

A Green's Function Analysis of Defect States in Periodic Hamiltonians

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December 1, 2004

1.1 Introduction

In this report, I discuss the Green's function method applied to a periodic lattice described by the tight-binding Hamiltonian. I first discuss the homogeneous solution in a 1D, 2D, and 3D perfect periodic lattice, and then describe the more complex problem involving an impurity potential, which gives rise to bound and resonant (scattering) states. I calculate the eigenstates and eigenfunctions explicitly for a Green's function of the cubic lattice, and discuss the nature of the bound and resonant states in this system. Finally, I look at how the formalism can be developed in the context of Maxwell's equations, as I am interested in studying defect states in photonic crystals. The principal reference for the material was Economou's book on Green's functions, Ch. 1-6 [1].

To give a brief review, the Green's function satisfies the equation of motion,

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}(t)\right)\hat{G}(t, t_0) = \delta(t - t_0), \quad (1.1)$$

and, as we know, is given by,

$$\hat{G}(E) = \frac{1}{E - \hat{H} + i\eta} = \sum_n \frac{|n\rangle\langle n|}{E - E_n + i\eta} \quad (1.2)$$

The poles of the Green's function correspond to the spectrum of eigenenergies of the Hamiltonian, E_n , and the eigenfunctions are related to the residues. Moreover, as we shall see, the density of states (DOS) is given by the imaginary part of the Green's function. Therefore, if we know the Green's function, we have a handle on the essential physics of the problem.

1.2 Green's functions for tight-binding Hamiltonians

1.2.1 One-dimensional result

The one-dimensional (1D) tight-binding Hamiltonian is defined as

$$\hat{H} = \sum_{n=1}^N \varepsilon_0 |n\rangle\langle n| - t \sum_{n=1}^N (|n\rangle\langle n+1| + |n+1\rangle\langle n|), \quad (1.3)$$

where ε_0 is an on-site energy, and t is the hopping energy to nearest neighbours. This model can be used to describe a periodic chain of atoms whose atomic orbitals weakly overlap with their neighbours. In the first question of Problem Set 1, we found that the continuous spectrum of energies in the band is given by

$$E(k) = \varepsilon_0 - 2t \cos(ka). \quad (1.4)$$

The corresponding Green's function is

$$G(n_2, n_1; E) = \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dk \frac{e^{ik(n_2 - n_1)a}}{E - \varepsilon_0 + 2t \cos(ka) + i\eta}, \quad (1.5)$$

with solution

$$G(n_2, n_1; E) = \frac{-i}{2t\sqrt{1-x^2}} (x - i\sqrt{1-x^2})^{|n_2 - n_1|}, \quad (1.6)$$

where

$$x = \frac{E - \varepsilon_0}{2t} \quad (1.7)$$

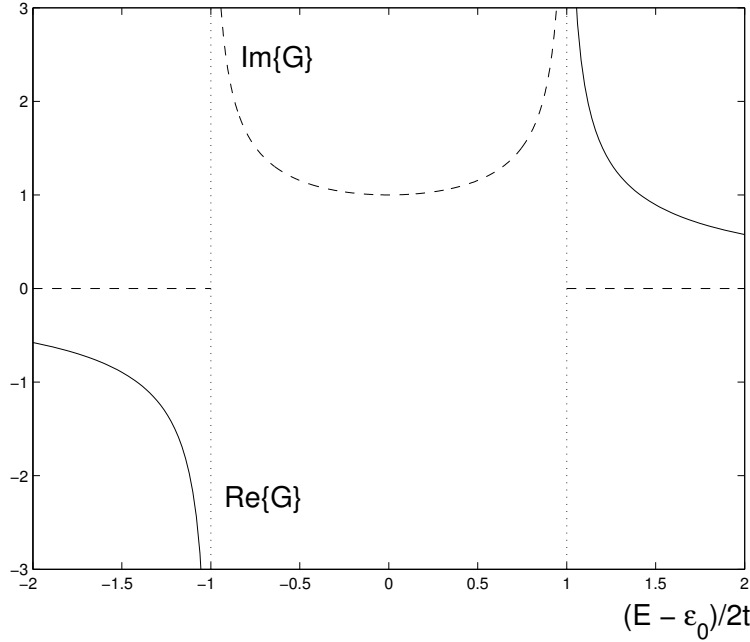


Figure 1.1: 1D tight-binding Green's function. The spectrum extends from $-1 < x < 1$.

The energy spectrum is defined by the band $-1 < x < 1$. The real and imaginary parts of the diagonal matrix element ($n_2 = n_1$) for the 1D Green's function are plotted in Figure 1.1. Note that the function is purely imaginary within the band, and outside the band, where $|x| > 1$, $G(n, n; E)$ is real. Both real and imaginary parts have square root singularities at the band edges, which is typical of a 1D system.

1.2.2 Two dimensional result

The 2D tight-binding Green's function for a square lattice is directly analogous to (1.5), except \vec{k} is now the vector $\vec{k} = k_x \hat{x} + k_y \hat{y}$. It is given by

$$G(\vec{l}, \vec{m}; E) = \frac{a^2}{(2\pi)^2} \int_{\text{1BZ}} d^2\vec{k} \frac{e^{i\vec{k}(\vec{l}-\vec{m})}}{E - \varepsilon_0 + i\eta - 2t[\cos(k_x a) + \cos(k_y a)]} \quad (1.8)$$

where $\vec{l} = l_x \hat{x} + l_y \hat{y}$, $\vec{m} = m_x \hat{x} + m_y \hat{y}$, and l_x, l_y, m_x, m_y are integers. The integral is over the 1st Brillouin zone, defined by $-\pi/a \leq k_x, k_y < \pi/a$. To find the solution, we start by keeping only the even terms in the integral, since the domain is symmetric:

$$G(\vec{l}, \vec{m}; E) = \frac{a^2}{\pi^2} \int_0^{\pi/a} dk_x \int_0^{\pi/a} dk_y \frac{\cos((l_x - m_x)k_x a) \cos((l_y - m_y)k_y a)}{E - \varepsilon_0 + i\eta - 2t[\cos(k_x a) + \cos(k_y a)]}. \quad (1.9)$$

