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2003 J. Phys. A: Math. Gen. 36 9827

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Floquet–Green function formalism for harmonically driven Hamiltonians

D F Martinez

Center for Statistical Mechanics, The University of Texas at Austin, 1 University Station, C1609
Austin, TX 78712-0264, USA

Received 2 July 2003, in final form 31 July 2003

Published 10 September 2003

Online at stacks.iop.org/JPhysA/36/9827

Abstract

A method is proposed for the calculation of the Floquet–Green function of a general Hamiltonian with harmonic time dependence. We use matrix continued fractions to derive an expression for the ‘dynamical effective potential’ that can be used to calculate the Floquet–Green function of the system. We demonstrate the formalism for the simple case of a space-periodic (in the tight-binding approximation) Hamiltonian with a defect whose on-site energy changes harmonically with time. We study the local density of states for this system and the behaviour of the localized states as a function of the different parameters that characterize the system.

PACS numbers: 73.21.–b, 73.23.–b, 72.10.–d, 32.80.–t

1. Introduction

The study of the effect of periodic driving in a system is almost as old as physics. The study of resonance, as it occurs in so many different physical systems, from musical instruments to planetary motion, plays a central role in the development of classical mechanics. With the discovery of electromagnetic induction and Maxwell’s equations, a description of the interaction between matter and electromagnetic radiation became possible; once again, central to this description lies the understanding of the effects of a harmonic drive in the atomic states. Furthermore, in the field of solid state, a microscopic description of electrons inside a crystal requires the study of the effect on the electron motion due to vibrations in the atomic potentials (phonons). These vibrations, which have a well defined frequency, can be thought to act, within a certain approximation (classical approximation), as a harmonically driven (HD) potential in the electron Hamiltonian (our method can also be used for the quantum solution of this problem, where the vibrations are treated as harmonic oscillator modes). The study of HD Hamiltonians is therefore of significant importance because of the enormous field of applications in solid state, atomic physics and many other fields. Despite their obvious relevance, theoretical studies of HD Hamiltonians have been traditionally perturbative, with

only lowest-order effects having been considered. With technological advances, high strength HD fields have become more accessible and provide us with the possibility of new applications, for which perturbative approaches are increasingly difficult to use.

In the last two decades, HD potentials have been studied considerably and many interesting effects have been found theoretically (and some have been observed experimentally) such as dynamical localization (mini-band collapse) [1, 2], photon-assisted tunnelling [3], quantum Hamiltonian ratchets [4, 5], chaos-assisted tunnelling [6–11] and atom stabilization [12]. They have also been used to study quantum tunnelling time [13–15], ionization [16, 17], electronic transmission [18–22] and quantum chaos [23].

The pioneering work of Shirley [24], Zel'dovich [25] and in particular the work of Sambe [26] laid down the theoretical foundations for a complete treatment of time-periodic potentials, based on the same mathematical tools already developed for time-independent potentials. Of great importance among these tools is the Green function, whose definition and application for time-periodic systems has not been clear until recently. A Floquet–Green function method for the solution of radiative electron scattering in a strong laser field was introduced by Faisal [27]. More recently, the $t-t'$ method [28] for treating time-dependent systems was developed with great success. For the case of a periodic potential, this formalism provides a natural way of defining and using the Floquet–Green function which can be used to study scattering through this kind of potential [28]. For the case of a harmonic driving (HD) potential, we find the Floquet Hamiltonian and derive the Floquet–Green function of the system using matrix continued fractions (MCF). This same approach can be used to derive the Green function of a phonon-coupled system, given the close resemblance between these two systems [29, 30]. It has in fact been used for the case of a two state system coupled to a harmonic oscillator [31].

As an application of our method, we calculate the Floquet–Green function for a system whose Hamiltonian is periodic in space (we use the tight-binding approximation) and has a defect at a particular location in the lattice. We characterize the defect by its on-site energy, which changes harmonically in time as $V_0 + V_1 \cos(\omega t)$. This Hamiltonian could be realized experimentally in a 1D heterostructure where a metal contact has been placed covering a small region and is connected to an oscillating voltage source. We also believe that the problem of conduction through a molecule placed between two metal contacts could be modelled with a similar Hamiltonian.

In section 2 we introduce the Floquet Hamiltonian and the Floquet–Green function for a time-periodic system. In section 3 we derive the Floquet–Green function for the case of a HD potential using matrix continued fractions. In section 4, as an illustration of the technique developed in section 3, we study a tight-binding Hamiltonian with a defect energy which depends harmonically on time. We calculate the local density of states (LDOS) and study the existence of localized states and their behaviour as a function of the different parameters of the model. Finally, in section 5, we make some concluding remarks.

2. $t-t'$ method and Floquet–Green function

In our approach we use the (t, t') method [28] where the time variable t' is treated as a spatial coordinate, and a new quasi-time variable t is introduced. Using this approach we derive the expression for the Floquet–Green function of a general time-periodic system.

We introduce the Floquet Hamiltonian, H^F , which is defined as

$$H^F(x, t') = H(x, t') - i\hbar \frac{\partial}{\partial t'} \quad (1)$$

and the (t, t') -Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \chi(x, t, t') = H^F(x, t') \chi(x, t', t). \tag{2}$$

It is easy to show that if $\chi(x, t', t)$ satisfies equation (2), then

$$\phi(x, t) \equiv \chi(x, t, t) \tag{3}$$

is a solution to the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \phi(x, t) = H(x, t) \phi(x, t). \tag{4}$$

The great advantage of the $t-t'$ method is that, since the Hamiltonian (equation (2)) is independent of t , $\chi(x, t', t)$ can be found using the standard techniques developed for the time-independent Hamiltonian. For example, calculation of the time propagator of the system can then be performed without any time-ordering procedures.

By using the method of separation of variables, we can write

$$\chi(x, t, t') = e^{-i\epsilon t/\hbar} \psi(\epsilon|x, t') \tag{5}$$

and using this into equation (2) gives a t -independent Schrödinger equation

$$H^F(x, t') \psi(\epsilon|x, t') = \epsilon \psi(\epsilon|x, t') \tag{6}$$

As a consequence of Floquet’s theorem, if $H(x, t')$ is periodic in t' (period τ), $\psi(\epsilon|x, t')$ is also periodic in t' . We define the Green function corresponding to this Floquet Hamiltonian as

$$[\epsilon - H^F(x, t')] G^F(\epsilon|x, x', t', t'') = \delta(x - x') \delta_\tau(t' - t'') \tag{7}$$

where $\delta_\tau(x)$ is the τ -periodic delta function. Because of the periodicity of the Hamiltonian, the Floquet eigenfunctions as defined by equation (6) are periodic in time. The solution of equation (7) can be written as

$$G^F(\epsilon|x, x', t', t'') = \int d\epsilon' \sum_n \frac{\psi_n^*(\epsilon'|x, t') \psi_n(\epsilon'|x', t'')}{\epsilon - \epsilon'} \tag{8}$$

where $\{\psi_n(\epsilon'|x, t)\}$ is the complete set of eigenfunctions of the Floquet–Hamiltonian (equation (6)). From this expression it can be seen that $G^F(\epsilon|x, x', t', t'')$ is periodic in both t' and t'' ; therefore, it can be written as

$$G^F(\epsilon|x, x', t', t'') = \sum_{\alpha, \beta=-\infty}^{\infty} G_{\alpha, \beta}^F(\epsilon|x, x') e^{i\alpha t'} e^{-i\beta t''}. \tag{9}$$

