RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 27, NUMBER 2 15 JANUARY 1983

Real-space rescaling method for the spectral properties of tight-binding systems

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(Received 19 November 1982)

Exact real-space rescaling transformations are used to calculate the spectral properties of tight-binding Hamiltonians with arbitrary range of interaction on a linear chain. Singularities of the spectral functions within the band of extended states are associated with fixed points of the rescaling transformation. The fixed points separate regions of energy in which the behavior of the system is qualitatively different. The method is not restricted to one dimension and can also be used to treat single-impurity problems.

Real-space rescaling methods have been quite successful in describing the singularities which occur in thermodynamic quantities at a phase transition.[1] More recently, these scaling methods have also been employed to obtain information about the spectral properties of disordered tight-binding systems.[2–5] We have developed an exact rescaling transformation for ordered systems described by tight-binding Hamiltonians with arbitrary range of interaction on a linear chain and show how the lattice Green's functions of the system can be evaluated using this approach. The conventional treatment of this system uses Fourier transformation to obtain the dispersion function and then expresses the spectral functions in terms of Brillouin-zone integrals. In general, the evaluation of these integrals requires numerical quadrature with inherent grid size effects. There are some exceptions where analytic results can be found, notably for nearest-neighbor problems,[6,7] but for real materials longer-ranged interactions are present and "quasianalytic" numerical methods[8] are frequently used. Our rescaling approach is computationally very efficient and is not necessarily restricted to translationally invariant systems.

The one-dimensional tight-binding Hamiltonian for a single band is

$$\mathcal{H}=\sum_i \epsilon |i\rangle\langle i| + \sum_{i,n} V_n(|i\rangle\langle i+n| + |i+n\rangle\langle i|) \ , \tag{1}$$

in obvious notation. Most studies of this system restrict the hopping matrix elements to nearest-neighbor sites but for reasons to be discussed later we are interested in the problem with arbitrary hopping range.

The spectral properties of this system are obtained by solving the following set of equations for the lattice Green's functions[7] G_{ij}:

$$(E-\epsilon)G_{ij}=\delta_{ij}+\sum_n V_n G_{ij+n} \ , \tag{2}$$

where

$$G_{ij}(E+i0^+)=\left\langle i\left|\frac{1}{E+i0^+-\mathcal{H}}\right|j\right\rangle \ .$$

Equations of this same form describe many different types of elementary excitation, e.g., electron quasiparticles, magnons, and phonons.

Our basic approach to solving these equations is to eliminate a fraction of the degrees of freedom from the set (2) and rewrite the resulting sets of equations in the same form as the original set but with renormalized parameters. The simplest rescaling transformation on the set (2), which involves N sites, would correspond to the elimination of alternate sites to form two new sets of equations which are completely decoupled from each other and each involving only $N/2$ sites. However, the elimination process generates additional inhomogeneous terms in the new sets, and these must be included in the initial set (2) if the procedure is to be iterated. We must replace the Kronecker δ in (2) by a matrix z_{ij}, which is only δ_{ij} initially. At any stage of the procedure the equations can be written in terms of reduced variables and have the following general form:

$$G_j=\alpha_j+\sum_n x_n G_{j+n} \ , \tag{3}$$

where

$$\alpha_j=\frac{z_{ij}}{E-\epsilon}, \quad x_n=\frac{V_n}{E-\epsilon} \ ,$$

and the first subscript i of the G_{ij} has been dropped for convenience. All α_j are initially zero except α_0. For each value of j, we multiply the equation for G_{j+m} by a factor $(-1)^{m+1}x_m$ and add them to G_j. This yields "even" and "odd" sets having the same general form as (3) but with renormalized parameters

α_j' and x_n' given by

$$\alpha_j' = \frac{\alpha_j + \sum_{m\neq 0} (-1)^{m+1} x_m \alpha_{j+m}}{\left(1 + \sum_{m\neq 0} (-1)^m x_m x_{-m}\right)} , \tag{4a}$$

$$x_{2n}' = \frac{2x_{2n} + \sum_{m\neq 0} (-1)^{m+1} x_m x_{2n-m}}{\left(1 + \sum_{m\neq 0} (-1)^m x_m x_{-m}\right)} . \tag{4b}$$

If we now perform a scaling of all lattice distances in each set by a factor $b=2$, then we can identify x_{2n}' as the effective x_n' and α_{j+2n}' as the effective α_{j+n}' in these new sets. The elimination of degrees of freedom and the rescaling of distances together constitute the rescaling tranformation. With the renormalized parameters, the procedures can now be repeated for the new sets to generate twice as many sets of decoupled equations. As the process is iterated, each G_j belongs to a smaller and smaller set until finally each set contains only one G_j. In this limit the renormalized equations can be solved exactly since they are now diagonalized. Each G_j is obtained as the limiting value of its inhomogeneous term α_j'.