An arbitrary matrix element $G(\vec{l}, \vec{m}; E)$ can be determined through recurrence relations in terms of the diagonal elements, $G(\vec{l}, \vec{l}; E)$ [2]. Along the diagonal, the numerator in (1.9) is 1, and using the sum and difference trigonometric identities, we can convert the sum into a product of cosines in the denominator:

$$G(\vec{l}, \vec{m}; E) = \frac{1}{\pi^2} \int_0^{\pi/a} dk_x \int_0^{\pi/a} dk_y \frac{1}{E - \varepsilon_0 + i\eta - 4t[\cos((k_x - k_y)/2a) \cos((k_x + k_y)/2a)]}, \quad (1.10)$$

This function can be expressed in terms of the elliptic integral of the first kind, which is defined as:

$$\mathbb{K}(\lambda) = \int_0^\pi \frac{d\phi}{(1 - \lambda^2 \cos^2 \phi)^{1/2}}. \quad (1.11)$$

So eqn. (1.10) becomes [2]:

$$G(\vec{l}, \vec{l}; E) = \frac{2}{\pi(E - \varepsilon_0)} \mathbb{K}\left(\frac{4t}{E - \varepsilon_0}\right), \quad |E - \varepsilon_0| > 4t \quad (1.12)$$

This expression holds for energies outside the band, where $\hat{G}(E)$ is real. But for E within the band, i.e. $|E - \varepsilon_0| < 4t$, $E \rightarrow E + i\eta$, so we must use the analytic continuation of \mathbb{K} , defined as [2]

$$\mathbb{K}(1/k) = k[\mathbb{K}(k) + i\mathbb{K}(\sqrt{1 - k^2})]. \quad (1.13)$$

Within the continuum, the real and imaginary parts of the Green's function are

$$\begin{aligned} \text{Re}\{G(\vec{l}, \vec{l}; E)\} &= -\frac{2}{\pi(4t)} \mathbb{K}\left(\frac{E - \varepsilon_0}{4t}\right), & -4t < E - \varepsilon_0 < 0 \\ \text{Re}\{G(\vec{l}, \vec{l}; E)\} &= \frac{2}{\pi(4t)} \mathbb{K}\left(\frac{E - \varepsilon_0}{4t}\right), & 0 < E - \varepsilon_0 < 4t \\ \text{Im}\{G(\vec{l}, \vec{l}; E)\} &= -\frac{2}{\pi(4t)} \mathbb{K}\left(\sqrt{1 - (E - \varepsilon_0)^2/(4t)^2}\right), & |E - \varepsilon_0| < 4t \end{aligned} \quad (1.14)$$

This rather cumbersome series of expressions is more easily appreciated in graphical form, as shown in Figure 1.2. The real part has a discontinuity when $E = \varepsilon_0$, and diverges logarithmically at the band edges. The imaginary part diverges at $E = \varepsilon_0$, and is discontinuous at the band edges.

1.2.3 Simple cubic lattice

The diagonal matrix element of the Green's function for the simple cubic lattice is the 3D generalization of the 2D result given in (1.8):

$$G(\vec{l}, \vec{m}; E) = \frac{a^2}{(2\pi)^3} \int_{-\pi/a}^{\pi/a} dk_x \int_{-\pi/a}^{\pi/a} dk_y \int_{-\pi/a}^{\pi/a} dk_z \frac{1}{E - \varepsilon_0 + i\eta - 2t[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]} \quad (1.15)$$

where again the integrals are over the 1st Brillouin zone, defined by $-\pi/a \leq k_x, k_y, k_z < \pi/a$.

The result is again in terms of elliptic functions:

$$G(l, l; E) = \frac{1}{2\pi^2 t} \int_0^{\pi/a} dk_1 v \mathbb{K}(v), \quad (1.16)$$

where

$$v = 4t/(E - \varepsilon_0 + i\eta - 2t \cos(k_1 a)). \quad (1.17)$$

For many purposes, one is mainly interested in the qualitative behaviour of the Green's functions, particularly at the band edges, and so it is convenient to approximate this result with an expression

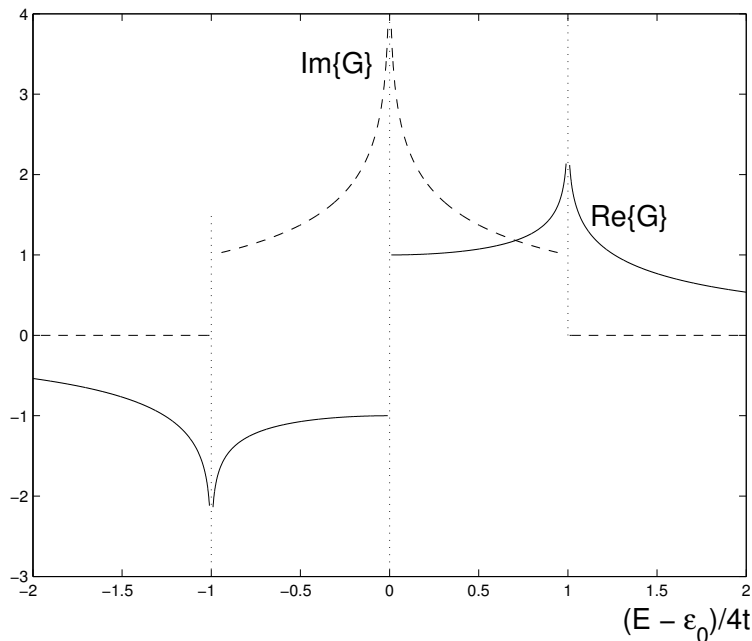


Figure 1.2: 2D tight-binding Green's function.

which has the correct analytic behaviour at the band edges, and gives one state per site. An approximate Green's function, which is plotted in Figure 1.3, is given by:

$$G(\vec{l}, \vec{l}; E) = \frac{2}{E - \varepsilon_0 + i\eta + \sqrt{(E - E_0)^2 - (6t)^2}}, \quad (1.18)$$

where the sign of $\sqrt{(E - E_0)^2 - (6t)^2}$ is negative for $(E - E_0)/6t < -1$. The main feature not reproduced in the approximation is the presence of van Hove singularities (kinks) within the band of the exact result. We shall do a quantitative analysis of this approximation in Section 1.4.