Similarly for $H^F(x, t')$, we write

$$H^F(x, t') = \sum_{\gamma=-\infty}^{\infty} H_{\gamma}^F(x) e^{i\gamma t'}. \tag{10}$$

Using equations (9) and (10) in (7) and equating components, we get

$$\epsilon G_{\alpha, \beta}^F(\epsilon|x, x') - \sum_{\gamma=-\infty}^{\infty} H_{\alpha, \gamma}^F(x) G_{\gamma, \beta}^F(\epsilon|x, x') = \delta(x - x') \delta_{\alpha, \beta} \tag{11}$$

where $H_{\alpha, \gamma}^F \equiv H_{\alpha-\gamma}^F$.

In the next section we specialize equation (11) for the case of a HD Hamiltonian. We will use the method of MCF to derive an explicit solution for the Floquet–Green function assuming a potential that depends harmonically on time.

3. Harmonically driven potential and matrix continued fraction method

The Hamiltonian that we consider in this section is of the general form (with no particular representation chosen),

$$\mathcal{H} = \mathcal{H}^o + \mathcal{V}_o + 2\mathcal{V}_1 \cos(\omega t'). \quad (12)$$

This general class of Hamiltonians includes a great variety of physical systems of interest. We refer to this class of Hamiltonians as HD Hamiltonians. In section 4 we will apply the methods developed here to a simple but nonetheless interesting system: a tight-binding model with a defect on-site energy that depends harmonically on time. According to equations (1) and (10) and the definition after equation (11), the Floquet Hamiltonian corresponding to equation (12) is

$$\mathcal{H}_{\alpha,\gamma}^F = (\mathcal{H}^o + \mathcal{V}_o - \alpha\hbar\omega)\delta_{\alpha,\gamma} + \mathcal{V}_1(\delta_{\alpha+1,\gamma} + \delta_{\alpha-1,\gamma}). \quad (13)$$

Using this in equation (11), we get

$$(1E_\alpha - \mathcal{H}^S)\mathcal{G}_{\alpha,\beta} - \mathcal{V}_1(\mathcal{G}_{\alpha+1,\beta} + \mathcal{G}_{\alpha-1,\beta}) = 1\delta_{\alpha,\beta} \quad (14)$$

where

$$E_\alpha \equiv \varepsilon + \alpha\hbar\omega \quad \mathcal{H}^S \equiv \mathcal{H}^o + \mathcal{V}_o \quad \langle x|\mathcal{G}_{\alpha,\beta}|x'\rangle \equiv G_{\alpha,\beta}^F(\varepsilon|x, x'). \quad (15)$$

To solve equation (14), we use MCF. It basically follows the procedure introduced by Martinez *et al* [18, 32] which has also been used by Moskalets and Büttiker [33] for the solution of three-term recurrence relations in a HD system. Similar approaches using continued fractions have also been used before in the solution of time-independent Hamiltonians (tight-binding type) [34–36]. To begin, we define the operator

$$\mathcal{F}_{\alpha,\beta} \equiv \mathcal{G}_{\alpha,\beta}\mathcal{G}_{\alpha+1,\beta}^{-1} \quad (16)$$

from which we can write

$$\mathcal{F}_{\alpha,\beta}^{-1}\mathcal{G}_{\alpha,\beta} = \mathcal{G}_{\alpha+1,\beta} \quad \mathcal{F}_{\alpha-1,\beta}\mathcal{G}_{\alpha,\beta} = \mathcal{G}_{\alpha-1,\beta}. \quad (17)$$

Using these equations in equation (14), we get

$$(1E_\alpha - \mathcal{H}^S)\mathcal{G}_{\alpha,\beta} - (\mathcal{V}_1\mathcal{F}_{\alpha,\beta}^{-1} + \mathcal{V}_1\mathcal{F}_{\alpha-1,\beta})\mathcal{G}_{\alpha,\beta} = 1\delta_{\alpha,\beta}. \quad (18)$$

Let us consider this equation for the case $\alpha \neq \beta$,

$$(1E_\alpha - \mathcal{H}^S)\mathcal{G}_{\alpha,\beta} - (\mathcal{V}_1\mathcal{F}_{\alpha,\beta}^{-1} + \mathcal{V}_1\mathcal{F}_{\alpha-1,\beta})\mathcal{G}_{\alpha,\beta} = 0 \quad \text{for } \alpha \neq \beta. \quad (19)$$

A trivial solution of this equation is $\mathcal{G}_{\alpha,\beta} = 0$, for $\alpha \neq \beta$; that is, the off-diagonal components vanish. This is expected only for the case $V_1 = 0$. For $V_1 \neq 0$ we assume that in general the off-diagonal elements do not vanish (at least not all of them) and therefore, from equation (19), we get

$$1E_\alpha - \mathcal{H}^S = (\mathcal{V}_1\mathcal{F}_{\alpha,\beta}^{-1} + \mathcal{V}_1\mathcal{F}_{\alpha-1,\beta}) \quad \text{for } \alpha \neq \beta. \quad (20)$$

Evaluating this equation for $\alpha = \beta + 1$, we get

$$\mathcal{V}_1\mathcal{F}_{\beta,\beta} = \mathcal{C}_{\beta+1} - \mathcal{V}_1(\mathcal{V}_1\mathcal{F}_{\beta+1,\beta})^{-1}\mathcal{V}_1 \quad (21)$$

where, to simplify notation, we defined $\mathcal{C}_\beta \equiv 1E_\beta - \mathcal{H}^S$. Iterating equation (21), we get

$$\mathcal{V}_1\mathcal{F}_{\beta,\beta} = \mathcal{C}_{\beta+1} - \mathcal{V}_1 \frac{1}{\mathcal{C}_{\beta+2} - \mathcal{V}_1 \frac{1}{\mathcal{C}_{\beta+3} - \mathcal{V}_1 \frac{1}{\ddots} \mathcal{V}_1}} \mathcal{V}_1. \quad (22)$$

Here, the notation $\frac{1}{A}$ instead of A^{-1} has been used for clarity. Evaluating equation (19) for $\alpha = \beta - 1$, we get

$$\begin{aligned}\mathcal{V}_1 \mathcal{F}_{\beta-1,\beta}^{-1} &= \mathcal{C}_{\beta-1} - \mathcal{V}_1 (\mathcal{F}_{\beta-2,\beta} \mathcal{V}_1^{-1}) \mathcal{V}_1 \\ &= \mathcal{C}_{\beta-1} - \mathcal{V}_1 \frac{1}{\mathcal{V}_1 \mathcal{F}_{\beta-2,\beta}^{-1}} \mathcal{V}_1.\end{aligned}\quad (23)$$

