

Spectrum of an N -state tight-binding Hamiltonian in a Bethe lattice

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By means of a canonical transformation the problem of the electronic structure in a Bethe lattice with N states per site, which normally requires a complicated numerical solution of a quadratic transfer-matrix equation, is reduced to the solution of an $(N \times N)$ eigenvalue-eigenfunction equation. The simplification achieved is considerable and great insight is obtained on the nature of the electronic spectrum by analytical means. The case $N=2$ is solved in its general form and the nature of the spectrum, mainly the existence of a gap and the number and location of the singularities in the density of states, is studied analytically.

I. INTRODUCTION

Bethe lattices, also known as Cayley trees, are useful mathematical devices which find ready applications in condensed-matter physics.¹ They are defined as an infinite set of points, each connected to z neighbors, such that no closed loops exist, and such that any two points in the lattice are joined by one and only one connectivity path. The $z=2$ lattice is a simple one-dimensional string; $z \geq 3$ corresponds to systems not susceptible to real three-dimensional realization, and which share some features of one-dimensional structures (single connectivity) and some features of infinite-dimensional bodies (the number of lattice points within a distance of R steps from the origin is $(z-2)^{-1}[z(z-1)^R - 2]$, of which $z(z-1)^{R-1}$ are at the "surface" of that hypersphere).

Bethe lattices have been successfully used in the study of ordered and disordered systems: semiconductors,² alloys,³ and dilute magnets⁴ in particular. They are instrumental in the study of many properties: electronic,^{2,3} vibrational,⁵ magnetic,^{4,6} surface-related,⁶ localization,⁷ etc. A Bethe lattice makes a simple "effective" medium of infinite extent, one which reproduces throughout the immediate local arrangement of an atom—the coordination number—and which is susceptible to exact and fairly simple mathematical treatment.

In this contribution we find some exact results which apply to the study of systems with N electronic states per atom in a Bethe lattice. We find a transformation which allows us to convert an N -band problem into a single-band Hamiltonian, thus simplifying all calculations by a great amount. The formulation of the problem and the main result are included in Sec. II. The particular case of $N=2$ and its exhaustive analysis are the subject of Sec. III.

II. THE CANONICAL TRANSFORMATION

If we define a creation-operator row N vector by

$$\underline{\psi}_i^\dagger = (C_{1i}^\dagger, C_{2i}^\dagger, \dots, C_{Ni}^\dagger), \quad (2.1)$$

where C_{Ji}^\dagger creates a Wannier state $|J, i\rangle$, the J th electron-

ic state ($J=1, 2, \dots, N$) at the site i in the Bethe lattice, and a corresponding column N vector for the destruction operator ψ_i , then the Hamiltonian under consideration can be written

$$H = \sum_i \psi_i^\dagger \underline{E} \psi_i + \sum_{\langle ij \rangle} \psi_i^\dagger \underline{V} \psi_j. \quad (2.2)$$

In (2.2) both \underline{E} and \underline{V} are $(N \times N)$ matrices and the summation $\langle ij \rangle$ is over nearest-neighbor pairs. The matrix \underline{E} gives the energy values and the intra-atomic overlapping energies of the N states. We choose the zero of the energy scale such that \underline{E} is traceless, $\text{Tr } \underline{E} = 0$. The $(N \times N)$ matrix \underline{V} gives the nearest-neighbor interatomic overlapping energies,⁸ and allows any of the N Wannier states in a site to overlap with any of the corresponding states in the neighboring sites. Without loss of generality we assume that \underline{V} is nonsingular, $\det \underline{V} \neq 0$ (all nonoverlapping states can be removed from the problem at the onset), and we choose our energy units such that $\text{Tr } \underline{V} = 1$.