1.3 Single Impurity Scattering

In this section, I describe in detail a calculation to determine the eigenstates of a single impurity in a tight-banding Hamiltonian. The formalism generalizes to any dimension.

1.3.1 Finding the Green's function

Suppose we have a Hamiltonian,

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \quad (1.19)$$

where the unperturbed part, \hat{H}_0 , is the tight-binding Hamiltonian

$$\hat{H}_0 = \sum_m |m\rangle \varepsilon_0 \langle m| + V \sum_{nm} |n\rangle \langle m|, \quad (1.20)$$

and the perturbation due to the impurity potential at site $|l\rangle$ is

$$\hat{H}_1 = |l\rangle \varepsilon \langle l|. \quad (1.21)$$

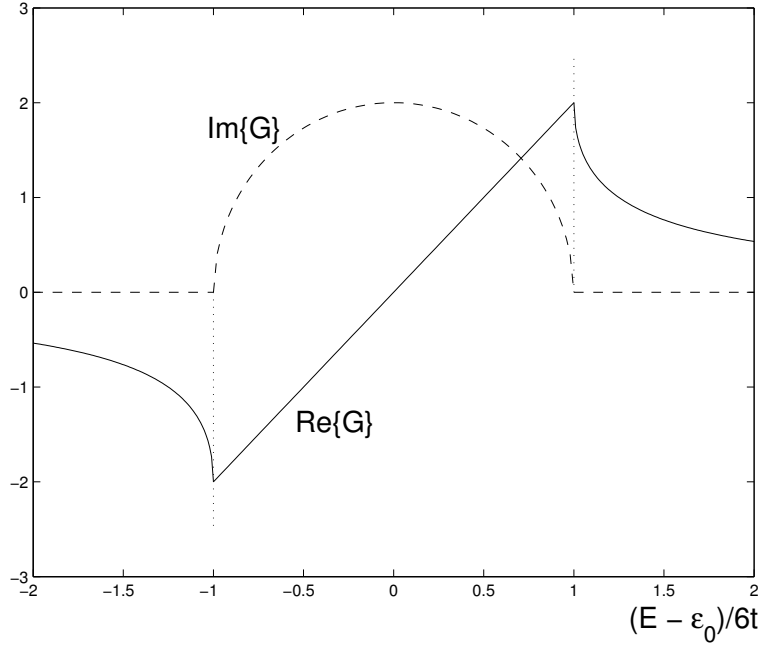


Figure 1.3: Approximate Green's function for the 3D tight-binding Hamiltonian

The Green's function (1.2) can be expressed in terms of the unperturbed (or free particle) Green's function, $\hat{G}_0(E) = 1/(E - \hat{H}_0 + i\eta)$, according to Dyson's equation:

$$\hat{G}(E) = \hat{G}_0(E) + \hat{G}(E)\hat{V}\hat{G}_0(E) \quad (1.22)$$

or, with the aid of the T-matrix, as we saw in Problem Set 4,

$$\hat{G}(E) = \hat{G}_0(E) + \hat{G}_0(E)\hat{T}(E)\hat{G}_0(E) \quad (1.23)$$

The T-matrix has a Dyson-like equation of its own:

$$\hat{T}(E) = \hat{H}_1 + \hat{H}_1\hat{G}_0(E)\hat{H}_1 + \hat{H}_1\hat{G}_0(E)\hat{H}_1\hat{G}_0(E)\hat{H}_1 + \dots \quad (1.24)$$

The advantage of using the T-matrix formalism is that, once the T-matrix is known, the Green's function can be computed directly. And with knowledge of the Green's function, we can compute the excitation spectrum, and more importantly, the density of states.

By substituting for H_1 , we get

$$T = |l\rangle\varepsilon\langle l| + |l\rangle\varepsilon\langle l|\hat{G}_0|l\rangle\varepsilon\langle l| + |l\rangle\varepsilon\langle l|\hat{G}_0|l\rangle\varepsilon\langle l|\hat{G}_0|l\rangle\varepsilon\langle l| + \dots \quad (1.25)$$

$$= |l\rangle\varepsilon\{1 + \varepsilon G_0(l, l; E) + [\varepsilon G_0(l, l; E)]^2 + \dots\}\langle l| \quad (1.26)$$

$$= |l\rangle\frac{\varepsilon}{1 - \varepsilon G_0(l, l; E)}\langle l| \quad (1.27)$$

where we have used the notation $G_0(l, l; E) = \langle l|\hat{G}_0(E)|l\rangle$.

This gives the Green's function

$$\hat{G}(E) = \hat{G}_0(E) + \hat{G}_0(E)\hat{T}(E)\hat{G}_0(E) \quad (1.28)$$

$$= \hat{G}_0(E) + \hat{G}_0(E)|l\rangle\frac{\varepsilon}{1 - \varepsilon G_0(l, l; E)}\langle l|\hat{G}_0(E) \quad (1.29)$$

The poles of $\hat{G}(E)$ are given by the real value

$$G_0(l, l; E_p) = 1/\varepsilon. \quad (1.30)$$

These poles must be bound states lying outside the energy band, as $G_0(l, l; E)$ is complex within the band.

1.3.2 Eigenstates

The eigenstates can be found from a calculation at each pole E_n of the residue, which, from the definition (1.2), is given in the \vec{r} -representation by

$$\text{Res}(G(\vec{r}, \vec{r}'; E_n)) = \sum_n \langle \vec{r} | n \rangle \langle n | \vec{r}' \rangle = \sum_{i=1}^p \phi_i(\vec{r}) \phi_i^*(\vec{r}'), \quad (1.31)$$

where the last sum is over the p degenerate eigenstates of the bound state.

