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1991 J. Phys. A: Math. Gen. 24 L1405

(http://iopscience.iop.org/0305-4470/24/24/004)

J. Phys. A: Math. Gen. 24 (1991) L1405-L1414. Printed in the UK

LETTER TO THE EDITOR

Mixed impurities in a tight-binding model

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Received 23 July 1991

Abstract. The Green function of a tight-binding model with mixed impurities is calculated exactly. The spectral properties of the one-dimensional lattice, including both extended and localized states, are also analysed exactly. We find at most two localized states which are always non-degenerate. The density of states per site in the continuum is calculated. Using a constructive procedure we obtain the localized eigenfunctions for the infinite and semi-infinite chain. Some results for three-dimensional lattices are presented.

The effects of defects on the spectrum of elementary excitations of crystals have been examined extensively [1]. Using the standard perturbation expansions for the Green function the properties of systems with few defects can be exactly expressed in terms of the known results in the perfect case. Thus, crystals containing only a low concentration of such defects can be interpreted in terms of those properties. These effects must be reproduced by disordered systems in the dilute (low concentration of defects) limit.

Recently, very much attention was given to the influence of off-diagonal disorder and its correlations with diagonal disorder in the density of states and transport properties of electronic systems, described by a tight-binding Hamiltonian [2]. However, up to now, very little has been done in examining in detail the effects of a single defect containing both diagonal and off-diagonal impurities. Any exact result on this problem, even in a very simple model, will be very useful in the implementation of approximate calculation schemes for strongly disordered systems. In this letter, we consider the most simple defect of this kind, that is, a tight-binding Hamiltonian containing one impure energy site and an impure hopping constant between this site and one nearest neighbour (mixed impurities). We analyse exactly the spectral properties, and calculate the density of states (DOS).

We consider a tight-binding (TB) Hamiltonian of the form

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_I \tag{1}$$

with

$$\mathbf{H}_0 = \varepsilon_0 \sum_{\boldsymbol{R}} |\boldsymbol{R}\rangle\langle\boldsymbol{R}| + V_0 \sum_{\boldsymbol{R},i} |\boldsymbol{R}\rangle\langle\boldsymbol{R}+\boldsymbol{\lambda}_i| \tag{2}$$

$$\mathbf{H}_I = \varepsilon|\boldsymbol{l}\rangle\langle\boldsymbol{l}| + V[|\boldsymbol{l}\rangle\langle\boldsymbol{l}+\boldsymbol{\delta}| + |\boldsymbol{l}+\boldsymbol{\delta}\rangle\langle\boldsymbol{l}|] \tag{3}$$

where each state $|\boldsymbol{R}\rangle$ corresponds to a Wannier orbital centred at the site $\boldsymbol{R}$. The sites $\{\boldsymbol{R}\}$ form an arbitrary Bravais lattice of dimension d. The vectors $\{\boldsymbol{\lambda}_i;\ i = 1, 2, \ldots, q\}$ are lattice vectors which connect each site with its nearest neighbours, and q is the coordination number of the lattice. $\mathbf{H}_0$ describes a homogeneous TB model, with ε_0 the

0305-4470/91/241405+10$03.50

electronic energy of an isolated orbital and V_0 the transition probability amplitude (hopping constant) between any pair of nearest-neighbour sites (we will take $V_0 \geqslant 0$). $\mathbf{H}_I$ is the contribution of the impurities to the energy, with $\varepsilon = \varepsilon' - \varepsilon_0$ and $V = V' - V_0$; ε' is the impure site energy associated with the site $\boldsymbol{l}$, and V' is the impure hopping constant between the particular sites $\boldsymbol{l}$ and $\boldsymbol{l}+\boldsymbol{\delta}$; $\boldsymbol{\delta}$ is an arbitrary and fixed vector selected from the set $\{\boldsymbol{\lambda}_i\}$.

