On Eigenvalues and Eigenfunctions Absent in the Actual Solid State Theory

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Abstract

In this letter new, closed and compact analytic expressions for the evaluation of resonant energies, resonant bound-states, eigenvalues and eigenfunctions for both scattering and bounded n-cell systems are reported. It is shown that for (scattering and bounded) 1-D systems the eigenfunctions $\Psi_{\mu,\nu}(z)$ are simple and well defined functions of the Chebyshev polynomials of the second kind $U_n$, and the energy eigenvalues $E_{\mu,\nu}$ (in the $\mu$-th band) are determined by the zeros of these polynomials. New insights on the energy gap and the localization effect induced by phase coherence are shown.

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Different techniques and approaches have been developed to determine, as exactly as possible, eigenvalues and eigenfunctions. In quantum theory the knowledge of these quantities represents a central aim and afford the possibility of evaluating other quantities. It is well known that, except for a small number of cases, it is not easy to obtain eigenvalues with the precision that one would like to have and to deduce explicit analytical expressions for the eigenfunctions. In the actual solid state physics theory, the eigenfunctions and eigenvalues are in some sense beyond it, and the theory is basically designed to describe systems in the continuous spectrum limit. The famous and widely accepted Bloch function \( e^{ik_B \cdot r} u_{\mu,k}(r) \), strictly valid only for infinite periodic systems[1], becomes the obvious and natural starting point for almost any approach of periodic systems, even though the periodic function \( u_{\mu,k_B}(r) \) remains in general practically unknown. Calculations based on the Bloch function lead also, almost automatically, to introduce the reciprocal space that inexorably, aside from text books’ didactic presentations, may obscure the analysis. As a consequence, great efforts and imagination had to be bestowed to explain the vast world of mechanisms, effects and properties discovered and populating the actual solid state and condensed matter physics[2-6]. The allowed and forbidden energy bands, which should not be confused with the energy eigenvalues of finite systems, are usually determined after a complex and perhaps painful numerical calculations with the aid of experimental input to fit parameters. On the other hand, high precision experiments and energy dependent applications, as those related to optical excitations, require one to solve the fine structure in the bands. This has been so far difficult for the actual theory. It is the purpose of this letter to extend the analytic methods of the scattering theory, for finite periodic systems with arbitrary potential shape, to determine compact and general expressions for an easy and simple evaluation of the eigenvalues and eigenfunctions, which are neither the energy bands nor the Bloch functions. In other words, the present approach allows one to solve the fine structures in bands completely.

Concerning band structures and electronic properties, there is an abundant literature and great contributions extending from the nearly free electron model to pseudopotential methods and Local Density Approximations. Important attempts were made forty years ago
by Kohn to study the analytic properties of Bloch waves and Wannier functions[2]. Since those years, the complexity of involved Green’s function and matching methods[7], together with a complete zoo of effective masses, perturbative methods, envelope functions, dispersion relations, and much more, have dominated the theory of real periodic systems[8-11].

A completely different and natural approach to deal with finite (or locally) periodic systems is being developed[12]. In this approach the Bloch functions, reciprocal spaces, Brillouin zones, and other intricate concepts and knotty theoretical structures are not needed at all in order to calculate fundamental quantities. The theory of finite periodic systems (TFPS), based on the transfer matrix method (originally proposed to calculate scattering amplitudes, and related properties in superlattices), will be expanded to include also the stationary properties and to deduce, new and closed formulas for quantities as fundamental and basic as the eigenvalues and eigenfunctions.

To encompass most of the various types of systems, I shall consider three representative cases, distinguished by their boundary conditions. Hence, I shall refer to open, bounded and quasi-bounded systems, as shown in figure 1. While for scattering systems (figure 1a)) I will refer to resonant energies and resonant bound-states, for bounded systems I will talk of energy eigenvalues and eigenfunctions. For the reasons of simplicity and lack of space, I will restrict to the widely used one channel (1-D) approximation. Some multichannel generalizations are almost straightforwardly obtained[13].

It is well known, in the scattering theory, that resonant transmission occurs precisely when the incident energy coincides with a bound-state energy in the scatterer system, which, for our purpose, is locally periodic with \( n \) cells (of length \( l_c \) each) in the transmission direction. For this kind of systems, the transmission amplitudes of \( N \)-propagating modes (\( N \)-channels) are obtained from[12]

\[
t_{N,n}^T = \frac{1}{p_{N,n} - \beta^{-1} \alpha \beta p_{N,n-1}}
\]

where the functions \( p_{N,n} \) are \( N \times N \) matrix polynomials fully determined in terms of the single-cell transfer matrix \( M \), which for time reversal invariant systems has the structure
\[ M = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} \]  

(2)

In the one channel (one propagating mode) approximation \( \alpha \) and \( \beta \) are complex scalars and \( p_{1,n} \) is the Chebyshev polynomial of the second kind \( U_n(\alpha_R) \) evaluated at the real part of \( \alpha \). Because of the close relation between the resonant structure and the spectral properties, we can determine simple expressions to evaluate the resonant energies. If we use the identity \( U_n U_{n-2} = U_{n-1}^2 - 1 \), the whole \( n \)-cell system transmission coefficient can be rewritten as

\[ |t_n|^2 = \frac{|t|^2}{|t|^2 + U_{n-1}^2(1 - |t|^2)}. \]  