To determine the degeneracy, we can integrate the residue of the diagonal matrix element $G(\vec{r}, \vec{r}; E_p)$ at the pole:

$$f_p = \int d^3\vec{r} \text{Res}(G(\vec{r}, \vec{r}; E_p)) \quad (1.32)$$

For the tight-binding model, where the basis states are localized to lattice sites $|n\rangle$, the degeneracy is

$$f_p = \sum_n \text{Res}(G(n, n; E_p)) \quad (1.33)$$

To progress further with the calculation of the Residue, we can expand the denominator in (1.29) for energies very near to the pole. So,

$$\begin{aligned} 1 - \varepsilon G_0(l, l; E - E_p + E_p) &= 1 - \varepsilon G_0(l, l; E_p) - \varepsilon(E - E_p)G'_0(l, l; E_p) \\ &= -\varepsilon(E - E_p)G'_0(l, l; E_p) \end{aligned} \quad (1.34)$$

The matrix element $\langle n | \hat{G}(E) | m \rangle$ from (1.29) is thus

$$G(n, m; E_p) = G(n, m; E_p) - \frac{G_0(n, l; E_p)G_0(l, m; E_p)}{(E - E_p)G'_0(l, l; E_p)} \quad (1.35)$$

which has a residue

$$\text{Res}(G(n, m; E_p)) = -\frac{G_0(n, l; E_p)G_0(l, m; E_p)}{G'_0(l, l; E_p)} \quad (1.36)$$

The degeneracy can now be calculated:

$$f_p = -\frac{1}{G'_0(l, l)} \sum_n G_0(n, l)G_0(l, n) \quad (1.37)$$

$$= -\frac{1}{G'_0(l, l)} \sum_n [G_0(n, n)]^2 \quad (1.38)$$

$$= -\frac{(E - H + i\eta)^{-2}}{G'_0(l, l; E_p)} \quad (1.39)$$

But note that, from the definition (1.2),

$$\frac{dG(n, n; E)}{dE} = - \left(\frac{1}{E - H + i\eta} \right)^2 \quad (1.40)$$

so

$$f_p = 1. \quad (1.41)$$

This shows that the degeneracy of the bound state in the tight-binding Hamiltonian is 1.

We can now determine the discrete eigenstate $|b_n\rangle$ at the pole E_p , using equation (1.31) for the complete states. An arbitrary matrix element can be written

$$\sum_n \langle n' | b_n \rangle \langle b_n | m' \rangle = \text{Res}\{G(n', m'; E_p)\}, \quad (1.42)$$

so, from (1.36),

$$\sum_n |b_n\rangle = \frac{G_0(E_p)|l\rangle}{\sqrt{-G'_0(l, l; E_p)}} \quad (1.43)$$

We can now rewrite the localized eigenstate in terms of the basis of eigenstates $|n\rangle$:

$$|b\rangle = \sum_n b_n |n\rangle, \quad (1.44)$$

where

$$b_n = \frac{G_0(n, l; E_p)|l\rangle}{\sqrt{-G'_0(l, l; E_p)}} \quad (1.45)$$

The denominator is assured of being real, since $G'_0(l, l; E_p)$ is negative for E outside the band of states, according to (1.40).

Thus we have determined the bound state energy, the degeneracy, and the eigenfunctions of the impurity state.

1.3.3 Density of States (and origin of the bound state)

The density of states of a system with energy levels denoted by E_n is given by

$$\rho(E) = \sum_n \delta(E - E_n) \quad (1.46)$$

This can be related to the imaginary part of the Green's function, using the identity

$$\lim_{\eta \rightarrow 0} \frac{1}{x + i\eta} = P(1/x) - i\pi\delta(x). \quad (1.47)$$

In the case of the unperturbed Green's function, $G_0(E)$, $x = E - E_n$, so we can find the DOS as follows:

$$-\frac{1}{\pi} \text{Im}\{G(n, n; E)\} = \sum_n \delta(E - E_n) = \rho(E). \quad (1.48)$$

In the \vec{r} -representation,

$$\rho(\vec{r}, E) = \sum_k |\langle \vec{r} | \vec{k} \rangle|^2 \delta(E - E_k) \quad (1.49)$$

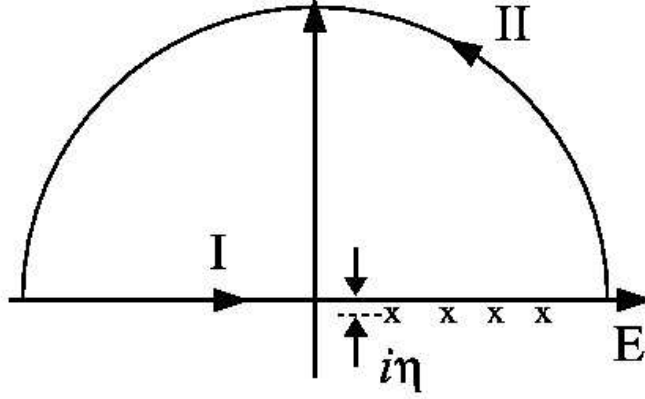


Figure 1.4: Two integration contours (I and II) for DOS expression, where x marks the positions of the poles of the continuous spectrum

Using eqn. (1.29) for the Green's function, we can write the partial DOS (“partial” in the sense that it refers to a specific site n), directly:

$$\rho(n; E) = \rho_0(n; E) - \frac{\text{Im}}{\pi} \left\{ \frac{\varepsilon \langle n | G_0(E) | l \rangle \langle l | G_0(E) | n \rangle}{1 - \varepsilon G_0(l, l; E)} \right\} \quad (1.50)$$

At the impurity site $|l\rangle$, the DOS is given by

$$\begin{aligned} \rho(l, E) &= -\frac{1}{\pi} \text{Im} \left\{ G(l, l; E) + \frac{\varepsilon [G_0(l, l; E)]^2}{1 - \varepsilon G_0(l, l; E)} \right\} \\ &= -\frac{1}{\pi} \frac{\rho_0(l; E)}{|1 - \varepsilon G_0(l, l; E)|^2} \end{aligned} \quad (1.51)$$