Continuing the fraction in an iterative way, we get

$$\mathcal{V}_1 \mathcal{F}_{\beta-1,\beta}^{-1} = \mathcal{C}_{\beta-1} - \mathcal{V}_1 \frac{1}{\mathcal{C}_{\beta-2} - \mathcal{V}_1 \frac{1}{\mathcal{C}_{\beta-3} - \mathcal{V}_1 \frac{1}{\ddots} \mathcal{V}_1}} \mathcal{V}_1. \quad (24)$$

We now rewrite equation (18), for $\alpha = \beta$, as

$$(1E_\beta - \mathcal{H}^S) \mathcal{G}_{\beta,\beta} - (\mathcal{V}_1 (\mathcal{V}_1 \mathcal{F}_{\beta,\beta})^{-1} \mathcal{V}_1 + \mathcal{V}_1 (\mathcal{V}_1 \mathcal{F}_{\beta-1,\beta}^{-1})^{-1} \mathcal{V}_1) \mathcal{G}_{\beta,\beta} = 1. \quad (25)$$

Using equations (22) and (24), we finally get

$$(1E_\beta - \mathcal{H}^S - \mathcal{V}_{\text{eff}}(E_\beta)) \mathcal{G}_{\beta,\beta}(E) = 1 \quad (26)$$

where

$$\mathcal{V}_{\text{eff}}(E_\beta) = \mathcal{V}_{\text{eff}}^\uparrow(E_\beta) + \mathcal{V}_{\text{eff}}^\downarrow(E_\beta) \quad (27)$$

with

$$\begin{aligned}\mathcal{V}_{\text{eff}}^\uparrow(E_\beta) &= \mathcal{V}_1 \frac{1}{\mathcal{C}_{\beta+1} - \mathcal{V}_1 \frac{1}{\mathcal{C}_{\beta+2} - \mathcal{V}_1 \frac{1}{\ddots} \mathcal{V}_1}} \mathcal{V}_1 \\ \mathcal{V}_{\text{eff}}^\downarrow(E_\beta) &= \mathcal{V}_1 \frac{1}{\mathcal{C}_{\beta-1} - \mathcal{V}_1 \frac{1}{\mathcal{C}_{\beta-2} - \mathcal{V}_1 \frac{1}{\ddots} \mathcal{V}_1}} \mathcal{V}_1.\end{aligned}\quad (28)$$

The off-diagonal components of the Floquet–Green function operator can be calculated by repeated multiplication by the operators $\mathcal{V}_{\text{eff}}^\uparrow$ and $\mathcal{V}_{\text{eff}}^\downarrow$.

Equation (26) is very interesting. It gives an expression for the diagonal part of the Floquet–Green function of the system (from which elastic transmission and density of states can be calculated), in which the effect of the coupling between different (Floquet) channels, generated by the HD potential, has been ‘summed up’ into a dynamical effective potential (DEP) that is energy dependent. This general result for the class of HD Hamiltonians is related to the ‘pruning’ technique developed by Haule and Bonča [37] for the treatment of electron–phonon interactions within a tight-binding lattice. Also, Pastawski and Medina [36] have developed a similar method (‘decimation’ technique) for the treatment of electron transport through a molecule.

It is interesting to note from equation (28) that to lowest order in E and \mathcal{V}_1 , $\mathcal{V}_{\text{eff}} = -\mathcal{V}_1 (\mathcal{H}^S)^{-1} \mathcal{V}_1$, which means that the harmonic potential generates an energy-independent DEP which is negative (in general it will lower the energy of the perturbed eigenstates as compared to the energy of the unperturbed ones) and is quadratic in \mathcal{V}_1 . The effect of this quadratic dependence of the effective potential has been reported before regarding the dependence of the transmission zero and pole with the amplitude of the oscillating potential for a δ -function potential [18] and also regarding the dynamics of the quasi-energy bands with lowest average energy in a chain of oscillating δ -function potentials [32]. This lowest-order correction to the potential experienced by a particle in an oscillating potential is similar to the

so-called Franck–Condon energy which is also negative and quadratic in the coupling constant between electrons in a lattice and phonons [38].

It is also worth noticing that our formalism goes beyond any perturbative approach in \mathcal{V}_1 since, even if we truncate the expression for \mathcal{V}_{eff} to lowest order in \mathcal{V}_1 , which gives $\mathcal{V}_{\text{eff}}(E_\beta) \sim \mathcal{V}_1 \left(\frac{1}{\mathcal{C}_{\beta+1}} + \frac{1}{\mathcal{C}_{\beta-1}} \right) \mathcal{V}_1$, the resulting expression for $\mathcal{G}_{\beta,\beta}$ contains all even powers of V_1 . This means that truncation of \mathcal{V}_{eff} to lowest order still gives a Floquet–Green function which includes contributions of an infinite number of diagrams. This feature makes equation (26) an ideal framework for the treatment of very strong HD potentials such as those produced by laser fields where multiphoton processes are common [39], and interesting effects such as atom stabilization have been reported [12].

Finally, we notice that the dependence of any quantity in equation (26) on the index β is only through the ‘channel’ energy $E_\beta = \varepsilon + \beta\hbar\omega$, where the quasi-energy ε (usually taken to be $\varepsilon \in [0, 1]\hbar\omega$) always accompanies the term $\beta\hbar\omega$. Because of this, the index β in E_β will be dropped. E represents the main channel energy, which, for example, for the scattering of a particle through this kind of potential, corresponds to the energy of the incoming particle. We can therefore simplify even further the notation in equation (26):

$$\mathcal{G}^D(E) = \frac{1}{(1E - \mathcal{H}^S - \mathcal{V}_{\text{eff}}(E))} \quad (29)$$

where $\mathcal{G}^D(E) = \mathcal{G}^D(\varepsilon + \alpha\hbar\omega) \equiv \mathcal{G}_{\alpha,\alpha}(\varepsilon)$.

Equation (29) can also be written making use of the Green function corresponding to the time-independent part of the Hamiltonian,

$$\mathcal{G}^D = \mathcal{G}^S \frac{1}{1 - \mathcal{V}_{\text{eff}}(E)\mathcal{G}^S} \quad (30)$$

with

$$\mathcal{G}^S \equiv \frac{1}{1E - \mathcal{H}^S}. \quad (31)$$

4. Tight-binding with defect. HD site-energy case

Electron localization in a crystal due to defects has been studied for many decades. In a space-periodic (time-independent) potential described in the tight-binding approximation, an irregularity in the atomic potential generates a bound state localized in the neighbourhood of the defect [40]. If the energy mismatch between the site-energy of the defect and that of the medium in which it is embedded is V_0 , the energy of the localized state is found to be $\text{sign}(V_0)\sqrt{4T^2 + V_0^2}$, where T is the tunneling parameter and the allowed band of extended states corresponds to energies between $-2T$ and $2T$.