The Green functions $\mathbf{G}_0(z)$ and $\mathbf{G}(z)$ associated with $\mathbf{H}_0$ and $\mathbf{H}$ respectively are defined by

$$(z-\mathbf{H})\mathbf{G}(z) = \mathbf{I} \tag{4}$$

where z is a complex number with $\operatorname{Re} z = E$ *and* $\operatorname{Im} z = \eta$. *On the real axis we must introduce the side limits*

$$\mathbf{G}^{\pm}(E) = \lim_{\eta \to 0^+} \mathbf{G}(E \pm \mathrm{i}\eta). \tag{5}$$

The Hamiltonian $\mathbf{H}_0$ given by (2) does not have discrete eigenvalues due to the translation invariance, and the continuous spectrum (band energy of extended eigenstates) is the branch cut of $\mathbf{G}_0$. $\mathbf{G}_0$ has been calculated for a great variety of Bravais lattices [4–8]. The continuous spectrum of $\mathbf{H}$ is the same as the continuous spectrum of $\mathbf{H}_0$ [9].

In order to calculate $\mathbf{G}(z)$ in terms of $\mathbf{G}_0(z)$ we introduce the t-matrix $T(z)$ by: $\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_0\mathbf{T}\mathbf{G}_0$. It is given in terms of H_I by [1]

$$\mathbf{T} = \mathbf{H}_I(1 - \mathbf{G}_0\mathbf{H}_I)^{-1} \tag{6}$$

From (6) we find after some matrix algebra

$$\begin{aligned}\mathbf{G} = \mathbf{G}_0 + \frac{1}{\Theta}\mathbf{G}_0[&|\boldsymbol{l}\rangle(\varepsilon + V^2\langle \boldsymbol{l}|\mathbf{G}_0|\boldsymbol{l}\rangle)\langle \boldsymbol{l}| + |\boldsymbol{l}+\boldsymbol{\delta}\rangle V^2\langle \boldsymbol{l}|\mathbf{G}_0|\boldsymbol{l}\rangle\langle \boldsymbol{l}+\boldsymbol{\delta}| \\ &+ |\boldsymbol{l}\rangle(V - V^2\langle \boldsymbol{l}+\boldsymbol{\delta}|\mathbf{G}_0|\boldsymbol{l}\rangle)\langle \boldsymbol{l}+\boldsymbol{\delta}| \\ &+ |\boldsymbol{l}+\boldsymbol{\delta}\rangle(V - V^2\langle \boldsymbol{l}+\boldsymbol{\delta}|\mathbf{G}_0|\boldsymbol{l}\rangle)\langle \boldsymbol{l}|]\mathbf{G}_0\end{aligned} \tag{7}$$

with

$$\begin{aligned}\Theta(z) = 1 &- \varepsilon\langle \boldsymbol{l}|\mathbf{G}_0(z)|\boldsymbol{l}\rangle - 2V\langle \boldsymbol{l}+\boldsymbol{\delta}|\mathbf{G}_0(z)|\boldsymbol{l}\rangle - V^2(\langle \boldsymbol{l}|\mathbf{G}_0(z)|\boldsymbol{l}\rangle)^2 \\ &+ V^2(\langle \boldsymbol{l}+\boldsymbol{\delta}|\mathbf{G}_0(z)|\boldsymbol{l}\rangle)^2.\end{aligned} \tag{8}$$

The analytical structure of $\mathbf{G}(z)$, which contains all the properties of the spectrum of $\mathbf{H}$, has been made explicit in $\Theta(z)$. It is worthwhile to note that $\Theta(z)$ is obtained from

$$\Theta(z) = \det[\mathscr{I} - \mathscr{G}_0(z)\mathscr{H}_I] \tag{9}$$

where $\mathscr{G}_0$ and $\mathscr{H}_I$ are the restriction of the operators $\mathbf{G}_0$ and $\mathbf{H}_I$ respectively, to the subspace spanned by the Wannier states related to the impure sites and those nearest-neighbour sites which are connected by impure hopping constants.

For $d = 1$ we have a simple chain. In this case the Wannier basis can be written as $\{|m\rangle;\ m = 0, \pm 1, \pm 2, \ldots\}$. The site l is the impure site and we have an impure hopping constant V' between the sites l and $l+1$.

