Chaotic renormalization approach to electronic systems

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We have proved the equivalence between the density of electronic states of a linear tight-binding chain and the density of chaotic visits along the energy axis for the map $\omega_n = \omega_{n-1}^2 - 2$, using a renormalization-group approach. Our results are generalized for other systems and for higher dimensions, providing a new, simple method for computing the density of states of *any* translationally invariant system with a known dispersion relation.

The local density of states for a linear chain of one-orbital identical atoms can be obtained[1,2] for a tight-binding first-neighbor hopping Hamiltonian by a real-space renormalization of the diagonal term of the Green's function and the hopping integral value. The method used in Refs. 1 and 2 consists in solving exactly the set of Eqs. (1),

$$(E-\epsilon)G_{i0} = \delta_{i0} + VG_{i+1,0} + VG_{i-1,0} \ , \tag{1}$$

where ϵ is the one-orbital energy (hereafter considered zero); V is the hopping integral, and G_{i0} is the Green's function between sites 0 and i of the numbered chain. The quantity E is defined in the usual way as $E = \omega - i\eta$, where ω is the frequency and η is a positive infinitesimal quantity included in order to guarantee the analytical properties of the retarded Green's functions. The diagonal Green's function related to the density of states can be obtained in an iterative process by eliminating the odd-numbered (odd i_s) equations from the system (1). After each complete elimination, the new system has the same form as the old one, with renormalized values for g and x defined by

$$g \equiv \frac{1}{E} \ , \tag{2}$$

$$x \equiv gV \ . \tag{3}$$

The renormalization equations are

$$x_n = \frac{x_{n-1}^2}{1-2x_{n-1}^2} \ , \tag{4}$$

$$g_n = \frac{1}{1-2x_{n-1}^2} g_{n-1} \ , \tag{5}$$

where n indicates the number of successive renormalizations. For each fixed value of the energy E which defines g_0 through Eq. (2), subsequent iterations of Eqs. (4) and (5) define two sequences that converge rapidly to the fixed point $x^* = 0$ and $g^* = r(\omega) + i\pi\rho(\omega)$, where $\rho(\omega)$ is the *exact* local density of states.

Let us now consider the chaotic behavior[3] of the renormalization process. Instead of renormalizing the hopping V (through x), Eq. (4) can be interpreted as an *energy* renormalization. Fixing $V = 1$ and defining

$$E_n = \frac{1}{x_n} \ , \tag{6}$$

Eqs. (4) and (5) can be rewritten as

$$E_n = E_{n-1}^2 - 2 \ , \tag{7}$$

$$g_n = \frac{E_{n-1}^2}{E_n} g_{n-1} \ . \tag{8}$$

While the energy E is renormalized through Eq. (7), g is a *captive variable* renormalized through a cascade of multiplicative factors depending only on E. Equation (7) has two fixed points $E^* = \omega^* = 2$ and $W^* = -1$. We will pay attention to the former. It divides the *real* axis into two distinct regions: $|\omega| < 2$, the *chaotic band,* and $|\omega| > 2$, the *non-chaotic* region. In this last case, renormalization (7) becomes monotonic and the whole region is attracted by $\omega = \infty$. These two regions are completely independent in the sense that Eq. (7) does not transform points from one region into the other. If we explicitly consider that E_0 has an infinitesimal imaginary part (it is a *quasi real* quantity), the iterative process produces a renormalization of the real and the imaginary parts of E such that

$$E_n = \omega_n - i\eta_n \ . \tag{9}$$

Let us start with an energy ω_0 ($0 < |\omega_0| < 2$) and follow the sequence E_0, E_1, E_2, etc. Equations (7) and (9) imply that E_n *is still quasi real up to iteration* $n = N$ *for which* $|\omega_N| < |\eta_N| \to 0$. In other words, the *phase* of the complex number E_n is near to 0 or π up to $n = N$, when there is a nonvanishing phase, $\alpha(\omega_0, \eta_0)$. Figure 1 shows the sequence $E_N \cong 0$, $E_{N+1} \cong -2$, $E_{N+2} \cong \omega^* = 2$, $E_{N+3} \cong \omega^* = 2$ in a schematic view. In this sequence, E_N is *arbitrarily* close to 0, E_{N+1} to -2, E_{N+2} and E_{N+3} to $\omega^* = 2$. The Jacobian