The system we are interested in also couples the electron at the impurity with a HD field. This system is similar to a tight-binding Hamiltonian with a defect that couples the electron states with the degrees of freedom of localized phonons [41]. As previously shown [29], the transmission in these two systems can be derived from a similar set of equations and therefore presents several features in common. The main differences are: (1) the harmonic oscillator spectrum of the phonons is bounded from below, which implies that it is impossible for an electron to gain energy when interacting with a HO in the ground state. For a HD potential, the electron can always gain energy (or lose it). (2) The coupling between a state with the HO in the eigenstate N and a state with a HO state $N + 1$ or $N - 1$ depends on N : for initial electron energy E and initial phonon state N , the probability amplitude to be scattered into the electron state $E - \hbar\omega$ and phonon state $N + 1$ is proportional to $\sqrt{N + 1}$; for

$E + \hbar\omega$ and phonon state $N - 1$ it is \sqrt{N} . This is not the case for the time-periodic field for which these probability amplitudes do not depend on any parameter except the amplitude of the HD field. (3) Phonons are usually due to thermal vibrations, which means that temperature is an additional variable to be considered in electron–phonon coupled systems. It is not a consideration for a HD potential which can be realized only by the application of an external field onto the electron system. Despite these differences, the two systems can be solved in an almost identical way, and the differences can only be attributed to the thermal averaging (necessary in the phonon case) when the oscillator state, before the interaction with the electron, has a large N .

We will now apply the method developed in the last section for the case of a Hamiltonian which has its matrix elements in the site representation given by

$$\mathcal{H} = \mathcal{H}^0 + (V_0 + V_1 \cos(\omega t))|0\rangle\langle 0| \tag{32}$$

with

$$\mathcal{H}^0 \equiv -T \sum_j (|j+1\rangle\langle j| + |j-1\rangle\langle j|) \tag{33}$$

where t is associated with the tunnelling probability between adjacent sites in the lattice, V_0 characterizes the defect on-site energy and V_1 is the amplitude of the external HD field, which is assumed to exist only at the defect site ($j = 0$ site). We have taken the on-site energy throughout the lattice to be zero except at the defect location.

In the notation of equations (12) and (15), we have

$$\mathcal{H}^D = \mathcal{H}^0 + V_0|0\rangle\langle 0| \quad \mathcal{V}_1 = \frac{1}{2}V_1|0\rangle\langle 0|. \tag{34}$$

From this, and using equations (27) and (29) we get

$$\begin{aligned} \mathcal{V}_{\text{eff}}^\uparrow(E) &= \frac{1}{4}V_1^2|0\rangle\langle 0| \frac{1}{C_1(E) - \frac{1}{4}V_1^2|0\rangle\langle 0| \frac{1}{C_2(E) - \frac{1}{4}V_1^2|0\rangle\langle 0| \frac{1}{\vdots} |0\rangle\langle 0|}} |0\rangle\langle 0| \\ &= \frac{1}{4}V_1^2|0\rangle\langle 0| \frac{1}{C_1(E) - |0\rangle\langle 0|\mathcal{V}_{\text{eff}}^\uparrow(E+1)|0\rangle\langle 0|} |0\rangle\langle 0| \\ &= V_{\text{eff}}^\uparrow(E)|0\rangle\langle 0| \end{aligned} \tag{35}$$

where the function $V_{\text{eff}}^\uparrow(E)$ is defined as

$$V_{\text{eff}}^\uparrow(E) \equiv \frac{1}{4}V_1^2\langle 0| \frac{1}{C_1(E) - V_{\text{eff}}^\uparrow(E+1)|0\rangle\langle 0|} |0\rangle. \tag{36}$$

Similarly for $\mathcal{V}_{\text{eff}}^\downarrow(E)$, we get

$$\begin{aligned} \mathcal{V}_{\text{eff}}^\downarrow(E) &= \frac{1}{4}V_1^2|0\rangle\langle 0| \frac{1}{C_{-1}(E) - |0\rangle\langle 0|\mathcal{V}_{\text{eff}}^\downarrow(E-1)|0\rangle\langle 0|} |0\rangle\langle 0| \\ &= V_{\text{eff}}^\downarrow(E)|0\rangle\langle 0| \end{aligned} \tag{37}$$

where the function $V_{\text{eff}}^\downarrow(E)$ is defined as

$$V_{\text{eff}}^\downarrow(E) \equiv \frac{1}{4}V_1^2\langle 0| \frac{1}{C_{-1}(E) - V_{\text{eff}}^\downarrow(E-1)|0\rangle\langle 0|} |0\rangle. \tag{38}$$

Accordingly, the operator $\mathcal{V}_{\text{eff}}(E)$ can be written as

$$\mathcal{V}_{\text{eff}}(E) = V_{\text{eff}}(E)|0\rangle\langle 0| = (V_{\text{eff}}^\downarrow(E) + V_{\text{eff}}^\uparrow(E))|0\rangle\langle 0|. \tag{39}$$

Using this in equation (29), we get

$$\mathcal{G}^D(E) = \frac{1}{(1E - \mathcal{H}^0 - (V_0 + V_{\text{eff}}(E))|0\rangle\langle 0|)}. \quad (40)$$

In terms of the Green function for the operator \mathcal{H}^0 , we write

$$\mathcal{G}^D(E) = \mathcal{G}^0 \frac{1}{(1 - H_1(E)\mathcal{G}^0)} \quad (41)$$

where

$$\mathcal{G}^0 = \frac{1}{(1E - H^0)} \quad \text{and} \quad H_1(E) = (V_0 + V_{\text{eff}}(E))|0\rangle\langle 0| = V(E)|0\rangle\langle 0|. \quad (42)$$

The operator $(1 - H_1(E)\mathcal{G}^0)^{-1}$ can be evaluated easily,

$$\begin{aligned} \frac{1}{(1 - H_1(E)\mathcal{G}^0)} &= 1 + V(E)|0\rangle\langle 0|\mathcal{G}^0 + V(E)^2\mathcal{G}_{0,0}^0|0\rangle\langle 0|\mathcal{G}^0 + \dots \\ &= 1 + \frac{V(E)}{1 - V(E)\mathcal{G}_{0,0}^0}|0\rangle\langle 0|\mathcal{G}^0 \end{aligned} \quad (43)$$

and therefore,

$$\mathcal{G}^D = \mathcal{G}^0 + \frac{V(E)}{1 - V(E)\mathcal{G}_{0,0}^0}\mathcal{G}^0|0\rangle\langle 0|\mathcal{G}^0. \quad (44)$$

In the site representation, this equation reads

$$\mathcal{G}_{i,j}^D = \mathcal{G}_{i,j}^0 + \frac{V(E)}{1 - V(E)\mathcal{G}_{0,0}^0}\mathcal{G}_{i,0}^0\mathcal{G}_{0,j}^0 \quad (45)$$

and for $i = j = 0$, we get

$$\begin{aligned} \mathcal{G}_{0,0}^D &= \mathcal{G}_{0,0}^0 + \frac{V(E)}{1 - V(E)\mathcal{G}_{0,0}^0}\mathcal{G}_{0,0}^0\mathcal{G}_{0,0}^0 \\ &= \frac{\mathcal{G}_{0,0}^0}{1 - V(E)\mathcal{G}_{0,0}^0}. \end{aligned} \quad (46)$$