The Green function for the homogeneous problem $\mathbf{G}_0(z)$ has the following matrix elements

$$\langle m|\mathbf{G}_0|n\rangle = F\rho^{|m-n|} \tag{10}$$

where

$$F=\frac{1}{2V_0R} \qquad x=\frac{z-\varepsilon_0}{2V_0}$$

$$\rho=x-R \qquad R=\sqrt{x^2-1}$$

and $\sqrt{x^2-1}$ denotes the square root whose imaginary part has the same sign as that of $\mathrm{Im}\{x\}$ (in which case the real parts of $\sqrt{x^2-1}$ and x have the same sign). The continuous spectrum of the model (branch cut of $\mathbf{G}_0$) corresponds to $|x|\leqslant 1$ with x real. We use the notation: $G(m,n)\equiv\langle m|\mathbf{G}|n\rangle$ for the matrix elements of the operator $\mathbf{G}$. Taking matrix elements of (4) and using (1)-(3) we obtain the recursion relations for the matrix elements of $\mathbf{G}$

$$(z-\varepsilon')G(l,h)-V'G(l+1,h)-V_0G(l-1,h)=\delta_{lh} \tag{11}$$

$$(z-\varepsilon_0)G(l+1,h)-V_0G(l+2,h)-V'G(l,h)=\delta_{l+1\,h} \tag{12}$$

for all h. And for $m\neq l, l+1$ and for all h

$$(z-\varepsilon_0)G(m,h)-V_0[G(m+1,h)+G(m-1,h)]=\delta_{mh}. \tag{13}$$

Similarly from the equation $\mathbf{G}(z-\mathbf{H})=\mathbf{I}$ we obtain for all m

$$(z-\varepsilon')G(m,l)-V'G(m,l+1)-V_0G(m,l-1)=\delta_{ml} \tag{14}$$

$$(z-\varepsilon_0)G(m,l+1)-V_0G(m,l+2)-V'G(m,l)=\delta_{ml+1} \tag{15}$$

and for $h\neq l, l+1$

$$(z-\varepsilon_0)G(m,h)-V_0[G(m,h+1)+G(m,h-1)]=\delta_{mh}. \tag{16}$$

Therefore from (11)-(16) all the matrix elements of $\mathbf{G}$ can be obtained from the three elements $G(l,l)$, $G(l+1,l+1)$, and $G(l,l+1)$.

From (7) and (8) we obtain

$$G(l,l)=F/\Theta \tag{17}$$

$$G(l+1,l+1)=\frac{1}{\Theta}[F+F^2\varepsilon(\rho^2-1)] \tag{18}$$

$$G(l,l+1)=\frac{F}{\Theta}[\rho+FV(\rho^2-1)] \tag{19}$$

$$\Theta=1-\varepsilon F-2V\rho F+V^2(\rho^2-1)F^2. \tag{20}$$

The diagonal matrix elements of $\mathbf{G}$ are:

$$G(l+n,l+n)=F+\begin{cases}[G(l+1,l+1)-F]\rho^{2(n-1)} & \text{if } n\geqslant 1\\ [G(l,l)-F]\rho^{-2n} & \text{if } n\leqslant 0.\end{cases} \tag{21}$$

All the simple poles of $\mathbf{G}$ are on the real axis, with $|x|>1$. Defining the parameters $\alpha'\equiv V'/V_0$ and $\delta\equiv\varepsilon/2V_0$ the equation $\Theta=0$ in equivalent to

$$(\alpha'^2+1)R=(\alpha'^2-1)x+2\delta. \tag{22}$$

We find at most two solutions of equation (22). Putting

$$X^{\pm}=\frac{1}{2\alpha'}[(\alpha'^2-1)\delta\pm(\alpha'^2+1)\sqrt{\delta^2+\alpha'^2}] \tag{23}$$

$X^+ > 1$ and $X^- < -1$; moreover:

$$\begin{aligned} &X^+ \text{ is a solution if } \delta > -\gamma \\ &X^- \text{ is a solution if } \delta < \gamma \end{aligned} \tag{24}$$

where $\gamma = \frac{1}{2}(\alpha'^2 - 1)$. We can thus distinguish different regions in the parameter-space (α', δ) according to the number of localized states present, as depicted in figure 1. Figure 2 shows the energy of the localized eigenstates as a function of α' for some values of δ. From (20) and (21) we calculate the residue of $G(l+n, l+n)$ at the poles $X^\pm$, and summing over all sites n we obtain $\mathrm{Tr}[\mathrm{Res}\{\mathbf{G}(X^\pm)\}] = 1$. Hence, the levels $X^\pm$ are non-degenerate.