The integral of the DOS $\rho(n; E)$ over all energies should yield 1; to check this, we can use Cauchy's theorem on the contour I shown in Fig. 1.4. Because I and II define a simply closed contour, Cauchy's theorem says that the contour integral of an analytic function along I and II should be 0. We observe that $\lim_{E \rightarrow \infty} G_0(E) \rightarrow 1/E$ (see (1.2)). As a result, from (1.29), $\lim_{E \rightarrow \infty} G(E) \rightarrow 1/E$ as well. Therefore,

$$\int_{-\infty}^{\infty} \rho(n; E) dE \equiv -\frac{\text{Im}}{\pi} \left\{ \int_{-\infty}^{\infty} G(n, n; E) dE \right\} = -\frac{1}{\pi} \lim_{E \rightarrow \infty} \text{Im} \left\{ \int_{II} \frac{dE}{E} \right\} \quad (1.52)$$

By making the substitution $E = Re^{i\theta}$, and integrating from $\theta = \pi$ to 0, the last integral in the brackets $\{ \}$ in (1.52) is $-i\pi$. Therefore,

$$\int_{-\infty}^{\infty} \rho(n; E) dE = 1. \quad (1.53)$$

We can now make use of the result 1.49 to separate the DOS as follows:

$$\int_{E_l}^{E_u} \rho(n; E) dE + \sum_p |\langle n | b_n \rangle|^2 = 1, \quad (1.54)$$

where E_l and E_u refer to the lower and upper energies bounding the band. By virtue of our equation for the localized eigenstates (1.45), this can be written

$$\int_{E_l}^{E_u} \rho(n; E) dE + \sum_p |b_n|^2 = 1. \quad (1.55)$$

Summing over n sites, and using $N(E)$ to denote the total DOS, N to be the number of lattice sites, and P the number of poles, this can be rewritten:

$$\int_{E_l}^{E_u} N(E) dE + P = N. \quad (1.56)$$

Since there is one state in the Hilbert space for each of the N lattice sites, this shows that the bound states are formed at the expense of the continuum. The impurity site plucks a state from the continuum, and, as (1.54) shows, receives a weight from each continuum site $|n\rangle$ according to the overlap $|b_n|^2$ of the discrete state with the site $|n\rangle$.

1.3.4 Scattering eigenstates

Assuming a Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$, the wavefunctions $|\psi\rangle$ are determined by the time-independent Schrodinger equation

$$(E - \hat{H}_0)|\psi\rangle = \hat{H}_1|\psi\rangle. \quad (1.57)$$

The general solution is

$$|\psi\rangle = |\psi_0\rangle + \hat{G}_0(E)\hat{H}_1|\psi\rangle. \quad (1.58)$$

where $|\psi_0\rangle$ is the solution to $(E - \hat{H}_0)|\psi_0\rangle = 0$. By iterating this self-consistent equation, we get the wavefunction in terms of the free particle Green's function and the T-matrix:

$$|\psi\rangle = |\psi_0\rangle + \hat{G}_0(E)\hat{T}(E)|\psi_0\rangle. \quad (1.59)$$

In the continuum, the scattering eigenstates are Bloch states, given by

$$|\vec{k}\rangle = \frac{1}{\sqrt{N}} \sum_l e^{i\vec{k}\cdot\vec{l}} |\vec{l}\rangle, \quad (1.60)$$

and so eqn. (1.59) is

$$|\psi\rangle = |\vec{k}\rangle + \hat{G}_0(E)\hat{T}(E)|\vec{k}\rangle. \quad (1.61)$$

In the \vec{r} -representation, the amplitude of probability of finding the particle at \vec{r} is (using (1.27):

$$\langle \vec{r} | \psi \rangle = \langle \vec{r} | \vec{k} \rangle + \frac{\langle \vec{r} | \hat{G}_0(E) | \vec{l} \rangle \varepsilon \langle \vec{l} | \vec{k} \rangle}{1 - \varepsilon G_0(\vec{l}, \vec{l}; E)}. \quad (1.62)$$

The amplitude of probability at the impurity site, \vec{l} , is

$$\langle \vec{l} | \psi \rangle = \frac{\langle \vec{l} | \vec{k} \rangle}{1 - \varepsilon G_0(\vec{l}, \vec{l}; E)}. \quad (1.63)$$

In scattering theory, the scattering cross section $|f|^2$ is proportional to $|\langle \vec{k}_f | T(E) | \vec{k}_i \rangle|^2$, where the T-matrix connects an incident state $|\vec{k}_i\rangle$ to a final scattered state $|\vec{k}_f\rangle$. Using our expression for T (1.27), the scattering cross section is thus proportional to (see Economou pp.61-62):

$$|f|^2 \propto \frac{\varepsilon^2}{|1 - \varepsilon G_0(\vec{l}, \vec{l}; E)|^2} \quad (1.64)$$

Inside the band, $G_0(\vec{l}, \vec{l}; E)$ is complex, so the denominator cannot equal 0, but for certain energies, it can become very small, leading to a large enhancement in the wavefunction around the impurity site, $|\vec{l}\rangle$. As we will see in the next section, this can occur in association with a bound state being split off from the continuum.

1.4 Quantitative 3D model

In Section 1.2.3, we proposed the approximate Green's function for the cubic lattice:

$$G_0(l, l; E) = \frac{2}{E - \varepsilon_0 + i\eta + \sqrt{(E - E_0)^2 - B^2}}, \quad (1.65)$$

where $B = 6t$ is half the bandwidth. To find the unperturbed density of states, note that within the band, the square root is imaginary. Multiplying the top and bottom by the complex conjugate of the denominator and taking the imaginary part gives

$$\rho_0(E) = \Theta(B - |E - \varepsilon_0|) \frac{2\sqrt{B^2 - (E - \varepsilon_0)^2}}{\pi B^2}. \quad (1.66)$$

From (1.51), the DOS at the impurity site in the band is

$$\begin{aligned} \rho(l, E) &= \frac{\rho_0}{\left|1 - 2\varepsilon \left(E + i\sqrt{B^2 - E^2}\right)^{-1}\right|^2} \\ &= \frac{\rho_0}{1 - 4\varepsilon E/B^2 + 4\varepsilon^2/B^2} \\ &= \frac{2}{\pi B} \left\{ \frac{\sqrt{1 - E^2/B^2}}{1 - 4\varepsilon E/B^2 + 4\varepsilon^2/B^2} \right\}, \end{aligned} \quad (1.67)$$

where we have set $\varepsilon_0 = 0$ for clarity.