The only remaining task is to find the function $V(E) = V_0 + V_{\text{eff}}(E)$, with $V_{\text{eff}}(E) = V_{\text{eff}}^\uparrow(E) + V_{\text{eff}}^\downarrow(E)$. Let us begin with $V_{\text{eff}}^\uparrow(E)$ defined in equation (36):

$$\begin{aligned} V_{\text{eff}}^\uparrow(E) &= \frac{1}{4}V_1^2\langle 0|\frac{1}{\mathcal{C}(E+1) - V_{\text{eff}}^\uparrow(E+1)|0\rangle\langle 0|}|0\rangle \\ &= \frac{1}{4}V_1^2\langle 0|\frac{1}{(\mathcal{G}^0(E+1))^{-1} - (V_0 + V_{\text{eff}}^\uparrow(E+1))|0\rangle\langle 0|}|0\rangle \\ &= \frac{1}{4}V_1^2\langle 0|\frac{\mathcal{G}^0(E+1)}{1 - (V_0 + V_{\text{eff}}^\uparrow(E+1))|0\rangle\langle 0|\mathcal{G}^0(E+1)}|0\rangle \end{aligned} \quad (47)$$

this last expression, following the procedure beginning with equation (41), is easily found to give a result very similar to equation (46),

$$\begin{aligned} V_{\text{eff}}^\uparrow(E) &= \frac{1}{4}V_1^2\frac{\mathcal{G}_{0,0}^0(E+1)}{1 - (V_0 + V_{\text{eff}}^\uparrow(E+1))\mathcal{G}_{0,0}^0(E+1)} \\ &= \frac{\frac{1}{4}V_1^2}{(1/\mathcal{G}_{0,0}^0(E+1) - V_0) - V_{\text{eff}}^\uparrow(E+1)}. \end{aligned} \quad (48)$$

Iterating this equation, we get the final expression

$$V_{\text{eff}}^\uparrow(E) = \frac{\frac{1}{4}V_1^2}{(1/\mathcal{G}_{0,0}^0(E+1) - V_0) - \frac{\frac{1}{4}V_1^2}{(1/\mathcal{G}_{0,0}^0(E+2) - V_0) - \frac{\frac{1}{4}V_1^2}{\vdots}}}. \tag{49}$$

Similarly for $V_{\text{eff}}^\downarrow(E)$, we find

$$V_{\text{eff}}^\downarrow(E) = \frac{\frac{1}{4}V_1^2}{(1/\mathcal{G}_{0,0}^0(E-1) - V_0) - \frac{\frac{1}{4}V_1^2}{(1/\mathcal{G}_{0,0}^0(E-2) - V_0) - \frac{\frac{1}{4}V_1^2}{\vdots}}}. \tag{50}$$

For the \mathcal{H}^0 given in equation (33), it is well known that $1/\mathcal{G}_{0,0}^0(E) = \pm\sqrt{E^2 - 4T^2}$ (the sign choice will be discussed later). With this, the Floquet–Green function for the system in equation (32) is completely solved in terms of the parameters (T, V_0, V_1, E) . Explicitly,

$$\mathcal{G}_{0,0}^D(E) = \frac{2/V_1}{a(E) - \frac{2}{V_1}V_{\text{eff}}(E)} \tag{51}$$

where

$$V_{\text{eff}}(E) = \frac{V_1/2}{a(E+1) - \frac{1}{a(E+2) - \frac{1}{\vdots}}} + \frac{V_1/2}{a(E-1) - \frac{1}{a(E-2) - \frac{1}{\vdots}}} \tag{52}$$

and to simplify the notation we defined the function

$$a(E) = \pm \frac{2\sqrt{E^2 - 4T^2}}{V_1} - 2\frac{V_0}{V_1}. \tag{53}$$

The choice in the sign of the function $\pm\sqrt{E^2 - 4T^2}$ is not a trivial one. For a system with perfect spatial periodicity, it is irrelevant; however, our system does not have such periodicity; the presence of the defect potential does force a choice in the sign. One can show that $\mathcal{G}_{0,i}^D = \mathcal{G}_{0,0}^D R_\pm(E)^{|i|}$ where $R_\pm(E) = \frac{E}{2T} \pm \sqrt{(E/2T)^2 - 1}$. When $E > 2T > 0$, $R_+ > 1$ and $R_- < 1$. The first choice (+) is not physical since it gives a Green function that diverges in space; this forces us to choose the negative sign for the square root in the case $E > 2T > 0$. A similar analysis shows that for $E < -2T < 0$, the plus sign in the square root is required. This sign change can be accomplished if we replace $\sqrt{(E/2T)^2 - 1}$ by $(E/2T)\sqrt{1 - (2T/E)^2}$. Using this, the correct form for equation (53) is

$$a(E) = \frac{2E}{V_1} \sqrt{1 - \left(\frac{2T}{E}\right)^2} - 2\frac{V_0}{V_1}. \tag{54}$$

It could be argued that one does not have to bother about taking care of the proper sign in $\mathcal{G}_{0,0}^0(E)$ for $|E| > 2T$ because it is outside the band $-2T < E < 2T$ where there might not even be any states. This is not true because of the possible existence of bound states outside the band (which is clearly the case for $V_0 \neq 0, V_1 = 0$). Another argument is that some of the off-diagonal (in Floquet index) elements of the Floquet–Green function will necessarily have energies outside the band, i.e., if $E = \alpha\hbar\omega$ is inside the band, $E + n\hbar\omega$ is obviously not necessarily in it, and therefore, the matrix elements $\mathcal{G}_{\alpha+n,\alpha}(0, j) = \mathcal{G}_{\alpha+n,\alpha}(0, 0)(1/R(E+n))^j$ when $|E + n\hbar\omega| > 2T$ will not converge as $j \rightarrow \infty$ unless the previously mentioned selection of sign is made for the square root in $R(E+n)$ and $a(E+n)$.

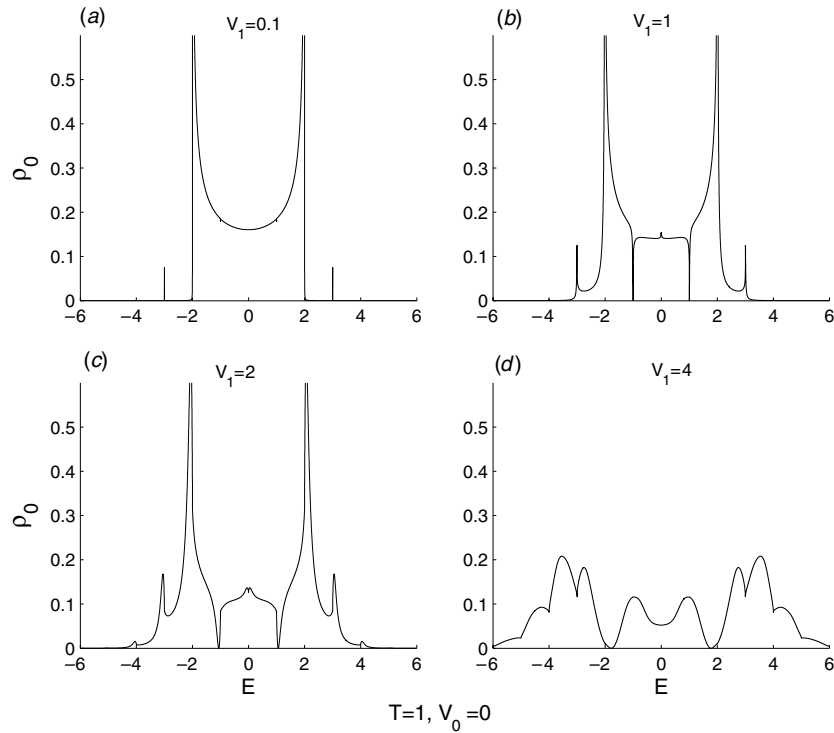


Figure 1. LDOS for a tight-binding Hamiltonian with a defect energy oscillating in time. $T = 1$, $V_0 = 0$ (units of $\hbar\omega$). The width of the band ($4T$) is larger than $\hbar\omega$.

