\begin{bmatrix}0&6&0&0\\0&0&4&0\\0&0&0&2\\0&0&0&0\end{bmatrix}\qquad X=\begin{bmatrix}0&0&0\\2&0&0\\0&4&0\\0&0&6\end{bmatrix}$$
$$Y=\begin{bmatrix}2&0&0&0\\0&2&0&0\\0&0&2&0\end{bmatrix}\qquad Z=\begin{bmatrix}-2&0&0\\0&-2&0\\0&0&-2\end{bmatrix}\qquad S=\begin{bmatrix}0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix}. \tag{4.26}$$

Differentiating (4.23) and eliminating ψ leads to

$$(z-U)\phi'+V\phi=0 \tag{4.27}$$

with

$$U=\begin{bmatrix}0&6&0&0\\2&0&4&0\\0&4&0&2\\0&0&6&0\end{bmatrix}\qquad V=\begin{bmatrix}1&0&0&0\\0&0&0&0\\0&0&-1&0\\0&0&0&-2\end{bmatrix}. \tag{4.28}$$

Since V is of rank 3, three coupled equations may be derived from (4.27) and a single equation for $g(z)=$ constant $I(0,0,0;z)$ is obtained, namely

$$(z^4-40z^2+144)g^{(3)}+(6z^3-120z)g^{(2)}+(7z^2-48)g^{(1)}+zg=0. \tag{4.29}$$

4.3. Kagomé lattice

This lattice is based on a triangular lattice with three sites (nearest neighbours) per unit cell. Thus $\nu=2$, A is as in (4.1) but $\eta=3$. To describe nearest-neighbour interactions, we take

$$\begin{aligned}&D(\mathbf{0})_{ij}=\delta_{ij}\qquad D(\boldsymbol{l})_{ij}=0\qquad \boldsymbol{l}\neq\mathbf{0}\\&B(\mathbf{0})_{ij}=1\qquad i,j=1,2,3\\&B(1,1)_{12}=B(-1,-1)_{21}=B(0,1)_{13}=B(0,-1)_{31}\\&\qquad=B(-1,0)_{23}=B(1,0)_{32}=1\\&B(\boldsymbol{l})_{ij}=0\qquad\text{otherwise.}\end{aligned} \tag{4.30}$$

Using (2.3) with (4.5) and (4.30) we find that $g(z)$ may be written

$$g(z)=\int_0^{2\pi}\mathrm{d}\theta_1\int_0^{2\pi}\mathrm{d}\theta_2\,N(z,\boldsymbol{\theta})/P(z,\boldsymbol{\theta}) \tag{4.31}$$

where

$$P(z,\boldsymbol{\theta})=\sum_{\boldsymbol{l}}(\cos\boldsymbol{\theta})^{\boldsymbol{l}}q(\boldsymbol{l};z). \tag{4.32}$$

Here

$$\begin{aligned}&q(0,0;z)=z^3-4z=a\qquad\text{say}\\&q(2,0;z)=q(1,1;z)=-4z-8=b\qquad\text{say}\\&q(\boldsymbol{l};z)=0\qquad\text{otherwise}\end{aligned} \tag{4.33}$$

and

$$N(z, \boldsymbol{\theta}) = \frac{1}{12\pi^2} \frac{\partial P(z, \boldsymbol{\theta})}{\partial z}. \tag{4.34}$$

We construct equations coupling $I(\boldsymbol{l}; z)$, $J(\boldsymbol{l}; z)$, where

$$\begin{aligned} I(\boldsymbol{l}; z) &= I(\boldsymbol{l}, \mathbf{0}; z) = \int (\cos \boldsymbol{\theta})^{\boldsymbol{l}} P(z, \boldsymbol{\theta})^{-1} \\ J(\boldsymbol{l}; z) &= J(\boldsymbol{l}, \mathbf{0}; z) = \int (\cos \boldsymbol{\theta})^{\boldsymbol{l}} P(z, \boldsymbol{\theta})^{-2}. \end{aligned} \tag{4.35}$$

We take (3.6) and (3.7) for $\boldsymbol{l} = (0, 0)$, $(2, 0)$, $(1, 1)$, $(0, 2)$ and (3.8) for $\boldsymbol{l} = (2, 0)$, $(0, 2)$ and $(1, 1)$ with $i = 1, 2$. With

$$\begin{aligned} \phi(z) &= [I(0, 0; z), I(2, 0; z), I(1, 1; z), I(0, 2; z)]^{\mathrm{T}} \\ \psi(z) &= [J(0, 0; z), J(2, 0; z), J(1, 1; z), J(0, 2; z), J(4, 0; z), \\ &\qquad J(3, 1; z), J(2, 2; z), J(1, 3; z)]^{\mathrm{T}} \end{aligned} \tag{4.36}$$

these equations may be written as

$$W\phi + X\psi = 0 \tag{4.37}$$

$$\phi' + Z\psi = 0 \tag{4.38}$$

where

$$W = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 2 \end{bmatrix} \quad X = \begin{bmatrix} a & b & b & 0 & 0 & 0 & 0 & 0 \\ 0 & a & 0 & 0 & b & b & 0 & 0 \\ 0 & 0 & a & 0 & 0 & b & b & 0 \\ 0 & 0 & 0 & a & 0 & 0 & b & b \\ 0 & 2b & b & 0 & -2b & -b & 0 & 0 \\ 0 & 0 & 2b & b & 0 & -2b & -b & 0 \\ 0 & b & 0 & 0 & 0 & 0 & -b & 0 \\ 0 & 0 & b & 0 & 0 & 0 & 0 & -b \end{bmatrix} \tag{4.39}$$

$$Z = \begin{bmatrix} a' & b' & b' & 0 & 0 & 0 & 0 & 0 \\ 0 & a' & 0 & 0 & b' & b' & 0 & 0 \\ 0 & 0 & a' & 0 & 0 & b' & b' & 0 \\ 0 & 0 & 0 & a' & 0 & 0 & b' & b' \end{bmatrix}.$$

It may be checked that $\det X$ is not identically zero, so that (4.37) may be solved to give

$$\psi = -X^{-1} W\phi. \tag{4.40}$$

Substitution in (4.38) leads to

$$\phi' - ZX^{-1} W\phi = 0 \tag{4.41}$$

four coupled equations for the four quantities making up ϕ. It is found that

$$\det X = 1024 z^2 (z+2)^9 (z-1)^2 (z-2)^2 (z-4) \tag{4.42}$$

the zeros of $\det X$ being singular points of (4.41).