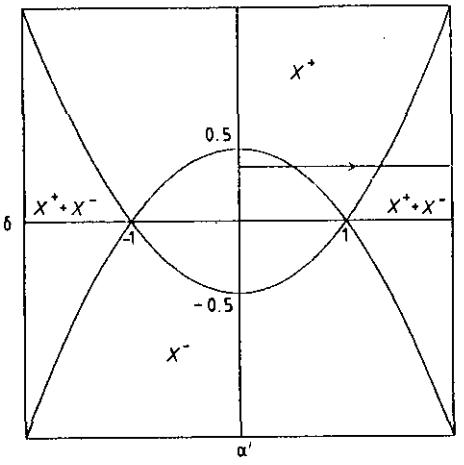

Figure 1. Regions of localized states in the space (α', δ) for the 1D case. X^+ (X^-) corresponds to a localized eigenstate above (below) the band. In the central region confined by the parabolic curves there is no localization. The oriented path shown at the right corner runs for $\delta = \frac{3}{8}$.

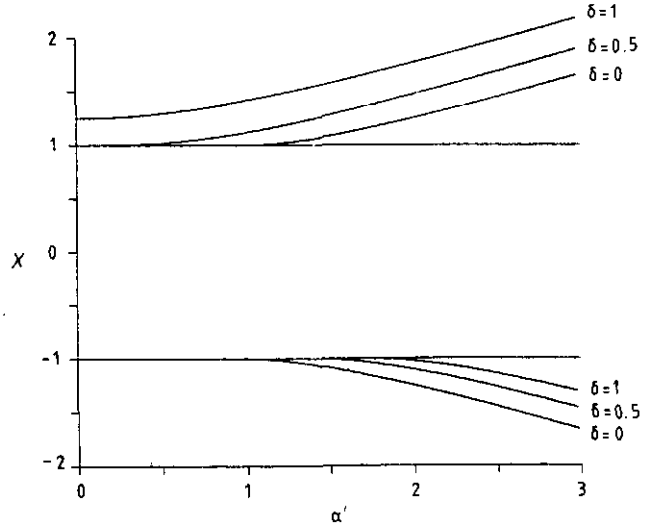

Figure 2. Normalized energy x of the localized eigenstates as a function of α' for the 1D case. The band is located at $|x| \leq 1$.

Let us analyse two simple particular cases. Firstly, for $\alpha' = 1$ we recover the results of the single diagonal impurity case (one impure site-energy). In figure 1 this case corresponds to the vertical line $\alpha' = 1$. We see that there is always only one localized eigenstate, without restriction on the parameter δ, with energy $\sqrt{1+\delta^2}$ if $\delta > 0$ and $-\sqrt{1+\delta^2}$ if $\delta < 0$. Secondly, for $\delta = 0$ we get a single off-diagonal impurity case (one impure hopping constant). In figure 2 this case corresponds to the $\delta = 0$ axis. Note that for $|\alpha'| < 1$ we do not have localized eigenstates. For $|\alpha'| > 1$ we have always two symmetrical localized states with energies:

$$X^{\pm} = \pm\frac{1}{2}\left(|\alpha'| + \frac{1}{|\alpha'|}\right).$$

We use a simple constructive procedure [10] to derive the localized eigenfunctions $|\psi_X\rangle$, which also leads to the localization length, a quantity of physical interest. Expanding

$$|\psi_X\rangle = \sum_{n=-\infty}^{\infty} C_n |n\rangle \tag{25}$$

the Schrödinger equation corresponding to the Hamiltonian (1) becomes

$$\begin{aligned} xC_n &= \tfrac{1}{2}(C_{n+1} + C_{n-1}) \qquad \text{for all } n \neq l, l+1 \\ xC_{l+1} &= \tfrac{1}{2}(\alpha' C_l + C_{l+2}) \\ (x-\delta)C_l &= \tfrac{1}{2}(C_{l-1} + \alpha' C_{l+1}). \end{aligned} \tag{26}$$