The LDOS at the defect location can be calculated from the diagonal elements of the Green function with the usual formula,

$$\rho_0(E) = \mp \frac{1}{\pi} \text{Im}(\mathcal{G}_{0,0}^D(E \pm i\gamma)). \quad (55)$$

In the derivation of this equation, which relates the density of states to the Green function, it is necessary to include $\pm i\gamma$ in the energy to get the contribution, in the density of states, of the discrete part of the spectrum (poles). In our numerical calculations, $\gamma = 10^{-7}$ unless otherwise specified.

Figure 1 shows a plot of $\rho_0(E)$, for different values of V_1 , where all parameters are given in units of $\hbar\omega$, and $V_0 = 0$, $T = 1$. In (a) it can be seen that the LDOS is very close to the expected LDOS for the static part of the Hamiltonian (\mathcal{H}^0), with the allowed energy band located between $-2T$ and $2T$. As the value of V_1 is increased, one can see some of the eigenstates leaking out of the band and populating the region outside the interval $[-2, 2]$. The first ones to do so are the unperturbed eigenstates in ‘resonance’ with the oscillating potential; that is the ones with energy close to $\pm\hbar\omega$. For $V_1 = 2$ the distribution is even broader with the features of the unperturbed Hamiltonian still recognizable. At $V_1 = 4$ the density of states has significantly spread over the region $-6 < E < 6$. For no value of V_1 do we find any poles (localized states) in the system.

Figure 2 shows the LDOS for $T = 1$, $V_0 = 1$ and various values of V_1 . For a very small V_1 we see the LDOS expected for a tight-binding model with an impurity, where the impurity produces a localized state (pole in the density of states) at an energy $\text{sign}(V_0)\sqrt{4T^2 + V_0^2}$.

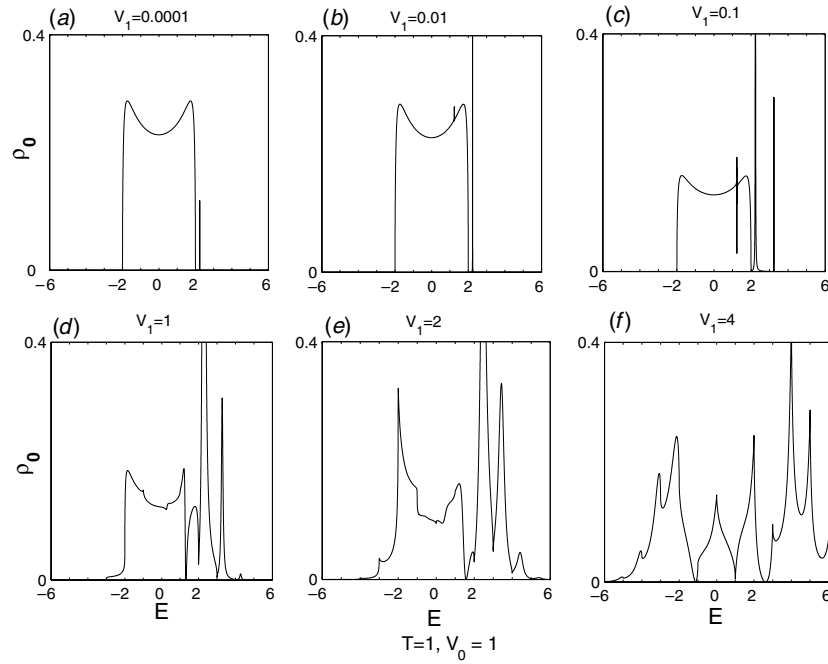


Figure 2. LDOS for different values of the amplitude of the oscillation. As in figure 1, $T = 1$ and the defect has a static on-site energy $V_0 = 1$. No poles were obtained at any value of V_1 .

A ‘pole’ can be seen in (a) at the expected value $\sqrt{4T^2 + V_0^2} = \sqrt{5}$. Closer analysis of this peak near $\sqrt{5}$ reveals that this is actually not a true pole. If this peak in the LDOS were truly a pole, its height should be proportional to $1/\gamma$ and therefore it should go to infinity as $\gamma \rightarrow 0$. For all the values of V_1 shown in figure 2, the height of the peak eventually saturates as γ is made smaller. For $V_1 = 0.0001$ the height as a function of γ saturates for $\gamma = 10^{-11}$; for $V_1 = 0.01$ we get a $\gamma \sim 10^{-7}$. For larger values of V_1 , saturation occurs for even smaller values of γ . This implies that the bound state of the static potential, in the presence of the oscillating potential, acquires a finite lifetime and therefore one can say that the oscillating potential ‘ionizes’ the bound state of the static part of the Hamiltonian.

It has been shown before [17] that, for an attractive δ -function potential, the addition of a time-periodic perturbation to the strength of the δ -function always ‘ionizes’ the bound state. It is actually easy to understand why this is so. The time-periodic perturbation couples the unperturbed Hamiltonian’s bound state (energy E_B) with all the unperturbed states at energies $E_B + n$ (in units of $\hbar\omega$). Clearly, for any E_B there is a value of n above which the unperturbed states will be in the continuum ($E_B + n > 0$). That means that the bound state has a finite probability to transit into those states and escape. Because of this, the resonance associated with it has an intrinsic non-zero width given by the inverse of the lifetime. In our case, in addition to the localized time-independent potential (the V_0 part of the defect energy), we have the tight-binding Hamiltonian, which has a continuum in the energy interval $[-2T, 2T]$. The argument that justifies the absence of a bound state in the δ -function case, applies also for our Hamiltonian: if the width of the energy band of \mathcal{H}^0 ($4T$) is greater than 1 ($\hbar\omega$), irrespective of the energy of the bound state (E_B) associated with V_0 , there will be at least one energy $E_B + n$ (for some n) that will fall inside the extended state band (the continuum). The bound state of the time-independent Hamiltonian, due to the time-harmonic potential, is therefore