If we let $y = B\rho(l, E)$ and $x = (E - \varepsilon_0)/B$, the DOS at the impurity site within the band is given by

$$y = \frac{2}{\pi} \left\{ \frac{\sqrt{1 - x^2}}{1 + 4x\alpha + 4\alpha^2} \right\}, \quad (1.68)$$

where $\alpha = -\varepsilon/B$ is the strength of the impurity potential.

This function is plotted for a range of α in Figure 1.5. As the impurity potential increases, states are pushed down towards the band edge, where they peak and form a resonant state. At a critical value of 0.5, they form a pole and a discrete level is split from the continuum into the gap. Above this value, the pole moves further from the band edge (not shown), and the resonant state diminishes in strength.

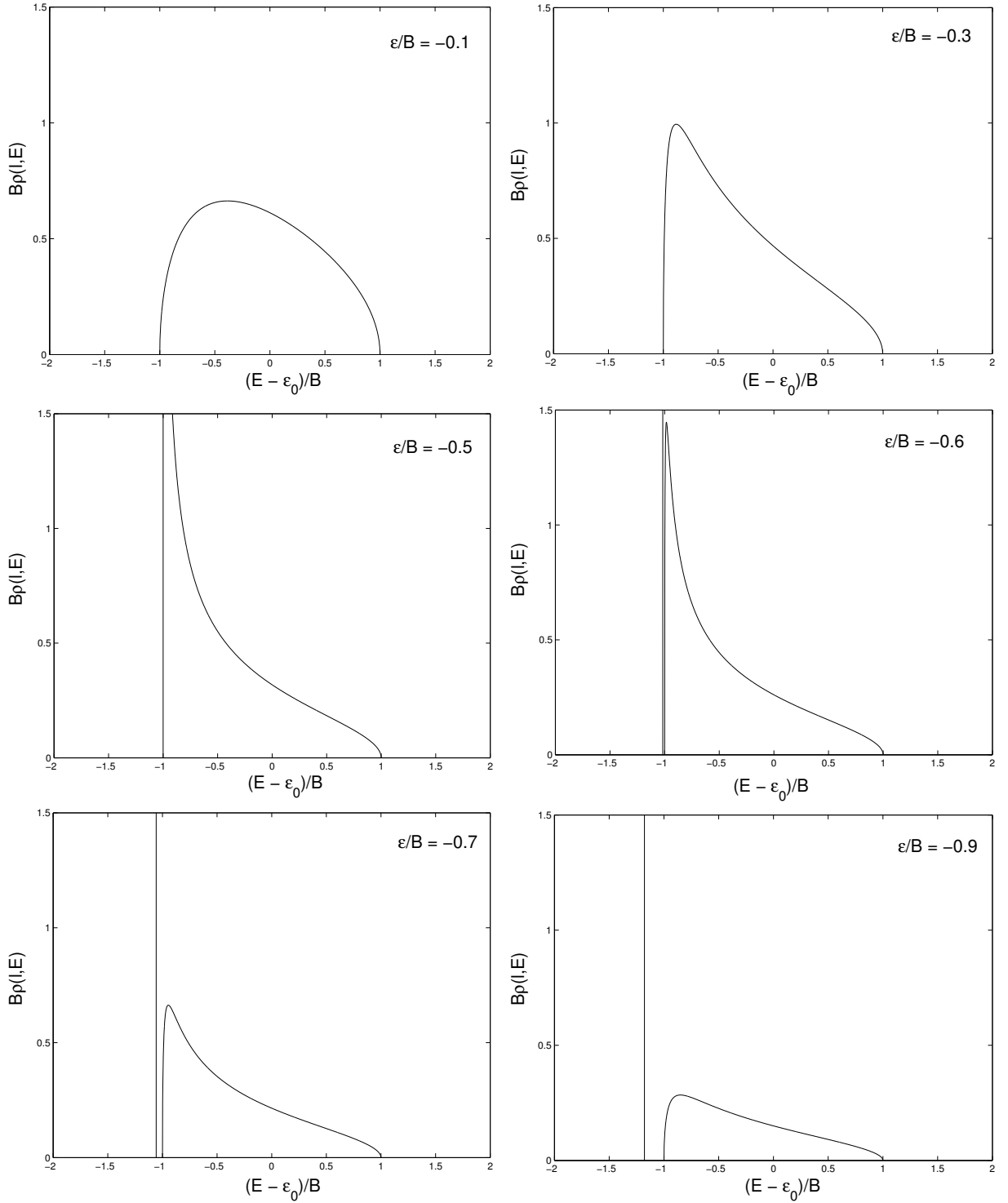


Figure 1.5: Impurity DOS $\rho(\vec{l}; E)$ as a function of energy for a range of attractive impurity potential strengths. The energy band extends from $-1 < (E - \epsilon_0)/B < 1$. The DOS clusters towards the lower band edge as $-\epsilon/B$ increases from 0.1 to 0.5. At this threshold, a bound state is split off from the continuum.