The Green's-function matrix of the system $\underline{G}_{ij}(\omega)$ is defined by Dyson's equation

$$\sum_k (\omega \underline{I} \delta_{ik} - \underline{H}_{ik}) \underline{G}_{kj}(\omega) = \underline{I} \delta_{ij}, \quad (2.3)$$

where \underline{I} is the $(N \times N)$ unit matrix. The density of electronic states $\rho(\omega)$ can be obtained from the usual equation

$$\rho(\omega) = -\pi^{-1} \text{Im Tr } \underline{G}_{ij}(\omega). \quad (2.4)$$

Our main result can be stated as follows: The Green's-function matrix can be written as

$$\underline{G}_{ij}(\omega) = \underline{V}^{-1} \underline{D}(\omega) \underline{\Gamma}_{ij}(\omega) \underline{D}^{-1}(\omega), \quad (2.5)$$

where each $\underline{\Gamma}_{ij}(\omega)$ is a *diagonal* $(N \times N)$ matrix whose elements are the simple Green's function $g_{ij}(\Omega)$ of the one-state Hamiltonian

$$h = \sum_{\langle ij \rangle} |i\rangle \langle j|, \quad (2.6)$$

given by

$$\sum_k (\Omega \delta_{ik} - h_{ik}) g_{kj}(\Omega) = \delta_{ij}, \quad (2.7)$$

evaluated at the values $\Omega = \lambda_K(\omega)$, $K = 1, 2, \dots, N$, which are the roots of the characteristic equation

$$\det(\underline{E} + \lambda \underline{V} - \omega \underline{I}) = 0. \quad (2.8)$$

In other words, the (J, K) matrix element of $\underline{\Gamma}_{ij}(\omega)$ is given by

$$[\underline{\Gamma}_{ij}(\omega)]_{JK} = \delta_{JK} g_{ij}(\lambda_K(\omega)). \quad (2.9)$$

The matrix $\underline{D}(\omega)$, of the same $(N \times N)$ dimension, diagonalizes the matrix

$$\underline{L}(\omega) \equiv (\omega \underline{I} - \underline{E}) \underline{V}^{-1} \quad (2.10)$$

to the eigenvalue form given by λ_K . Once $\underline{D}(\omega)$ and the set $\{\lambda_K\}$ are found, application of (2.5) and (2.4) solves the problem. Proof of these results are given in the Appendix.

Several points should be remarked about the method.

(a) The problem of an N -state Bethe-lattice Hamiltonian is separated into a canonical one-state Bethe lattice problem

$$g_{ii}(\Omega) = \frac{2(z-1)}{(z-2)\Omega + [\Omega^2 - 4(z-1)]^{1/2}}, \quad (2.11)$$

and the solution of an $N \times N$ diagonalization problem as a function of the energy ω , i.e., the eigenvectors and eigenvalues of $\underline{L}(\omega)$.

(b) Since in general \underline{D} and \underline{V}^{-1} do not commute, the product

$$\underline{D}^{-1}(\omega) \underline{V}^{-1} \underline{D}(\omega)$$

is a function of ω . Because this product appears in the trace, (2.4) and (2.5), the density of states, $\rho(\omega)$, is not a linear combination of the one-state densities of states of the simple Hamiltonian (2.6).

(c) The variable λ is the energy of the one-state problem; ω is the energy variable of the N -state problem.

Equation (2.8) gives the relationship between them. As seen in (2.11), there are allowed one-state energy levels for $|\lambda| < \mu$, where $\mu = 2(z-1)^{1/2}$.

Equation (2.8) is a polynomial of order N in ω so, for each real value of λ , there are N real solutions for ω . In other words, if (2.8) is interpreted as an implicit equation for $\omega(\lambda)$, that function has N real branches in the region of interest, and therefore N allowed energy bands for the Hamiltonian (2.2). As an example, for $z=5$, $N=3$ with

$$\underline{E} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \quad \underline{V} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

the Hamiltonian (2.6) has a spectrum bound by

$$-4 \leq \lambda \leq 4,$$

the solution of (2.8) yields three branches

$$\begin{aligned} \omega_1 &= 2 + \lambda, \\ \omega_{2,3} &= -1 \pm (1 + \lambda^2)^{1/2}, \end{aligned}$$

which yields for the spectrum of (2.2) three bands:

$$\begin{aligned} -2 &\leq \omega_1 \leq 6, \\ 0 &\leq \omega_2 \leq 3.123, \\ -5.123 &\leq \omega_3 \leq -2. \end{aligned}$$

By replacing

$$\begin{aligned} \Omega_1 &= \omega - 2, \\ \Omega_2 &= +(\omega^2 + 2\omega)^{1/2}, \\ \Omega_3 &= -(\omega^2 + 2\omega)^{1/2} \end{aligned}$$

into (2.11) and using the fact that

$$\underline{D}^{-1}(\omega) \underline{L}(\omega) \underline{D}(\omega) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & (\omega+1)(\omega^2+2\omega)^{-1/2} & -(\omega^2+2\omega)^{-1/2} \\ 0 & (\omega^2+2\omega)^{-1/2} & -(\omega+1)(\omega^2+2\omega)^{-1/2} \end{pmatrix},$$

analytic expressions for the three branches of the density of states (2.4) can be obtained.