If we propose

$$C_n \begin{cases} e^{q(n-1)} & \text{if } n \leqslant l \\ \omega\, e^{-q(n-l-1)} & \text{if } n \geqslant l+1 \end{cases} \tag{27}$$

with parameters q and ω, then

$$q = \begin{cases} q^+ & \text{for } x = X^+ \\ q^- + i\pi & \text{for } x = X^- \end{cases} \tag{28}$$

where

$$q^{\pm} = \ln\left[\pm\frac{\alpha'}{\omega^{\pm}}\right] \tag{29}$$

$$\omega^{\pm} = \frac{1}{\alpha'}[-\delta \pm \sqrt{\delta^2 + \alpha'^2}] \tag{30}$$

$$X^{\pm} = \frac{1}{2}\left(\frac{\alpha'}{\omega^{\pm}} + \frac{\omega^{\pm}}{\alpha'}\right). \tag{31}$$

Therefore

$$X^{\pm} = \pm\cosh(q^{\pm}). \tag{32}$$

Now the physical meaning of the restrictions on the parameters (α', δ) (equation (24)) becomes clear. It can be seen from (29) and (30) that these restrictions ensure the localized character of the solutions given by (27), i.e. $q^{\pm} > 0$.

We see immediately from (32) that the localization length $1/q^{\pm}$ diverges at the band edges with an inverse power law whose exponent is $\frac{1}{2}$. This kind of behaviour can be observed in other one-dimensional localization problems [11].

The density of states per site, for energies inside the band, is given by

$$\rho(x, m) = \mp\frac{1}{\pi}\,\mathrm{Im}\{G^{\pm}(m, m)\}. \tag{33}$$

From (21) we obtain

$$\rho(x, l+n) = \frac{1}{2\pi V_0\sqrt{1-x^2}}\left\{1+\frac{1}{\Omega}\left(\sqrt{1-x^2}(\gamma x+\delta)\sin(2n\phi(x))\right.\right.$$
$$\left.\left.-[(1-x^2)\gamma+\gamma^2+\delta(\delta+2\gamma x)\cos(2n\phi(x))]\right)\right\} \tag{34}$$

if $n \leqslant 0$, and

$$\rho(x, l+n) = \frac{1}{2\pi V_0\sqrt{1-x^2}}\left\{1-\frac{1}{\Omega}[\sqrt{1-x^2}(\gamma x-\delta(1-2x^2+2\gamma+2x\delta))\right.$$
$$\times\sin(2(n-1)\phi(x))$$
$$+(\gamma(1-x^2+\gamma)+\delta(\delta+2\gamma x+2(1-x^2)(x-\delta)))$$
$$\left.\times\cos(2(n-1)\phi(x))]\right\} \tag{35}$$

if $n \geqslant 1$, where

$$\Omega = (1-x^2)(1+2\gamma)+\gamma^2+\delta(\delta+2\gamma x) \tag{36}$$

and $\phi(x)$ satisfies: $\cos\phi(x) = x$, $\sin\phi(x) = +\sqrt{1-x^2}$.

In figure 3 we show $\rho(x, l)$ and $\rho(x, l+1)$ for α and δ following the path depicted in figure 1 ($\delta = 3/8$). Note that the DOS per site diverges at the band edges when the localized states appear, i.e. when the path reaches the parabolic frontiers ($\delta = \pm\gamma$). From (34) and (35) we get the asymptotic behaviour of $\rho(x, m)$ at the band edges $|z| \to 1$:

$$\rho(x, m) \sim \begin{cases} \sqrt{\dfrac{1+x}{1-x}} & \text{if } \delta = -\gamma \\ \sqrt{\dfrac{1-x}{1+x}} & \text{if } \delta = \gamma. \end{cases} \tag{37}$$