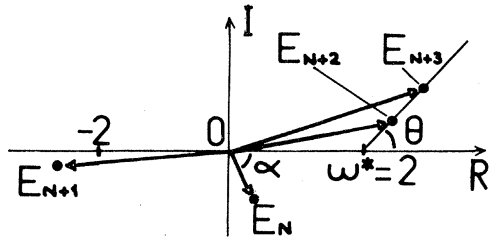

FIG. 1. Schematic view of the renormalized complex values $E_N, E_{N+1}, E_{N+2}, E_{N+3}$ under Eq. (7), after $E_N = \omega_N - i\eta_N$, where $|\omega_N| < |\eta_N| \to 0$.

matrix of (7) in the complex plane, calculated at $\omega^*=2$,

$$\begin{pmatrix} \frac{\delta\omega_n}{\delta\omega_{n-1}} & \frac{\delta\omega_n}{\delta\eta_{n-1}} \\ \frac{\delta\eta_n}{\delta\omega_{n-1}} & \frac{\delta\eta_n}{\delta\eta_{n-1}} \end{pmatrix} = \begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix} , \tag{10}$$

is degenerate (proportional to the unity matrix). This implies that all directions θ (see Fig. 1) are equivalent in the neighborhood of $\omega^*=2$. This is the central fact of our following argument. The value of θ is obviously related to α through the relation $\theta=2\alpha-\pi$. It is clear then that θ can take values arbitrarily close to zero, simply by taking α arbitrarily close to $-\pi/2$ choosing convenient values for N and η_0. It is possible to obtain the electronic density of states by relating it to the Green's function defined previously:

$$\rho(\omega_0)=\frac{1}{\pi}\,\mathrm{Im}g^*(\omega_0) \ . \tag{11}$$

The value $\theta=0$ is obtained starting from zero energy ($\omega_0=0$). As E_n and g_n acquire nonvanishing imaginary parts *only* for $n\geq N$ for which $|\omega_N|<|\eta_N|$, a simple iteration of Eq. (8) repeated $N-1$ times allows establishment of a relation between $\rho(\omega_0)$ and $\rho(0)$ given by

$$\rho(\omega_0)=\rho(0)\prod_{n=0}^{N-1}\omega_n \ . \tag{12}$$

The factorial-like Eq. (12) represents a new method for calculating $\rho(\omega_0)$. Using (7) *without imaginary part,* one generates the chaotic sequence $\omega_0, \omega_1, \omega_2$, etc. up to a certain ω_N close to zero within a predetermined tolerance. Equation (12) then determines $\rho(\omega_0)$. The value $\rho(0)$ can be calculated *a posteriori* by imposing the normalization condition $\int d\omega\,\rho(\omega)=1$.

Furthermore, if we restrict Eq. (12) to just one iteration,

$$\rho(\omega_{n-1})=\omega_{n-1}\rho(\omega_n) \ , \tag{13}$$

and take $\omega_{n-1}=2-\delta$ close to $\omega^*=2$, the linearization (10) shows that $\omega_n=2-4\delta$. Equation (13) becomes

$$\rho(2-\delta)\cong 2\rho(2-4\delta) \ . \tag{14}$$

Equation (14) implies that $\rho(\omega)$ diverges as $(2-\omega)^{-1/2}$ at $\omega=\omega^*=2$, where $\frac{1}{2}$ is a critical exponent. Using the fact that $\rho(\omega)$ is an even function, and so there is another divergence at $\omega=-2$, we obtain $\rho(\omega)\propto(4-\omega^2)^{-1/2}$ near the band edges which in this case turns out to be the exact analytical form for the density of states in the whole band.

The new method to obtain $\rho(\omega)$ introduced by the factorial-like Eq. (12) is computationally simpler than the previous one[1,2] because it requires only real numbers, but it does not introduce new qualitative features to the problem. We will now give a proof of a result[4] which allows a new interpretation for the density of states. We define the *density of visits* $\nu(\omega)$ through $N\nu(\omega)d\omega$, the number of visits to the interval $(\omega,\omega+d\omega)$ after $N\to\infty$ iterations of Eq. (7). The starting point ω_0 is a random real value ($|\omega_0|<2$).[5] Figure 2 shows a small interval δ_n around ω_n and two small intervals δ_{n-1} around ω_{n-1} and $-\omega_{n-1}$. By construction, the number of visits to δ_n is the same as the number of visits to both δ_{n-1}, because every visit to δ_{n-1} corresponds