The resonant peak in the DOS (1.68) can be found by differentiation to be

$$E_r = \frac{4\varepsilon B^2}{B^2 + 4\varepsilon^2}. \quad (1.69)$$

Similarly, we can find the energy of the pole outside the band, where both E and $G_0(l, l; E) = 2/(E + \sqrt{E^2 - B^2})$ are real. Solving $G_0(l, l; E) = 1/\varepsilon$ yields

$$E_p = \frac{4\varepsilon^2 + B^2}{4\varepsilon} \quad (1.70)$$

The trajectories of E_r and E_p as a function of impurity strength are shown in Figure 1.6. There is no bound solution E_p for $\varepsilon/B > -0.5$, as was also evident from the DOS plotted in Fig. 1.5. For impurity potentials stronger than this threshold, a bound state is split off from the continuum, and as the potential increases, both E_r and E_p diverge steadily away from E_l .

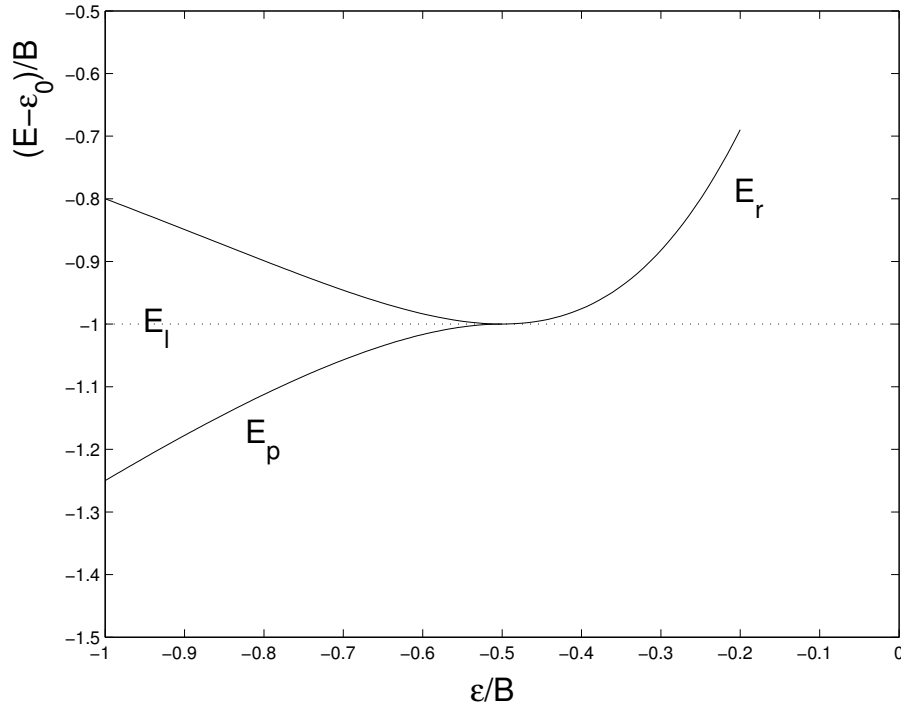


Figure 1.6: Resonant (E_r) and bound (E_p) state energy trajectories as a function of impurity strength. The lower band edge is marked E_l . At the threshold $\varepsilon/B = -0.5$, the bound and resonant state energies coincide.

1.5 Application to Maxwell's equations

My interest in the theory of defect states in a periodic Hamiltonian stems from my research into defect states in photonic crystals, which we are currently designing and fabricating in Ampel. In this section I will introduce the general and 2D photonic Green's function for dielectric materials.

The derivation is very similar to the electronic case, except now we are dealing with vector wave equations derived from Maxwell's equations rather than the Schrodinger equation. It is always

useful to start with the Maxwell's equations, so for completeness, I write them here:

$$\vec{\nabla} \cdot \vec{D}(\vec{r}, t) = 0 \quad (1.71)$$

$$\vec{\nabla} \cdot \vec{B}(\vec{r}, t) = 0 \quad (1.72)$$

$$\vec{\nabla} \times \vec{E}(\vec{r}, t)(\vec{r}, t) = -\frac{\partial \vec{B}(\vec{r}, t)}{\partial t} = -\mu_0 \frac{\partial \vec{H}(\vec{r}, t)}{\partial t} \quad (1.73)$$

$$\vec{\nabla} \times \vec{H}(\vec{r}, t)(\vec{r}, t) = \frac{\partial \vec{D}(\vec{r}, t)}{\partial t} = \epsilon_0 \epsilon(\vec{r}) \frac{\partial \vec{E}(\vec{r}, t)}{\partial t} \quad (1.74)$$

Solving equations 1.73 and 1.74 for either $\vec{E}(\vec{r}, t)$ or $\vec{H}(\vec{r}, t)$ gives the two wave equations:

$$\frac{1}{\epsilon(\vec{r})} \vec{\nabla} \times \{ \vec{\nabla} \times \vec{E}(\vec{r}, t) \} = -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} \vec{E}(\vec{r}, t) \quad (1.75)$$

$$\vec{\nabla} \times \left\{ \frac{1}{\epsilon(\vec{r})} \vec{\nabla} \times \vec{H}(\vec{r}, t) \right\} = -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} \vec{H}(\vec{r}, t), \quad (1.76)$$

where the speed of light in vacuum is

$$c = \frac{1}{\sqrt{\epsilon_0 \mu_0}} \quad (1.77)$$

1.5.1 Hermitian operator and eigenfunctions

If we define the Hamiltonian for eqn. (1.75) by

$$\hat{H} = \frac{1}{\sqrt{\epsilon(\vec{r})}} \vec{\nabla} \times \left(\vec{\nabla} \times \frac{1}{\epsilon(\vec{r})} \right) \quad (1.78)$$

and define a complex vector function

$$\vec{Q}(\vec{r}, t) = \sqrt{\epsilon(\vec{r})} \vec{E}(\vec{r}, t), \quad (1.79)$$

equation 1.75 can be rewritten as

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} + H \right) \vec{Q}(\vec{r}, t) = 0. \quad (1.80)$$