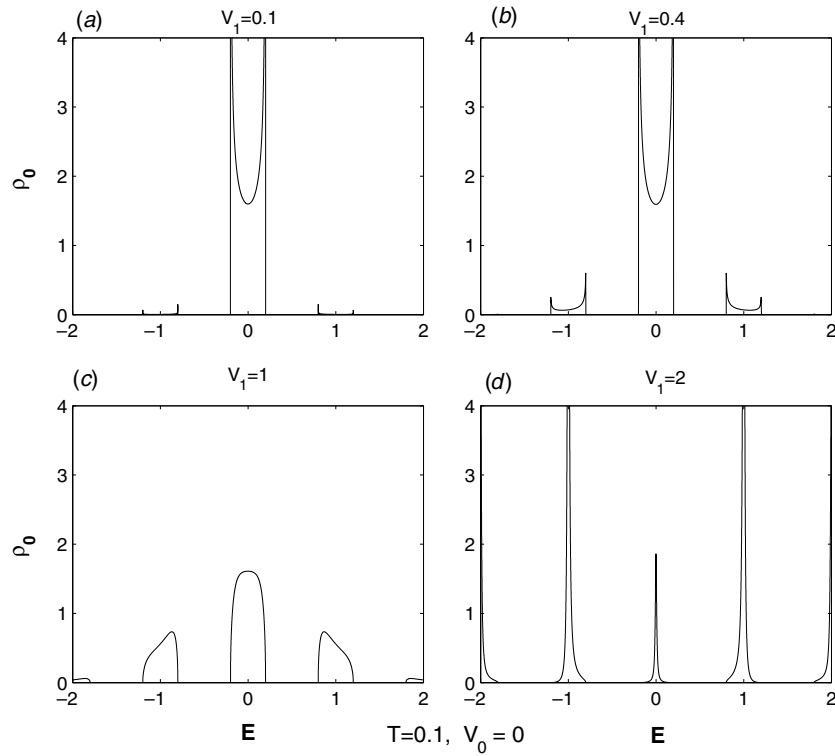


Figure 3. LDOS for a small band width. $T = 0.1(\hbar\omega)$ and therefore, the width of the band ($4T$) is smaller than $\hbar\omega$. No static on-site energy, $V_0 = 0$.

coupled to at least one extended state and therefore no longer becomes bound (for $4T > 1$). For small values of V_1 , these kinds of narrow resonances associated with bound states are called quasi-bound states and are typical of multichannel Hamiltonians [42]. At $V_1 = 0.1$ it is interesting to notice the ‘daughter’ resonances on both sides of the bound state resonance at $\sqrt{5} \pm 1$. In fact there is an infinite number of these ‘daughter’ resonances at $\sqrt{5} + n$ with an amplitude that decays quickly with $|n|$. For large values of V_1 , a complex structure of peaks has developed, separated in energy by integer values of $\hbar\omega$. This is what would be expected if instead of a HD potential we had a harmonic oscillator coupled to the electron. For large coupling (V_1), the density of states of the oscillator becomes dominant in the LDOS of the electron.

In figure 3 we study an interesting regime. For $T = 0.1$, the width of the energy band of \mathcal{H}^0 ($4T = 0.4$) is smaller than 1. In this figure, $V_0 = 0$, and we look at different values of V_1 . In (a) the density of states is very close to the well known LDOS for a tight-binding model without a defect. Very small replica bands can be observed around $E = \pm 1$. In (b) these replica bands are more noticeable. For $V_1 = 1$ in (c), the shape of the LDOS inside the bands is starting to change. For $V_1 = 2$ and higher, the LDOS looks very much like the LDOS for a harmonic oscillator, highly peaked around $E = n(\hbar\omega)$.

For figure 4 we chose again $T = 0.1$, and $V_0 = 0.1$. This gives an energy of the bound state of \mathcal{H}^S of $E_B = \sqrt{0.04 + 0.01} = 0.2236$. Because the band width is smaller than 1, the bound state is coupled to unperturbed states with energies $E_B + n$ which are all outside the extended state band. This means one would expect that, for small V_1 , as in figure 4(a),

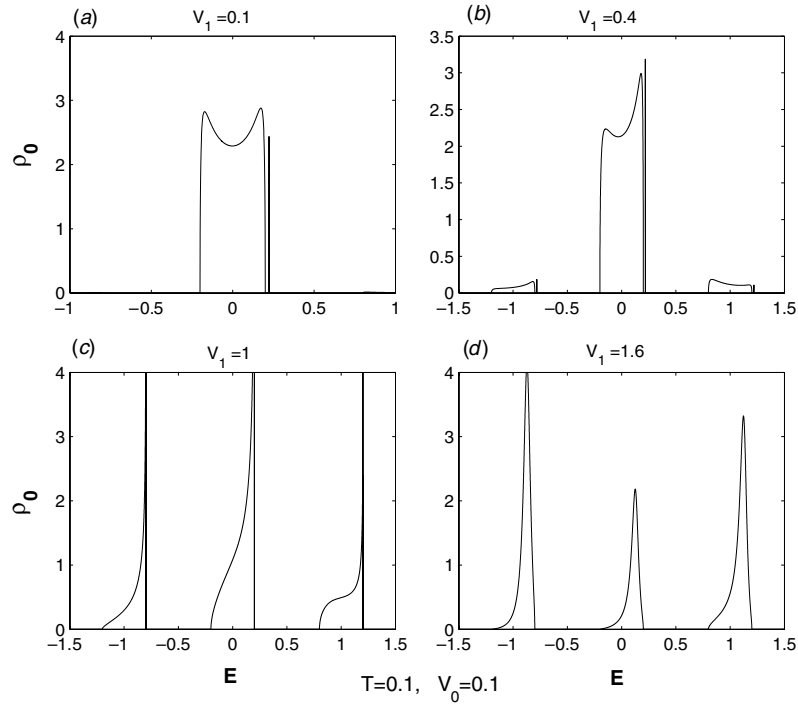


Figure 4. LDOS for $T = 0.1$, $V_0 = 0.1$ and different values of V_1 . There is a pole on the right of the extended state band for $V_1 < 1$.

there will be a true pole in the density of states at an energy $E_B \sim 0.223$. Indeed, within our numerical possibilities, no saturation in the height of the peak was detected with decreasing γ . In (b), $V_1 = 0.4$. We still have a pole on the right of the band, but its energy is down to $E_B = 0.2185$. The pole moves towards the extended state band as we increase V_1 . Notice that there are replica bands of extended states centred around $E = n$, as well as replica poles (too small to be seen in figure 3). In (c), for $V_1 = 1.0$ there is still a pole, located right next to the edge of the band. In the figure, this pole is too close to be discernible from the edge of the continuum of extended states. At $V_1 = 1.6$ in (d), the pole has already disappeared inside the band; there are no longer localized states in the system and the spectrum of the system resembles the spectrum of the harmonic oscillator, with density of states highly peaked near $E = 0.1 + n$.