(d) The problem has been considerably simplified with respect to the standard procedure. In particular, there is no need to calculate the complicated $(N \times N)$ transfer matrix T (see the Appendix). Also, there are no complications in the choice of phases and roots; once the proper behavior is established for $g_{ii}(\lambda)$, Eq. (2.11), the phases and properties of $\underline{G}_{jj}(\omega)$ are also fixed.

(e) Our canonical transformation resembles somewhat that found by Thorpe and Weaire⁹ for¹⁰ the specific four-state Hamiltonian of the tetrahedrally bonded semiconductors. But, while their $\omega(\lambda)$ quadratic function only applies to the s - p hybridized states in the diamond struc-

ture, our transformation is general, applies to any number N of states, but can only be applied to Bethe lattices where the lack of closed rings allows the introduction of a transfer matrix for the Green's function.

(f) The spectral limits can be very easily determined by finding the values of ω , called ω_l , that satisfy either the equation

$$\det(\underline{E} \pm \mu \underline{V} - \omega_l \underline{I}) = 0, \quad (2.12)$$

or the equation

$$\frac{d\omega}{d\lambda} = 0, \quad |\lambda_l| \leq \mu. \quad (2.13)$$

III. ANALYSIS OF THE TWO-BAND CASE

For $N=2$ the matrices \underline{E} and \underline{T} of (2.2) take the general form

$$\underline{E} = \begin{pmatrix} \epsilon & V_1 \\ V_1 & -\epsilon \end{pmatrix}, \quad (3.1)$$

$$\underline{V} = \begin{pmatrix} \frac{1}{2}(1+t) & V_2 \\ V_2 & \frac{1}{2}(1-t) \end{pmatrix}. \quad (3.2)$$

It is more convenient to use, instead of the four parameters ϵ , t , V_1 , and V_2 , the following three invariants:

$$d_V \equiv \det \underline{V} = \frac{1}{4}(1-t^2) - V_2^2, \quad (3.3)$$

$$d_E \equiv -\det \underline{E} = \epsilon^2 + V_1^2, \quad (3.4)$$

$$r \equiv \text{Tr}(\underline{E}\underline{V}) = 2V_1V_2 + \epsilon t, \quad (3.5)$$

and the combinations

$$\delta \equiv d_E \mu^{-2} \geq 0, \quad \phi \equiv -d_V + \frac{1}{4} \geq 0, \quad \rho \equiv r \mu^{-1}. \quad (3.6)$$

The equation for $\omega(\lambda)$ given by (2.8) yields

$$\left(\frac{1}{2}\lambda - \omega\right)^2 = \left(\epsilon + \frac{1}{2}\lambda t\right)^2 + (V_1 + \lambda V_2)^2, \quad (3.7)$$

which in terms of

$$x \equiv \lambda \mu^{-1}, \quad y \equiv \omega \mu^{-1}, \quad (3.8)$$

and the definitions (3.3)–(3.6) above reduces to

$$\left(\frac{1}{2}x - y\right)^2 = \delta + \rho x + \phi x^2. \quad (3.9)$$

Equation (3.9) is that of an hyperbola. The positive-definite character of the right-hand side of (3.7) guarantees positive definiteness of the right-hand side of (3.9)—a positive-definite quadratic form—and therefore

$$\rho^2 \leq 4\phi\delta. \quad (3.10)$$

The asymptotes of the hyperbola (3.9) are

$$y_{as} = \left(\frac{1}{2} \pm \phi^{1/2}\right)x \pm \frac{1}{2}\rho\phi^{-1/2}, \quad (3.11)$$

which guarantee (a) two monotonically increasing branches of $y(x)$ for $\phi \leq \frac{1}{4}$, and (b) a gap in the y spectrum centered about $y_G = -\rho/4\phi$ for values of $\phi > \frac{1}{4}$.