(3)

Here \( |t|^2 \) is the single-cell transmission coefficient. It is clear from this expression that the transmission resonances occur when the polynomial \( U_{n-1} \) becomes zero. Therefore, the \( \nu \)-th resonant energy \( E_{\mu,\nu} \) is a solution of

\[ (\alpha_R)_\nu = \cos \frac{\nu \pi}{n} \]  

(4)

where \( (\alpha_R)_\nu \) is the \( \nu \)-th zero of the Chebyshev polynomial and \( \nu = 1, 2, \ldots, n - 1 \). The index \( \mu \) labels the bands, peculiar to periodic systems and entirely determined by the phase coherence. In the transfer matrix approach the allowed energy bands are those energies which satisfy the condition \( |\alpha_R| \leq 1 \). To illustrate the use of equation (4), let us consider the square-barrier superlattice of figure 1a). This is similar to the familiar Kronig-Penney model (except that here we have a finite number of cells \( n \)) with barrier height \( V_o \), and valley and barrier widths \( a \) and \( b \), respectively. In this case

\[ \cos k_{\nu} a \cosh q_{\nu} b - \frac{k_{\nu}^2 - q_{\nu}^2}{2k_{\nu}q_{\nu}} \sin k_{\nu} a \sinh q_{\nu} b = \cos \frac{\nu \pi}{n} \]  

(5)

with \( k_{\nu}^2 = 2m^* E_{\mu,\nu}/\hbar^2 \) and \( q_{\nu}^2 = 2m^*(V_o - E_{\mu,\nu})/\hbar^2 \). Notice that each energy band contains the same number of resonant energies as confining wells have the scatterer periodic system. In this case is \( n - 1 \). In figure 2, some of these energies and the associated level densities \( \rho(E) \) are plotted for different values of \( n \). The level density behavior tends rapidly, as a
function of \(n\), to that of the Kronig-Penney model, though the continuous spectrum limit is reached only when \(n \to \infty\).

An important extension of the scattering approach, and the transfer matrix method, is to studying stationary properties of bounded periodic systems. If we have systems like those shown in figures 1b-c), we can apply the main results of the TFPS and introduce the boundary conditions. For a periodic \(n\)-cell system (with length \(nl_c\)) bounded by infinite hard walls, it is easy to show that the energy eigenvalues are determined from

\[
(\alpha_n - \alpha_n^* + \beta_n^* - \beta_n) = 0
\]

which, using the relations\[12\] \(\alpha_n = U_n - \alpha U_{n-1}\) and \(\beta_n = \beta U_{n-1}\) can be written as \(U_{n-1}(\alpha_I - \beta_I) = 0\). Here the subscript \(I\) refers to the imaginary part. Notice that \(n - 1\) of the energy eigenvalues of the bounded system are the zeros of the Chebyshev polynomial \(U_{n-1}\). For the particular example shown in figure 1b), which length is \(nl_c + a\), the eigenvalues are obtained from

\[
U_n \sin ka + (\alpha_I \cos ka - \alpha_R \sin ka - \beta_I)U_{n-1} = 0.
\]

These eigenvalues are used below when evaluating the eigenfunctions.

Another type of system that I would also like to consider is a periodic \(n\)-cell system confined by finite potential walls as shown in figure 1c). In this case, assuming \(E < V_w\), the eigenvalues are obtained from

\[
h_wU_n - f_wU_{n-1} = 0
\]

with \(f_w = (\alpha_R - \alpha I \frac{q_w^2 - k_o}{2q_w k_o} + \beta_I \frac{q_w^2 + k_o}{2q_w k_o})\) and \(h_w = (1 + \frac{q_w^2 - k_o}{2q_w k_o})\). Here \(q_w^2 = 2m(V_w - E)/\hbar^2\) and \(k_o\) is the wave vector at \(z = z_o + 0^+\). Below, these eigenvalues are used to evaluate the corresponding eigenfunction for an specific system.

I shall now refer to the eigenfunctions \(\Psi_{\mu,\nu}(z)\) of finite periodic systems. For this purpose, it is convenient first to fix some notation. As shown in figure 1, the coordinates \(\{z_j\}\), with \(j = 0, 1, 2, ... n\), define a set of points separated by multiples of \(l_c\), i.e. \(z_j = jl_c\). If we are interested in evaluating functions at any point \(z\) in the \(j\)-th cell, it is useful to define the difference \(\delta z = z - z_j \leq l_c\). Taking into account the transfer matrix multiplicative
properties, the total transfer matrix $M_T(z_o \rightarrow z)$ relating the wave vectors $\Phi(z_o)$ and $\Phi(z)$, can be factorized as $M_j(z'_o \rightarrow z)M_{o\rightarrow o'}(z_o \rightarrow z'_o)$, with $z'_o = z_o + \delta z$, and subsequently, the wave vector can be written as

$$\Phi(z) = \begin{pmatrix} \varphi'(z) \\ \varphi(z) \end{pmatrix} = \begin{pmatrix} \alpha_j & \beta_j \\ -\beta_j^* & \alpha_j^* \end{pmatrix} \begin{pmatrix} \varphi'(z'_o) \\ \varphi(z'_o) \end{pmatrix}.$$ \hspace{1cm} (8)

