RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 30, NUMBER 3 1 AUGUST 1984

Renormalization-group decimation technique for spectra, wave functions, and density of states

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(Received 10 April 1984)

The renormalization-group decimation technique is exact for one-dimensional nearest-neighbor tight-binding models with or without translational invariance. Spectra, wave functions, and the density of states are calculated with little numerical work from the renormalized coefficients upon iteration. The method is used on the Soukoulis and Economou model.

Crystals containing a modulating potential of a period different from that of the underlying lattice (either commensurate or incommensurate with it),[1] electrons in a two-dimensional (2D) square lattice in a perpendicular magnetic field,[2] the Schrödinger equation with an arbitrary potential of atomic type (through the construction of the Poincaré map of the problem),[3] superconductive networks (de Gennes–Alexander theory)[4] lead to equations of the type

$$t_{n-1,n}\psi_{n-1}+t_{n,n+1}\psi_{n+1}=\epsilon_n\psi_n \ , \tag{1}$$

where ψ_n is an amplitude (wave function, amplitude of oscillation, etc.), $t_{n,n+1}$ is a nearest-neighbor coupling parameter (off-site coefficient), and ϵ_n includes the eigenvalue and possibly an on-site energy term (on-site coefficient). Our method to treat this problem is based on renormalization-group decimation (RGD), which is exact for the 1D problem. In that context we present a systematic procedure for the calculation of spectra, wave functions, and the density of states. RGD proceeds by eliminating every second site in this set of equations to obtain the equations for a chain of double spacing. Repeating this procedure r times, we obtain a chain of spacing 2^r, with the form-conserving equations

$$t^{(r)}_{n-k,n}\psi_{n-k}+t^{(r)}_{n,n+k}\psi_{n+k}=\epsilon^{(r)}_n\psi_n \ , \tag{2}$$

where $k=2^r$ and the recursion relations are[5]

$$\epsilon_n^{(r+1)}=(\epsilon_n-t^2_{n,n-k}/\epsilon_{n-k}-t^2_{n,n+k}/\epsilon_{n+k})^{(r)} \ ,$$
$$t^{(r+1)}_{n\pm 2k,n}=(t_{n\pm k,n}\pm k2\pm 1 t_{n\pm k,n}/\epsilon_{n\pm k})^{(r)} \ . \tag{3}$$

To *illustrate* the method we briefly discuss a simple, well-known example. For a 1D, one-band, tight-binding model with one impurity, the equation of motion reads $(\omega-\epsilon_n)\psi_n-t(\psi_{n+1}+\psi_{n-1})=0$ where $\epsilon_n=\epsilon$ for host sites and $\epsilon_n=\epsilon_i$ for the impurity site; ω is the eigenvalue. For this problem a localized state exists[6] as ω such that $1-(\epsilon_i-\epsilon)G_{00}(\omega)=0$, G_{00} being the local Green's function at the impurity site. In agreement with previous results[7] the RGD applied to this problem shows that for energies outside the band the on-site coefficient, as a function of iteration, saturates at a finite value. For an energy exactly equal to that of the localized state the coefficient tends to zero, whereas for energies within the extended band it shows oscillations. The saturation value of the on-site coefficient as a function of ω is monotonic outside the extended band, goes through zero for the localized ω, and oscillates inside the band of extended states. For energies inside the extended band, and if the order of iteration is low enough (for a given increment of ω), the on-site coefficient is a set of continuous branches, going through zero at different separations and diverging steeply. If the order of iteration is increased, more branches are present; beyond a certain limit, the function looks discontinuous because points from different branches are picked up. The zeros of this function are related to the eigenvalues; the inverse of the separation between them is proportional to the density of states. In fact, for $r=6$ this quantity already reproduces the square-root divergent density of states of the 1D tight-binding model. Increasing the order of iteration only varies the number of points available to draw the curve.

To illustrate the method on a more sophisticated example we choose the model of Soukoulis and Economou,[1] described by the following equations:

$$\epsilon_n\psi_n+t(\psi_{n+1}+\psi_{n-1})=E\psi_n$$

with

$$\epsilon_n=V_0[\cos(Qn)+V_1\cos(2Qn)] \ .$$

RGD gives the following results.

In Fig. 1 we plot the on-site coefficient at $n=0$ and iteration 12 (already saturated for gaps and for localized states) as a function of E. This is "rough" run with $\Delta E=0.1$. According to the previous analysis, whenever this function goes through zero or stops to be monotonic, either extended bands or localized states exist. The rectangles on the upper part mark the regions where states are present and show good rough agreement with Ref. 1 except that the localized peak around $E=2$ has not appeared. At saturation the computer will not collect information from distances beyond 2^r around the chosen one. Thus localized states can be "lost" if decimation is performed around some sites and can "appear" if the chosen site is changed. We performed the rough analysis positioning ourselves on sites 500, 1000, 1500, 2000, etc., and noticed the extended peaks at all

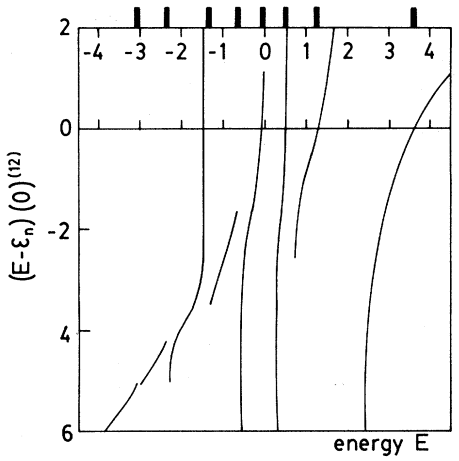

FIG. 1. On-site coefficient at $n=0$, iteration 12, as a function of E for the model of Ref. 4 with $\Delta E = 0.1$.