It should be noted that in the region of physical interest $|x| < 1$, there may be (and generally is) a gap in the y spectrum for values of $\phi < \frac{1}{4}$, but there is never a single-domain spectrum for $\phi \geq \frac{1}{4}$.

The properties of the hyperbola can now be used to study the ω spectrum. For $\phi < \frac{1}{4}$ the monotonically increasing properties of both branches yield the following results. The lower branch has the spectral limits $y_L(\pm 1)$,

$$\begin{aligned} y_{L-} &= -\frac{1}{2} - (\delta + \phi - \rho)^{1/2}, \\ y_{L+} &= \frac{1}{2} - (\delta + \phi + \rho)^{1/2}. \end{aligned} \quad (3.12)$$

Similarly the upper branch limits $y_U(\pm 1)$ are

$$\begin{aligned} y_{U-} &= -\frac{1}{2} + (\delta + \phi - \rho)^{1/2}, \\ y_{U+} &= \frac{1}{2} + (\delta + \phi + \rho)^{1/2}. \end{aligned} \quad (3.13)$$

The two branches overlap if

$$y_{L+} > y_{U-},$$

which reduces to

$$1 > (\delta + \phi + \rho)^{1/2} + (\delta + \phi - \rho)^{1/2}. \quad (3.14)$$

The exact solution of (3.14) gives (i) a single-domain spectrum for all allowed values (3.10) of ρ if $(\delta + \phi) \leq \frac{1}{4}$; (ii) a single-domain spectrum for $\frac{1}{4} < (\delta + \phi) < \frac{1}{2}$ and $(\phi + \delta - \frac{1}{4}) \leq \rho^2 \leq 4\phi\delta$; (iii) a two-domain spectrum with a gap for $\frac{1}{4} < (\delta + \phi) < \frac{1}{2}$ and $\rho^2 < (\phi + \delta - \frac{1}{4})$; (iv) a two-domain spectrum with a gap for any ρ and for $(\delta + \phi) > \frac{1}{2}$.

Finally the singularities in the density of states are, except for accidental degeneracies, at a minimum of four energies and a maximum of six. The four frequencies $\omega(\pm\mu)$, i.e., $y(\pm 1)$, given by (3.12) and (3.13), are always singular points in the density of states. In addition, one or two extra singularities appear between y_{L+} and y_{U-} whenever

$$(4\phi - 1)(\phi \pm \rho) + \rho^2 - \delta > 0, \quad \phi > \frac{1}{4}. \quad (3.15)$$

These spectral singularities are caused by the extrema in the $\omega(\lambda)$ curves which fall in the interval $|\lambda| < \mu$.

In summary, the complicated problem of a two-band Hamiltonian in a Bethe lattice, including the classical problem of two bands in a linear chain, can be solved in a completely analytic and simple fashion. Extensions to larger N would involve more parameters, more invariants, and the solution of an eigenvalue-eigenfunction equation of higher degree. But, as can be clearly seen in the $N=2$ case discussed in this section, the simplification achieved from the standard techniques is considerable, and the insight gained into the problem is a clear advantage.

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APPENDIX: PROOF OF RESULTS OF SEC. II

If we define

$$\tilde{\underline{G}}_{ij} \equiv \underline{V}\underline{G}_{ij}, \quad (A1)$$

replace this definition in Dyson's Eq. (2.3) for the Hamiltonian (2.2), and make use¹¹ of (2.10), we obtain

$$\underline{L}(\omega)\tilde{\underline{G}}_{ij} - \sum_k \Delta_{ik}\tilde{\underline{G}}_{kj} = \underline{I}\delta_{ij}, \quad (A2)$$

where

$$\Delta_{ik} = \begin{cases} 1 & \text{if } \langle ik \rangle \text{ are nearest neighbors} \\ 0, & \text{otherwise.} \end{cases} \quad (\text{A3})$$

The introduction of an $N \times N$ transfer matrix \underline{T} , defined by¹²

$$\begin{aligned} \sum_k \Delta_{ik} \tilde{\underline{G}}_{kj} &= z \underline{T} \tilde{\underline{G}}_{ij} \quad \text{for } i=j \\ &= [(z-1)\underline{T} + \underline{T}^{-1}] \tilde{\underline{G}}_{ij} \quad \text{for } i \neq j, \end{aligned} \quad (\text{A4})$$

yields

$$[\underline{L}(\omega) - z \underline{T}] \tilde{\underline{G}}_{ii} = \underline{I}, \quad (\text{A5})$$

$$[\underline{L}(\omega) - (z-1)\underline{T} - \underline{T}^{-1}] \tilde{\underline{G}}_{ij} = 0, \quad i \neq j. \quad (\text{A6})$$