The total density of states results

$$\rho(x) = \rho_0(x)\,\frac{(1-x^2)(1+2\gamma)-\gamma+\delta(\delta-(1-\gamma)x)}{(1-x^2)(1+2\gamma)+\gamma^2+\delta(\delta+2\gamma x)}. \tag{38}$$

Following [12], a resonance eigenstate centred at the energy X_r (X_r belonging to the band) exist if

$$\mathrm{Re}\{\Theta^{+}(X_r)\} = 0 \tag{39}$$

and

$$\Gamma = 2V_0\,\frac{\mathrm{Im}\{\Theta^{+}(X_r)\}}{\mathrm{d}/\mathrm{d}x\,\mathrm{Re}\{\Theta^{+}(X_r)\}} > 0 \tag{40}$$

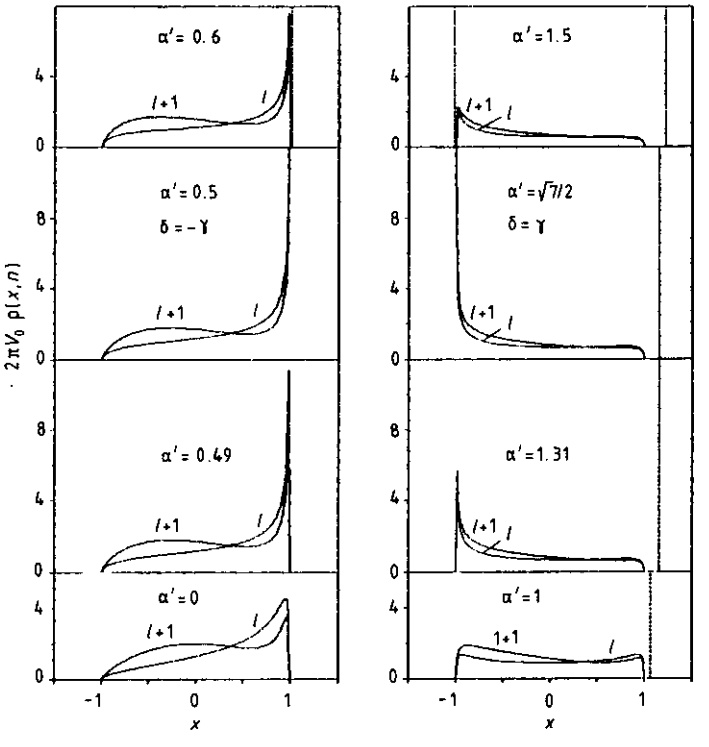

Figure 3. DOS per site $\rho(x, n)$ for the sites $n = l, l+1$ versus x for different values of (α', δ) over the path depicted in figure 2 ($\delta = \frac{3}{8}$). For $\alpha' = 0.5, \sqrt{7}/2$ the path crosses the parabolic curves and a discrete level is split off the band (vertical broken lines).

where Γ is called the width of the resonance state. From (20) we obtain

$$\Theta^{\pm}(x) = 1 + \gamma \pm i \frac{x(\gamma + \delta)}{\sqrt{1-x^2}}. \tag{41}$$

It is immediate that the resonance state does not exist. It is interesting to compare this with the problem of a chain with two diagonal impurities located at the lth and mth sites with strengths ε_1 and ε_2 respectively. From (9) we get in this case

$$\Theta = 1 - (\varepsilon_1 + \varepsilon_2)F + \varepsilon_1 \varepsilon_2 F^2 (1 - \rho^{|l-m|}). \tag{42}$$

If we consider $m = l+1$ then

$$\Theta^{+} = 1 - \frac{\delta_1 \delta_2}{1+x} + i \frac{\delta_1 + \delta_2 - \delta_1 \delta_2}{\sqrt{1-x^2}}$$

with $\delta_i = \varepsilon_i / 2V_0$, $i = 1, 2$. So it is possible to find a resonance eigenstate centred at the energy $X_r = \delta_1 \delta_2 - 1$ with width

$$\Gamma = 2V_0 \frac{\delta_1 + \delta_2 - \delta_1 \delta_2}{\sqrt{(2/\delta_1 \delta_2) - 1}}$$

if $0 < \delta_1 \delta_2 < 2$ and $\Gamma > 0$.