In one dimension the range of interaction at any stage is the same as the initial range. However, the transformation (4) does not rely on this property. As an illustration of the method, consider a tight-binding Hamiltonian with only nearest- and next-nearest-neighbor overlap. Only x_1' and x_2' are required at each stage and determined from the following recurrence relations:

$$x_1' = \frac{x_1^2 + 2x_2}{(1 - 2x_1^2 + 2x_2^2)} , \tag{5a}$$

$$x_2' = \frac{-x_2^2}{(1 - 2x_1^2 + 2x_2^2)} . \tag{5b}$$

The calculation of a particular G_j also involves the inhomogeneous terms of the other members of its set at each stage and these are determined from the following recurrence relations:

$$\alpha_{j+n}' = \frac{\alpha_{j+2n} + x_1(\alpha_{j+2n+1} + \alpha_{j+2n-1}) - x_2(\alpha_{j+2n+2} + \alpha_{j+2n-2})}{(1 - 2x_1^2 + 2x_2^2)} . \tag{6}$$

Before we describe the evaluation of the G_j in detail, consider the recurrence relations in (5). The behavior of the system at any value of the energy E and for given initial choices of the hopping elements V_1 and V_2 can be determined by studying the behavior of these recurrence relations alone. In general, if the value of E lies within a certain range, the parameters x_1 and x_2 oscillate in an apparently random fashion as the equations are iterated. However, if the value of E lies outside this range, the parameters iterate to zero monotonically. The various regions of E in which the behavior of the recurrence relations (5) is qualitatively different are shown in Fig. 1. In the central region I all initial values of x_1 and x_2 are eventually mapped into the origin. In region II, x_2 iterates to zero and only x_1 oscillates, whereas in region III both parameters oscillate. In this way the boundaries which separate the different regions of E can be mapped out in the x_1-x_2 plane. The curve which separates region I from either region II or III is, in fact, the locus of the band edge. The lines separating regions II and III correspond to internal singularities within the band which appear when the ratio of the second-neighbor to the first-neighbor coupling exceeds a critical value.[9]

The recurrence relations (5) possess certain fixed points, or special points where the values of x_1 and x_2 do not change under iteration. The recurrence relations can be linearized about these fixed points and the eigenvalues which describe their stability properties can be obtained.[1] In the present case there are two unstable fixed points whose coordinates and eigenvalues are listed in Table I. Fixed point A describes the change in behavior at the band edges and on the lines separating regions II and III in Fig. 1. Fixed point B describes this behavior for a special value of the ratio $|x_2/x_1| = \frac{1}{4}$ where the three different regions intersect. These changes in behavior from one region to another are similar to the bifurcation phenomena observed in some simple models of dynamical systems.[10,11]

Standard scaling arguments[1] indicate that the eigenvalues of these fixed points describe singularities of the G_j as we cross the boundaries in Fig. 1. Near these values of E, denoted E_c, the G_j behave as $G_j \propto |E - E_c|^{(d-y)/y}$, where d is the dimension of the lattice and y is an exponent corresponding to the largest eigenvalue of the associated fixed point. For a scaling factor b, the exponents are related to the eigenvalues as $\lambda = b^y$. Fixed point A describes the square-root singularities of the G_j at the band edges and at internal points in the band, whereas fixed point B describes a special case where the internal singularities merge with the band edge to give an $|E - E_c|^{-3/4}$ behavior and occurs when $|V_2/V_1| = \frac{1}{4}$. For values of V_2 smaller than this the G_j are singular only at the band edges but for values of V_2 which are larger, the group velocity can also vanish inside the band.[9] Fixed point B thus describes the onset of this new behavior as V_2 is increased.