Since $g(z)$ is a linear combination of the components of ϕ, a single fourth-order equation for $g(z)$ could be obtained.

We now summarise the results, obtained in the same way, for several other lattices. In each case $D(\mathbf{0}) = 1$, $D(\boldsymbol{l}) = 0$, $\boldsymbol{l} \neq \mathbf{0}$ and we assume only nearest-neighbour interactions. Unless noted $\eta = 1$.

4.4. Square lattice (Katsura and Inawashiro 1971)

$$A = \begin{bmatrix} 1, & 0 \\ 0, & 1 \end{bmatrix}$$

$B(\boldsymbol{l}) = 1 \qquad \boldsymbol{l} = (\pm 1, 0), (0, \pm 1)$

$B(\boldsymbol{l}) = 0 \qquad$ otherwise

$$(z^3 - 16z)g^{(2)} + (3z^2 - 16)g^{(1)} + zg = 0.$$

4.5. Honeycomb lattice

$$A = \begin{bmatrix} 1, & -1/2 \\ 0, & \sqrt{3}/2 \end{bmatrix}$$

$\eta = 2$

$B(\boldsymbol{l})_{12} = 1 \qquad \boldsymbol{l} = (1, 1), (-1, 0), (0, -1)$

$B(\boldsymbol{l})_{21} = 1 \qquad \boldsymbol{l} = (-1, -1), (1, 0), (0, 1)$

$B(\boldsymbol{l})_{ij} = 0 \qquad$ otherwise

$$(z^6 - 10z^4 + 9z^2)g^{(2)} + (3z^5 - 10z^3 - 9z)g^{(1)} + (z^4 - 2z^2 + 9)g = 0.$$

4.6. Body-centred cubic lattice (Joyce 1971)

$$A = \begin{bmatrix} t, & -t, & t \\ t, & t, & -t \\ -t, & t, & t \end{bmatrix} \qquad t = 1/\sqrt{3}$$

$B(\boldsymbol{l}) = 1 \qquad \boldsymbol{l} = (\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1), (1, 1, 1), (-1, -1, -1)$

$B(\boldsymbol{l}) = 0 \qquad$ otherwise

$$(z^4 - 64z^2)g^{(3)} + (6z^3 - 192z)g^{(2)} + (7z^2 - 64)g^{(1)} + zg = 0.$$

4.7. Face-centred cubic lattice

$$A = \begin{bmatrix} s, & 0, & s \\ s, & s, & 0 \\ 0, & s, & s \end{bmatrix} \qquad s = 1/\sqrt{2}$$

$B(\boldsymbol{l}) = 1 \qquad \boldsymbol{l} = (\pm 1, 0, 0), (0, \pm 1, 0), \quad (0, 0, \pm 1), (1, -1, 0), \quad (-1, 1, 0),$
$(1, 0, -1), (-1, 0, 1), (0, 1, -1), (0, -1, 1)$

$B(\boldsymbol{l}) = 0 \qquad$ otherwise

$$(z^4 - 4z^3 - 80z^2 - 192z)g^{(3)} + (6z^3 - 18z^2 - 240z - 288)g^{(2)} + (7z^2 - 12z - 96)g^{(1)} + zg = 0.$$

4.8. Diamond lattice

$$A=\begin{bmatrix} t & -t & t \\ t & t & -t \\ -t, & t, & t \end{bmatrix} \qquad t=1/\sqrt{3}$$

$$\eta=2$$

$$B(\boldsymbol{l})_{12}=1 \qquad \boldsymbol{l}=(1,0,0),(0,1,0),(0,0,1),(-1,-1,-1)$$

$$B(\boldsymbol{l})_{21}=1 \qquad \boldsymbol{l}=(-1,0,0),(0,-1,0),(0,0,-1),(1,1,1)$$

$$B(\boldsymbol{l})_{ij}=0 \qquad \text{otherwise}$$

$$(z^7-20z^5+64z^3)g^{(3)}+(6z^6-60z^4)g^{(2)}+(7z^5-32z^3+64z)g^{(1)}+(z^4-64)g=0.$$

4.9. Hypercubic lattice

$$A=\begin{bmatrix} 1, & 0, & 0, & 0 \\ 0, & 1, & 0, & 0 \\ 0, & 0, & 1, & 0 \\ 0, & 0, & 0, & 1 \end{bmatrix}$$

$$B(\boldsymbol{l})=1 \qquad \boldsymbol{l}=(\pm1,0,0,0),(0,\pm1,0,0),(0,0,\pm1,0),(0,0,0,\pm1)$$

$$B(\boldsymbol{l})=0 \qquad \text{otherwise}$$

$$(z^5-80z^3+1024z)g^{(4)}+(10z^4-480z^2+2048)g^{(3)}+(25z^3-608z)g^{(2)}$$
$$+(15z^2-128)g^{(1)}+zg=0.$$

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