We now consider a more complex situation: The semi-infinite chain with mixed impurities, where

$$\mathbf{H}_0 = \varepsilon_0 \sum_{n=-\infty}^{0} |n\rangle\langle n| + V_0 \sum_{n=-\infty}^{0} [|n-1\rangle\langle n| + |n\rangle\langle n-1|] \tag{43}$$

$$\mathbf{H}_I = \varepsilon |0\rangle\langle 0| + (V'' - V_0)[|-1\rangle\langle 0| + |0\rangle\langle -1|] \tag{44}$$

i.e., the diagonal impurity ε' is located at the end of the chain (site 0), and the off-diagonal impurity V'' is the hopping constant between the sites 0 and -1.

Using the expansion (25) for the localized eigenfunctions with $n \leqslant 0$ we obtain

$$C_n \begin{cases} \Omega & \text{if } n = 0 \\ e^{q(n+1)} & \text{if } n \leqslant -1 \end{cases} \tag{45}$$

with q given by (28) and

$$q^{\pm} = \ln[\pm\alpha''\Omega^{\pm}] \tag{46}$$

$$\Omega^{\pm} = \frac{1}{\alpha''}[\delta \pm \sqrt{\delta^2 + \alpha''^2 - 1}] \tag{47}$$

where $\alpha'' \equiv V''/V_0$. Then we re-obtain (32). The condition of localization $q^{\pm} > 0$ results in

$$\begin{aligned} &X^+ \text{ is a solution if } \delta > 1 - \tfrac{1}{2}\alpha''^2 \\ &X^- \text{ is a solution if } \delta < \tfrac{1}{2}\alpha''^2 - 1. \end{aligned} \tag{48}$$

As a particular case we consider the semi-infinite chain with only a diagonal impurity $\alpha'' = 1$. This problem has only one localized state with $\Omega = 2\delta$ for $|\delta| > \frac{1}{2}$. The energy of this state will be above or below the band according to the sign of δ. The corresponding inverse of the localization length is $q = \ln(2|\delta|)$.

The semi-infinite chain problem is equivalent to the infinite chain with mixed impurities after taking $\alpha' = 0$. For example, for the end site of the chain (taking $l = 0$ and $\alpha' = 0$ in (34)) we obtain for the DOS per site

$$\rho(x, 0) = \frac{\sqrt{1 - x^2}}{4\pi V_0[\frac{1}{4} + \delta(\delta - x)]}. \tag{49}$$

Again we have the singular behaviour given by (37) of the DOS per site at the band edges when the localized state appears.

Some of the results obtained for the one-dimensional model are also present in lattices of higher dimension. It is worth noting that the parabolic curves in the parameter-space (α', δ), like the ones depicted in figure 1, are present for many Bravais lattices. A localized state appears at the band edge when one crosses one of these curves, that is to say the equation $\Theta(x) = 0$ has a solution at one of the band edges. As long as the matrix elements of the Green function $\mathbf{G}_0$ are finite at the band edges (square lattice in $d = 2$, sc and bcc lattices in $d = 3$, etc) (8) shows that the equation $\Theta(x) = 0$ gives the parabolic shape of the curves.

In order to fix ideas we will consider from now on a simple cubic lattice. The TB band for the homogeneous problem at the sc lattice is located in the interval $|x| \leqslant 3$. To calculate Θ from (8) we choose the origin of the lattice as the impure site $\boldsymbol{l} = (0, 0, 0)$ and we take $\boldsymbol{\delta} = (1, 0, 0)$. The diagonal elements of $\mathbf{G}_0$ are given by

$$\langle \boldsymbol{R}|\mathbf{G}_0(x)|\boldsymbol{R}\rangle = \frac{1}{2V_0}\mathscr{F}(x) \tag{50}$$

where $\mathcal{F}(x)$ is the dimensionless diagonal matrix element of the Green function for the sc lattice usually tabulated [13]. The non-diagonal element present in (8) can be expressed as [4]