The Hamiltonian is not chosen as the differential operator from (1.75), because this operator is not Hermitian. Accordingly, its eigenfunctions $\vec{E}(\vec{r}, t)$ are neither complete nor orthogonal. The eigenfunctions corresponding to the Hermitian operator \hat{H} defined in (1.78) are given by (1.79). They are normalized by

$$\int_V d\vec{r} \vec{Q}_{kn}^{\alpha*}(\vec{r}) \cdot \vec{Q}_{k'n'}^{\beta}(\vec{r}) = V \delta_{\alpha\beta} \delta_{\vec{k}\vec{k}'} \delta_{nn'} \quad (1.81)$$

where $\alpha, \beta = T$ or L , for transverse or longitudinal. The only physical solutions to the wave equations in free space are transverse. In a dielectric such as a photonic crystal, the spatial variation of $\epsilon(\vec{r})$ mixes the solutions, so we can only describe the solutions as quasi-transverse and quasi-longitudinal. As in free space, the longitudinal solutions in the dielectric are unphysical, in that they do not

satisfy the first Maxwell equation 1.71. However, they are important in the following definition of completeness of the eigenfunctions:

$$\sum_{\vec{k}n} \vec{Q}_{\vec{k}n}^T(\vec{r}) \otimes \vec{Q}_{\vec{k}n}^{T*}(\vec{r}') + \sum_{\vec{k}n} \vec{Q}_{\vec{k}n}^L(\vec{r}) \otimes \vec{Q}_{\vec{k}n}^{L*}(\vec{r}') = V \mathbb{1} \delta(\vec{r} - \vec{r}') \quad (1.82)$$

The longitudinal solutions satisfy

$$\hat{H} \vec{Q}_{\vec{k}n}^L(\vec{r}) = 0 \quad (1.83)$$

and the transverse solutions

$$\hat{H} \vec{Q}_{\vec{k}n}^T(\vec{r}) = \frac{\omega_{\vec{k}n}^{(T)2}}{c^2} \vec{Q}_{\vec{k}n}^T(\vec{r}) \quad (1.84)$$

1.5.2 Green's Function

The operator and basis of eigenfunctions just introduced for Maxwell's equations leads to a retarded Green's function defined by

$$-\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} + \hat{H}\right) \vec{G}(\vec{r}, \vec{r}', t - t') = \mathbb{1} \delta(\vec{r} - \vec{r}') \delta(t - t'), \quad (1.85)$$

which is very similar to the equation of motion for fermionic Green's functions, except that it is a wave equation instead of Schrodinger's equation. The (linear) photonic case is simpler than the electronic case in that the photons are non-interacting. However, the problem is made more complex by the vectorial nature of the fields.

It is important to remember why we develop the Green's function formalism. The Green's function solves the homogeneous Maxwell's equations assuming a delta-function source term. Armed with the Green's function, it is easy to solve for the real fields $\vec{E}(\vec{r}, t)$, which are subject to the inhomogeneous equation

$$-\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} + \hat{H}\right) \vec{E}(\vec{r}, t) = f(\vec{r}), \quad (1.86)$$

because

$$\vec{E}(\vec{r}, t) = \int G(\vec{r}, \vec{r}', t - t') f(\vec{r}') d\vec{r}'. \quad (1.87)$$

Carrying on with our analysis, the Fourier transform of (1.85), using the usual definition we used in class, is

$$\left(\frac{\omega^2}{c^2} - \hat{H}\right) G(\vec{r}, \vec{r}', \omega) = \mathbb{1} \delta(\vec{r} - \vec{r}'). \quad (1.88)$$

We can find the Green's function in ω -space by rewriting (1.88), and expanding $\mathbb{1}$ in a complete set of states, according to (1.82):

$$\begin{aligned} G(\vec{r}, \vec{r}', \omega) &= \frac{\mathbb{1}}{\omega^2/c^2 - \hat{H}} = \frac{c^2 \sum_{\vec{k}} |Q_{\vec{k}}\rangle \langle Q_{\vec{k}}|}{\omega^2 - \omega_{\vec{k}}^2} \\ &= \frac{c^2}{V} \sum_{\vec{k}n} \left[\frac{\vec{Q}_{\vec{k}n}^T(\vec{r}) \otimes \vec{Q}_{\vec{k}n}^{T*}(\vec{r}')}{(\omega - \omega_{\vec{k}n}^T + i\delta)(\omega + \omega_{\vec{k}n}^T + i\delta)} + \frac{\sum_{\vec{k}n} \vec{Q}_{\vec{k}n}^L(\vec{r}) \otimes \vec{Q}_{\vec{k}n}^{L*}(\vec{r}')}{(\omega + i\delta)^2} \right] \end{aligned} \quad (1.89)$$

Using the residue theorem, it is easy to show that in the time domain, (1.89) becomes

$$G(\vec{r}, \vec{r}', t - t') = -\frac{c^2}{V} \sum_{\vec{k}n} \left\{ \frac{\sin \omega_{\vec{k}n}^T t}{\omega_{\vec{k}n}^T} \vec{Q}_{\vec{k}n}^T(\vec{r}) \otimes \vec{Q}_{\vec{k}n}^{T*}(\vec{r}') + t \vec{Q}_{\vec{k}n}^L(\vec{r}) \otimes \vec{Q}_{\vec{k}n}^{L*}(\vec{r}') \right\} \quad (1.90)$$

For 2-D photonic crystals, such as I am interested in for my research, the argument proceeds exactly as above, except we consider only in-plane \vec{r} and \vec{k} , denoted by \vec{r}_{\parallel} and \vec{k}_{\parallel} . We are usually interested in TE-like solutions, for which the \vec{E} -field is in-plane, so this plays the role of the transverse solutions in the general case, and there are no longitudinal solutions. The 2D TE-polarized Green's function is given by

$$G^{(2)}(\vec{r}_{\parallel}, \vec{r}_{\parallel}', t, t') = -\Theta(t - t') \frac{c^2}{V} \sum_{\vec{k}_{\parallel n}} \frac{\sin \omega_{\vec{k}_{\parallel n}}^E t}{\omega_{\vec{k}_{\parallel n}}^E} \vec{Q}_{z, \vec{k}_{\parallel n}}(\vec{r}_{\parallel}) \otimes \vec{Q}_{z, \vec{k}_{\parallel n}}^*(\vec{r}_{\parallel}'). \quad (1.91)$$

1.6 References

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