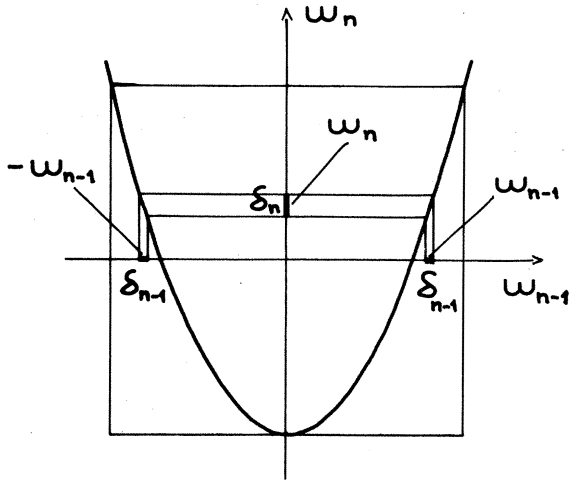

FIG. 2. Plot of Eq. (7) for relating $\nu(\omega_n)$ and $\nu(\omega_{n-1})$.

to a subsequent visit to δ_n,

$$\nu(\omega_n)\delta_n=\nu(\omega_{n-1})\delta_{n-1}+\nu(-\omega_{n-1})\delta_{n-1} \ . \tag{15}$$

Assuming that $\nu(\omega)$ is an even function,[6] we obtain

$$\nu(\omega_n)\delta_n=2\nu(\omega_{n-1})\delta_{n-1} \ . \tag{16}$$

Returning to Fig. 2, we can relate δ_n and δ_{n-1} through the derivative of (7), at ω_{n-1}, and rewrite (16) as

$$\nu(\omega_{n-1})=\omega_{n-1}\nu(\omega_n) \ . \tag{17}$$

Comparing (13) and (17) we obtain

$$\nu(\omega)=\rho(\omega) \ . \tag{18}$$

Equation (18) first presented by José[4] is now proved for the map (7). The same proof can be made, for instance, using the map $\omega_n=\omega_{n-1}^3-3\omega_{n-1}$ obtained by using length scale 3 (instead of 2 as used before) in solving the system (1). Actually, Eq. (18) is valid for other maps obtained by using different length scales.

We will now show how to obtain the density of states through the density of chaotic visits for other systems and for higher dimensions. The dispersion relation for the linear chain

$$\omega=2\cos(2\pi k) \tag{19}$$

together with the transformation $k_n=2k_{n-1}$ in the reciprocal space (corresponding to length scale 2) yields directly Eq. (7). Since the value of k can be restricted to the interval [0,1), we obtain

$$k_n=\mathrm{frac}(2k_{n-1}) \ , \tag{20}$$

where $\mathrm{frac}(x)$ is the fractionary part of x. This map together with the dispersion relation Eq. (19) generates a chaotic sequence for the energy which can also be obtained directly from the map (7). This allows us to conclude the following:

(i) Transformation (20) is mixing and ergodic (for aperiodic orbits).

(ii) The density of visits for the map (20) is uniform along the interval [0,1), i.e., every finite interval in this range is visited with the same frequency in an infinite

number of iterations.

(iii) The excluded periodic orbits of (7) or (20) corresponds to rational values of the seed k_0 as well as to periodic (in real space) Bloch functions.

Let us now consider the linear Heisenberg ferromagnetic chain for which the dispersion relation is $\omega = 2[1 - \cos(2\pi k)]$. Using (20) we get

$$\omega_n = \omega_{n-1}(4 - \omega_{n-1}) \ , \tag{21}$$

and from this map we can get, using (18), the magnon density of states. In the case of phonons in a chain we have $\omega^2 = 2[1 - \cos(2\pi k)]$ and the density of states for these excitations can be obtained by constructing a sequence $\omega_0, \omega_1, \omega_2, \ldots$ through (21), extracting the square root of each element, and then computing the density of visits along the interval [0,2]. For the first- and second-neighbor hopping tight-binding linear chain,[2] the dispersion relation is

$$\epsilon = 2\cos(2\pi k) + \gamma 2\cos(4\pi k) \ ,$$

where γ is the ratio between hoppings. Using a basic sequence $\omega_0, \omega_1, \omega_2, \ldots$ obtained by (7), we can construct a secondary sequence $\epsilon_n = \omega_n + \gamma\omega_{n+1}$ from which we get directly the density of states.