$$\langle(1,0,0)|\mathbf{G}_0(x)|(0,0,0)\rangle = \frac{1}{2V_0}\left[\frac{x}{3}\mathcal{F}(x) - \frac{1}{3}\right] \tag{51}$$

so that

$$\Theta(x) = 1 - \delta\mathcal{F}(x) - \alpha\left[\frac{x}{3}\mathcal{F}(x) - \frac{1}{3}\right] - \frac{\alpha^2}{4}\mathcal{F}(x)^2 + \frac{\alpha^2}{4}\left[\frac{x}{3}\mathcal{F}(x) - \frac{1}{3}\right]^2 \tag{52}$$

where $\alpha \equiv V/V_0 = \alpha' - 1$. The parabolic curves in the parameters space for the sc lattice are given by

$$\delta = \pm\frac{1}{g}\left[1 - \alpha\left(g - \frac{1}{3}\right) - \frac{\alpha^2}{12}\left(2g - \frac{1}{3}\right)\right] \tag{53}$$

where $g = \mathcal{F}(x=3)$. For $x > 3$ ($x < -3$) the equation $\Theta(x) = 0$ has at most one root above (below) the band. From the general asymptotic behaviour of $\mathbf{g}_0(z)$ [3] we see that $\lim_{x\to\pm\infty}\theta(x) = 1$, thus the sign of Θ at the band edge determines if a localized state exists, i.e. for $\Theta(x=3) < 0$ ($\Theta(x=-3) < 0$) we have localized state with energy X^+ (X^-) above (below) the band. Then we can distinguish the same kind of regions in the parameter space as in the one dimensional model. In figure 4 we show a numerical calculation of the energy of the localized eigenstate for two values of δ.

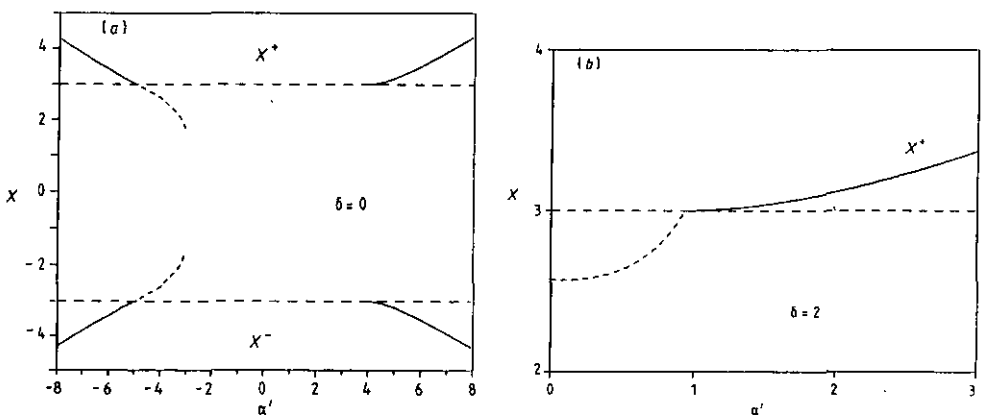

Figure 4. Normalized energy x for the localized (full lines) and resonant (broken lines) eigenstates for the sc lattice. The band is located at $|x| \leqslant 3$. (*a*) $\delta = 0$, (*b*) $\delta = 2$.

For the sc lattice we find that the equation $\mathrm{Re}\{\Theta\} = 0$ will have solutions inside the band depending on the values of the parameters α' and δ. For determined regions in the parameter space some of these solutions correspond to resonance eigenstates, according to the condition (40). We find that a resonance eigenstate appears at the band edge together with a localized eigenstate and goes to the centre of the band when varying α' and keeping δ constant; see the broken lines in figure 4. All the numerical results were done with the Chebyshev approximate formulas for $\mathcal{F}(x)$ [13].

Fruitful discussions with G A Raggio and D P Prato are acknowledged. This work was partially supported by grant PID 641/90 and 1707/90 from Consejo Provincial de Investigaciones Científicas y Technológicas de Córdoba (Argentina).

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