The real and imaginary parts of the lattice Green's functions G_j are calculated by iterating the recurrence

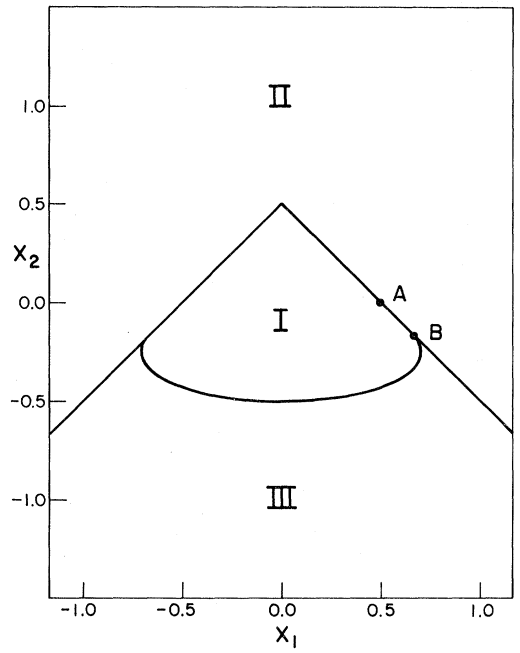

FIG. 1. I, II, and III label the regions of the x_1-x_2 plane in which the behavior of the recurrence relations (5) is qualitatively different. The positions of the fixed points are labeled by A and B.

formulas (5) and (6) for energy $E+i0^+$. The x_n now iterate to zero for all values of E although the distinct regions discussed earlier exhibit qualitative differences in how this occurs. When the inhomogeneous terms in (6) reach limiting complex values (dependent on the value of E) we have that $G_j=\alpha_j^{(\infty)}$.

The number of inhomogeneous terms depends on the value of j. For $j=0$, where the imaginary part of $G_0(E+i0^+)$ gives the local density of states, only α_0 and α_1 are needed at any stage and, by using the fact that $\alpha_1=\alpha_{-1}$, are determined from the following relations:

$$\alpha_0'=(\alpha_0+2x_1\alpha_1)/(1-2x_1^2+2x_2^2)\ ,$$
$$\alpha_1'=(x_1\alpha_1-x_2\alpha_0)/(1-2x_1^2+2x_2^2)\ . \tag{7}$$

Under iteration, α_1 changes but eventually tends to zero as α_0 reaches its limiting value. On the other hand, the calculation of G_1 involves three inhomogeneous terms which satisfy

$$\alpha_1'=[\alpha_1+x_1(\alpha_0+\alpha_2)]/(1-2x_1^2+2x_2^2)\ ,$$
$$\alpha_2'=(x_1\alpha_2-x_2\alpha_1)/(1-2x_1^2+2x_2^2)\ , \tag{8}$$
$$\alpha_0'=(x_1\alpha_0-x_2\alpha_1)/(1-2x_1^2+2x_2^2)\ .$$

In this case α_1 tends to a limiting value and the neighboring α's tend to zero. Other G_j can be calculated in a similar manner but involve larger numbers of inhomogeneous terms.

For G_0 and G_1 the number of iterations required for six-digit precision depends upon E but is of the order of ten and can be readily implemented on any programmable device. The results for the second-neighbor problem are in complete argeement with recent analytic results.[9]

TABLE I. Fixed points of the recurrence relations (5) and their corresponding eigenvalues.

Fixed points	x_1^*	x_2^*	λ_1	λ_2
A	$\frac{1}{2}$	0	4	0
B	$\frac{2}{3}$	$-\frac{1}{6}$	16	4

In the nearest-neighbor case it is easy to see for the calculation of G_0 from (7) (with $x_2=0$) that α_1 is always zero. In fact, the initial δ_{ij} in (2) never changes in this case. Thus the consideration of the inhomogeneous terms was not necessary in the recent calculations of the density of states for the nearest-neighbor chain.[5]

We have performed explicit calculations for the system with third-neighbor overlap where there are more distinct energy regions than for the second-neighbor case. However, it is the arbitrary range problem that we have formulated for one dimension (1D) in (4) that is important for extensions to higher dimensions. The reason is simply that, in contrast to the linear chain where the initial range of coupling does not effectively change, in two and three dimensions, even for only nearest-neighbor couplings initially, each successive elimination causes a proliferation of the range of interaction. For the 2D square lattice we have constructed an exact transformation similar to that given in (4) which has been successful in locating the band edges. The initial increase in the range of the couplings reverses under iteration as the x_n tend to zero. In the region of energy outside the band of extended states, fifth neighbors and ten iterations are typically involved. We are currently investigating the application of the present techniques to the evaluation of the lattice Green's functions for higher dimensional lattices with couplings which extend beyong nearest neighbors.

The present approach can also be used to study problems in which the couplings are not uniform. For example, the case of a single impurity in a chain can also be treated exactly. The method has potential applications to the study of problems with strong disorder such as Anderson localization and spin-glasses.

ACKNOWLEDGMENT

This research has been supported by the Natural Sciences and Engineering Research Council of Canada.

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