Since (A6) is valid for any $i \neq j$, it follows that

$$\underline{L}(\omega) = (z-1)\underline{T} + \underline{T}^{-1}, \quad (\text{A7})$$

i.e., \underline{L} is a simple function of \underline{T} and therefore \underline{L} and \underline{T}

commute. Similarly (A5) establishes that

$$\tilde{\underline{G}}_{ii} = [\underline{L}(\omega) - z \underline{T}]^{-1}, \quad (\text{A8})$$

that is, $\tilde{\underline{G}}_{ii}$ is also a simple function of \underline{T} and therefore $\tilde{\underline{G}}_{ii}$ commutes with both \underline{L} and \underline{T} . It then follows that $\underline{L}(\omega)$, $\underline{T}(\omega)$, and $\tilde{\underline{G}}_{ij}(\omega)$ can all be diagonalized simultaneously. Let $\underline{D}(\omega)$ be the matrix that diagonalizes all three and let $\underline{\lambda}(\omega)$ be the diagonal form of $\underline{L}(\omega)$:

$$\underline{\lambda}(\omega) = \underline{D}^{-1}(\omega) \underline{L}(\omega) \underline{D}(\omega), \quad (\text{A9})$$

$$\underline{g}_{ij} = \underline{D}^{-1}(\omega) \tilde{\underline{G}}_{ij}(\omega) \underline{D}(\omega). \quad (\text{A10})$$

If Eq. (A2) is now multiplied by \underline{D}^{-1} on the left and by \underline{D} on the right, one obtains

$$\underline{\lambda}(\omega) \underline{g}_{ij} - \sum_k \Delta_{ik} \underline{g}_{kj} = \underline{I} \delta_{ij}, \quad (\text{A11})$$

which corresponds to N -decoupled equations, each one identical to the one-state Green's-function equation (2.7) for $\Omega = \lambda_K(\omega)$. This proves the required result.

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¹An informative review of Bethe lattices—their history and development—can be found in the article by M. F. Thorpe, in *Excitations in Disordered Systems*, edited by M. F. Thorpe (Plenum, New York, 1982), pp. 85–107. See also C. Domb, *Adv. Phys.* **9**, 145 (1960).

²See, for instance, J. Oliva and L. M. Falicov, *Phys. Rev. B* **28**, 7366 (1983), and references therein. For a comprehensive review see J. D. Joannopoulos and M. L. Cohen, in *Solid State Physics: Advances in Research and Applications*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1976), Vol. 31, p. 71.

³See, for instance, M. O. Robbins and L. M. Falicov, *Phys. Rev. B* **25**, 2343 (1982); **29**, 1333 (1984), and references therein.

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⁸To avoid a cumbersome notation we have taken the elements of \underline{E} and \underline{V} to be real. Generalization to complex matrix elements, as long as Hermiticity is maintained, presents no difficulties.

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¹¹It should be remembered that, although \underline{V} and \underline{G}_{ij} are $N \times N$ matrices, \underline{V} is that part of the Hamiltonian which connects nearest neighbors and is independent of the particular site i . Formula (A1) defines $\tilde{\underline{G}}_{ij}$, regardless of the relative position of i and j , as the matrix product of the (i, j) -independent \underline{V} and the Green's-function matrix \underline{G}_{ij} .

¹²A transfer matrix, in the sense used here, “transfers” information (the amplitude and phase of the Green's function) between neighboring sites and in a single sense. It can be defined only for systems in which any two sites can be connected by *only one path*, i.e., a Bethe lattice. For an arbitrarily chosen origin in the lattice each site can be labelled by the number of steps necessary to reach it from the origin, and the transfer matrix \underline{T} is then defined by $\underline{G}_{(\alpha+1)\beta} = \underline{T} \underline{G}_{\alpha\beta}$. This standard definition is identical to our definition (A4), where $i = j$ is the origin.