In figure 5 we show a sequence of plots where $T = 0.1$, $V_0 = 0.4$ for different values of V_1 . In (a), $V_1 = 0.1$, and we find a pole very close to $E_B = \sqrt{4T^2 + V_0^2} = 0.447$, which is the location of the pole for the static potential case ($V_1 = 0$). For $V_1 = 0.4$ in figure 5(b), the pole has moved to $E_B \sim 0.443$ and the ‘replica bands’ are clearly seen on the right and left of the main band (near $E = 0$). Also two ‘daughter’ poles are large enough to be seen at $E = 0.443 \pm 1$. In (c) $V_1 = 1$, the poles have moved to $E = 0.424 + n\hbar\omega$, and the relative amplitude of the continuum part of the spectrum is growing smaller compared to the set of localized states (poles), for increasing V_1 values. The region of the energy axis where poles have significant residue to be observable in the figure grows with V_1 . For (d) $V_1 = 2$, the poles are now at $E \sim 0.3955 + n$. As the value of V_1 is increased further, the pole no longer moves from this location and the point spectrum (poles) becomes more and more important

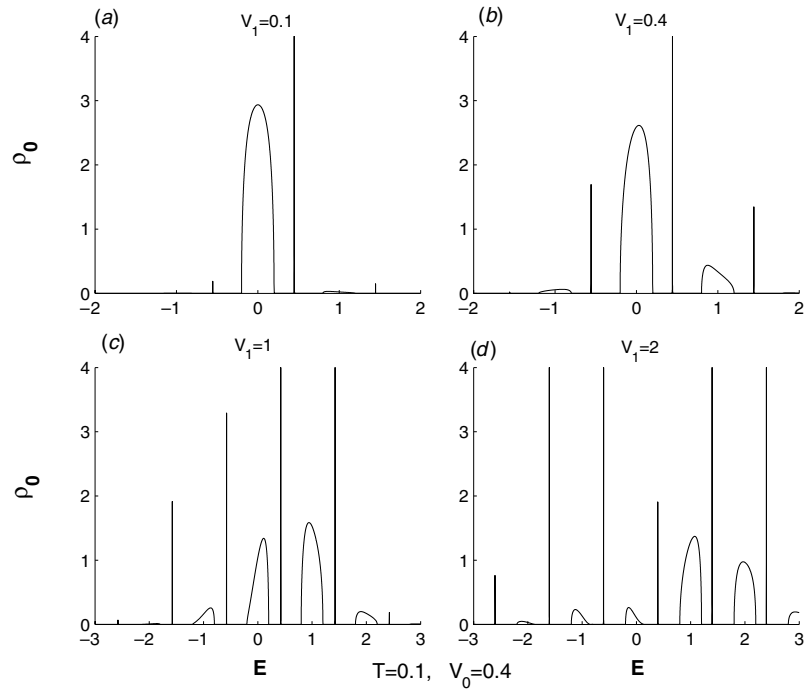


Figure 5. LDOS for $T = 0.1$, $V_0 = 0.4$ and different values of V_1 . There are poles for all values of V_1 . The pole location changes from $0.44 + n$ for $V_1 \rightarrow 0$ to $\sim 0.4 + n$ for $V_1 \rightarrow \infty$, with n any integer.

as compared to the continuum spectrum. For all values of V_1 , for $T = 0.1$ and $V_0 = 0.4$ there is a pole.

It can be proved easily that the location of the poles behaves in the following way for any values of V_0 , V_1 and T (provided $4T < 1(\hbar\omega)$):

$$E_B \rightarrow \sqrt{4T^2 + V_0^2} + n \quad \text{for } V_1 \rightarrow 0 \quad E_B \rightarrow V_0 + n \quad \text{for } V_1 \rightarrow \infty. \quad (56)$$

There would be no pole in any of these limits if the expected location of the pole (in this limit) falls inside the extended states band between $-2T, 2T$. This is the case in figure 4 ($T = 0.1$, $V_0 = 0.1$), where, when $V_1 \rightarrow 0$, pole location $\rightarrow \sqrt{4T^2 + V_0^2} = 0.223$ and for $V_1 \rightarrow \infty$, expected ‘pole’ location $\rightarrow V_0 = 0.1$, which is inside the band. Already for $V_1 > 1$ the pole has moved into that band (it is no longer a pole), generating a peak in the density of states, which continues to move inside the band for increasing values of V_1 until it settles at $E = V_0 + n \sim 0.1 + n$ for $V_1 > 2$.

5. Conclusions

Within the general framework of the $t-t'$ method, one can define the Floquet–Green function corresponding to a time-periodic Hamiltonian, from which transmission properties, density of states and wave packet propagation can be calculated. We have shown that in the general case of harmonic driving, the Floquet–Green function of any such system can be written in a compact way and calculated efficiently using MCF. We have also derived an expression for the (energy-dependent) dynamical effective potential (DEP) which includes the effect of the coupling to the different energy states due to the time periodicity of the system. The DEP allows one to

calculate, to any precision, the diagonal of the Floquet–Green function operator from which the density of states can be found easily. Calculation of the DEP could provide an interesting tool to help understand effects such as dynamical stabilization of atoms in a strong laser field [12].

We applied this formalism to the case of a tight-binding model with a defect energy which depends harmonically on time. The transmission through this defect potential has been calculated before and compared to the transmission through a tight-binding Hamiltonian with a defect that couples the electron with phonon degrees of freedom only present at the defect location [29]. We calculated the diagonal of the Floquet–Green function at the defect location ($\mathcal{G}_{0,0}^D$) and from it, the LDOS as a function of energy for different values of the parameters of the system. We found that there is a qualitative difference in the behaviour of the system for the regimes $4T > \hbar\omega$ and $4T < \hbar\omega$. In both cases we found that the LDOS spreads over a larger range of energies as the parameter V_1 is increased. However, in the first case there are no localized states for any values of the parameters V_0, V_1 . This result is due to the fact that the oscillating potential couples the bound state with at least one extended state of the unperturbed Hamiltonian, producing a finite probability of escape from the bound state. Turning on the oscillating potential will therefore, in all cases (provided $4T > \hbar\omega$), ‘ionize’ the bound state (if any) of the static part of the Hamiltonian. This result is consistent with the work of Costin *et al* [17] which shows that the bound state of an attractive δ -function potential does not remain bound when a time-periodic driving is turned on (except for a very particular class of non-harmonic periodic driving). For the case $4T < \hbar\omega$, there may or may not be any localized states in the system depending on the different values of V_0 and V_1 . A bound state outside the band can only be coupled to energy eigenstates of the static Hamiltonian which are all localized. The effect of the oscillating potential changes the location of the localized state energy, and produces an infinite chain of poles in the LDOS, all located at multiples of $\hbar\omega$ from each other. The pole location changes with the parameter V_1 according to equation (56) above. In both cases ($4T > \hbar\omega$ and $4T < \hbar\omega$), the LDOS makes a transition from the LDOS of the static defect problem, for small V_1 , to a harmonic-oscillator-like LDOS for V_1 large.

Acknowledgments

The author would like to thank L E Reichl for her support and for suggestions about this manuscript. The author also wishes to thank N V Kenkre for his kind invitation to spend several weeks at the University of New Mexico at the Consortium for the Americas, where he also enjoyed fruitful discussions with D H Dunlap. This work has been partially supported by the Welch Foundation, grant no F-1051, NSF grant INT-9602971 and DOE contract no DE-FG03-94ER14405.

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