times, whereas the "thinner" localized peaks sometimes were not noticed. Also for a peak around 3.6 decimating around $n=0$ the only zero is at $E = 3.639\,293\,698\,116\,315$. Changing to site 4000 the coefficient goes through zero at 3.629 756 647 46. We have to work with high precision because we do not pose boundary conditions and so we are picking up both the increasing and the decreasing solutions. In Fig. 2 we plot the inverse of the separation between zeros of the on-site coefficient as function of energy for the peak around -2.317. This should be compared with the density of states in Ref. 1. The peaks are obtained at iteration 12 where saturation occurs; the central region is drawn at iteration 7 because at iteration 12 too many points appear for our precision (no saturation even at iteration 12). The graph (except the last 5 peaks on the right) is obtained decimating around the site zero. In Fig. 3(a) we plot $\ln|\psi_n|^2$ as a function of position for $E = -2.317$. Agreement with the result of Ref. 1 is excellent and shows that the state is extended. In Fig. 3(b) we plot ψ_n for $E = -2.320\,377\,527\,580\,125$ (peak on left of Fig. 2). Precision for the eigenvalue is crucial. This and the fact that saturation is obtained suggests that the side regions are different from the center. The wave function looks like connected localized packets. This is a new result and we think that for the *first time* we were able to show what the wave

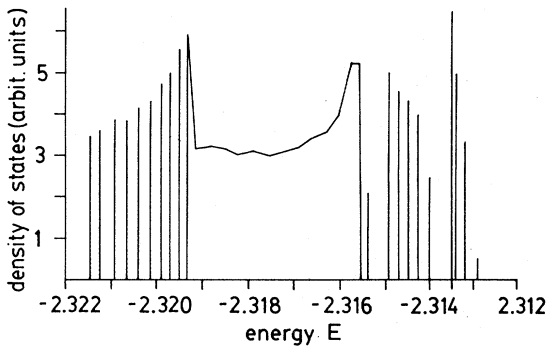

FIG. 2. Spectral analysis with our procedure of the extended peak around $E = -2.317$.

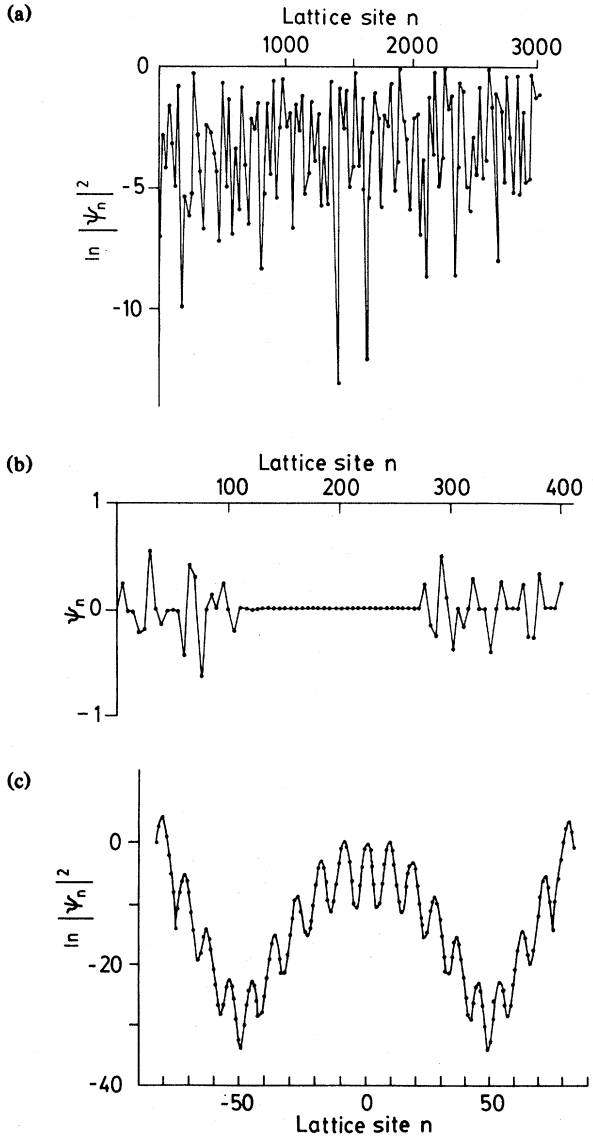

FIG. 3. Spatial extension of the wave function for different eigenvalues: (a) extended for $E = -2.317$; (b) connected localized packets at $E = -2.320\,377\,527\,580\,125$; (c) localized at $E = 3.639\,293\,698\,116\,315$.

function, which is neither localized nor extended, looks like. In Fig. 3(c) we show ψ_n for $E = 3.639\,293\,698\,116\,315$ (localized state). The behavior agrees with Ref. 1 (localization in 100 sites) but outside, we get a diverging wave function.

Goncalves da Silva and Koiller[8] and Oliveira, Continentino, and Anda[9] have worked along similar lines.

The authors acknowledge discussions with A. López, C. Balseiro, R. B. Stinchcombe, and M. P. Tosi. They thank Professor Abdus Salam, International Atomic Energy Agency (IAEA) and United Nations Educational, Scientific and Cultural Organization (UNESCO), for hospitality at the International Centre for Theoretical Physics, Trieste. C. Wiecko acknowledges financial support from Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina.

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