Let us now consider higher-dimensional systems. For the tight-binding square lattice we have

$$\epsilon = 2\cos(2\pi k_x) + 2\cos(2\pi k_y) \ .$$

Using *two independent* basic sequences $\omega_0^x, \omega_1^x, \omega_2^x, \ldots$ and $\omega_0^y, \omega_1^y, \omega_2^y, \ldots$ $(\omega_n^{(i)} = \omega_{n-1}^{(i)2} - 2)$ arising from two independent sequences in reciprocal space, one for each direction, we can construct another sequence[7] $\epsilon_n = \omega_n^x + \omega_n^y$ which yields the density of states for the system. For three-dimensional systems, we use three independent basic sequences ω_n^x, ω_n^x, and ω_n^z. For the simple cubic lattice, the secondary sequence $\epsilon_n = \omega_n^x + \omega_n^y + \omega_n^z$ gives the density of states, while for the bcc and fcc lattices the corresponding sequences are $\epsilon_n = \omega_n^x\omega_n^y\omega_n^z$ and $\epsilon_n = \omega_n^x\omega_n^y + \omega_n^x\omega_n^z + \omega_n^y\omega_n^z$, respectively. For illustration, Fig. 3 shows the density of states obtained for the fcc lattice using only 10 000 iterations and 40 interval divisions of the energy axis.

Note that the map (7) as well as the maps corresponding to other length scales ($\omega_n = \omega_{n-1}^3 - 3\omega_{n-1}$, for example) are in the critical situation of a boundary crisis.[8] We intend to investigate the scaling laws associated with that critical situation for applying the present method to disordered systems.

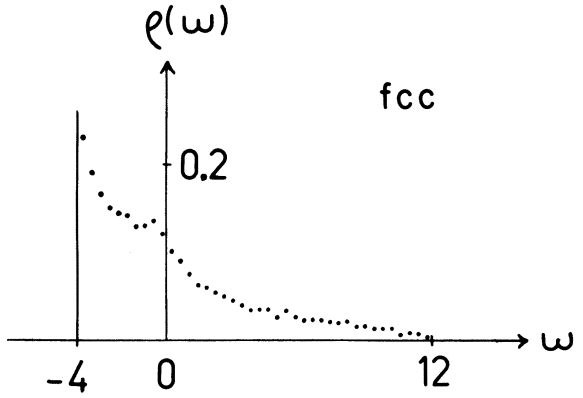

FIG. 3. Histogram of the density of states for a tight-binding fcc lattice obtained by our method with 10 000 interactions and 40 interval divisions of the energy axis.

Although the map (7) could have been obtained indirectly from the map (20) using its properties,[4,9] we believe that our proof for the equivalence between the density of states and the density of visits in the energy axis *without resorting to the k space* allows for the possibility of extending our results for disordered systems where k is no longer a good quantum number. In fact, this is currently being done for a disordered linear chain.

Note added. We have recently learned about the work by José[4] and that J. Langlois, A. Tremblay, and B. W. Southern as well as S. Alexander, D. Bensimon, E. Domany, and L. Kadanoff have also obtained similar results for the linear-chain case.

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[4]J. V. José, J. Phys. A 16, L205 (1983).

[5]From the chaotic interval $-2 < \omega < 2$ we exclude points such as 0, ± 1, $\pm\sqrt{2}$, etc., that follow periodic orbits.

[6]Alternatively, we can define $\bar{\nu}(\omega) \equiv [\nu(\omega) + \nu(-\omega)]/2$.

[7]Note that the sequence $\epsilon_0, \epsilon_1, \epsilon_2, \ldots$ is *not* Markovian, and *cannot* be constructed by itself $[\epsilon_n \neq f(\epsilon_{n-1})]$. It is necessary to resort to both sequences ω_n^x and ω_n^y. The seeds ω_0^x and ω_0^y must correspond to irrational values of k_0^x, k_0^y, and k_0^y/k_0^x. The last condition assures that all of the two-dimensional Brillouin zone will be uniformly visited.

[8]The map $\omega_n = \omega_{n-1}^2 - C$ presents no chaotic behavior for $C > 2$. Just for $C = 2$ it is nondissipative while it is dissipative for $C < 2$. See C. Grebogi, E. Ott, and J. A. Yorke, Phys. Rev. Lett. 48, 1507 (1982) and J. P. Eckmann, Rev. Mod. Phys. 53, 643 (1981).

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