Here $\alpha_j = U_j - \alpha^* U_{j-1}$, $\beta_j = \beta U_{j-1}$, and the functions $\varphi'(z)$ and $\varphi(z)$ represent, depending on the difference $E - V(z)$, the right and left propagating or exponentially increasing and decreasing functions, respectively\cite{12}. The eigenfunctions are easily obtained by using these relations, the boundary conditions and the general expressions for $\alpha_j$ and $\beta_j$.

For a scattering system like the one shown in Fig. 1a), the wave function at $z$ is given by

$$\Psi(z, E) = \varphi'(z'_o) \left[ \alpha_j + \beta_j^* - (\alpha_j^* + \beta_j) \frac{\beta_j^*}{\alpha_j^*} \right]$$ \hspace{1cm} (9)

It is clear that evaluating the function $\Psi(z, E)$ at $E_{\mu,\nu}$ we have the corresponding $\nu$-th resonant bound state in the $\mu$-th band

$$\Psi_{\mu,\nu}(z) = \Psi(z, E_{\mu,\nu}).$$ \hspace{1cm} (10)

In figures 3a-d) we plot four different functions for a system with the potential parameters of the superlattice $GaAs(Al_{0.3}Ga_{0.7}As/GaAs)$\cite{12}. In 3a) we have the function $|\Psi_2(z, E)|^2$ for an arbitrary energy $E \neq E_{\mu,\nu}$ within the second energy band. This is an extended aperiodic wave function with a complicated behavior along the superlattice. In figures 3b and 3c), we have instead the functions $|\Psi_{2,2}(z)|^2$ and $|\Psi_{4,3}|^2$ corresponding to the second and third resonant energies in the second ($\mu = 2$) and fourth ($\mu = 4$) energy bands. In these cases the bound-state functions are modulated by an oscillating envelope function with $\nu - 1$ minima plus those at $z_o = 0$ and $z_n = nl_c$. Notice that, since these wave functions describe not only extended but also transmitted states, they are, except for a few points in $|\Psi_{2,2}(z)|^2$, different from zero with the probability to find the particle at the two ends of the system different from zero. This will change for bounded systems, of course. Finally, in figure 3d)
we plot $|\Psi(z, E)|^2$ at some point in the gap between the second and third bands. The wave function behavior, for an incident energy in the gap, is not only compatible with the well known vanishing of the transmission coefficient, it makes also evident the localization effect induced by the phase coherence at the energy gap, as suggested in some sense by Kohn[2]. This is a very appealing result which may deserve further reflections.

To complete this discussion we shall now briefly refer to the other two types of systems. Consider first the system bounded by infinite hard walls. In this case, the $\mu, \nu$ eigenfunctions are evaluated from

$$\Psi_{\mu,\nu}(z) = \mathcal{V}(z')_0(\alpha_j + \beta_j^* - \alpha_j^* - \beta_j) \tag{11}$$

with $E = E_{\mu,\nu}$ and the matrix elements $\alpha_j$ and $\beta_j$ as mentioned above are simple functions of the Chebyshev polynomials of order $j$ and $j-1$. Care has to be taken when extra pieces of length $a/2$ are added to the system of length $nl_c$. For the particular case shown in figure 1b) the last two terms in Eq. (11) have to be multiplied by $((\alpha_n + \beta_n^*e^{-ika})/(\beta_n + \alpha_n^*e^{-ika})$. Two of these eigenfunctions ($|\Psi_{2,2}(z)|^2, |\Psi_{2,3}(z)|^2$) are plotted in figures 4a-b). Contrary to the scattering system, the wave function vanishes at the ends. An important difference between a periodic potential flanked by infinite hard walls and a constant potential flanked also by infinite hard walls, is the presence (in the periodic potential case) or absence (in the single well case) of phase interference effect responsible for energy splittings that in the former case develop the band structure and the energy eigenvalues.

Finally, for the system with finite walls mentioned above, the eigenfunctions are given by

$$\Psi_{\mu,\nu}(z) = \mathcal{V}(z')_0(\alpha_{jR} + \beta_{jR} + \frac{q_w}{k}(\beta_{jI} - \alpha_{jI})) \tag{12}$$

Here $E_{\mu,\nu}$ is obtained from equation (7). Some of these eigenfunctions are plotted in figures 5a-c). Although imperceptible, the wave functions decrease exponentially inside the potential walls. As in previous figures, we distinguish two main characteristics: a strongly oscillating behavior, which frequency grows with $\mu$ and $\nu$, and a periodic modulation, with period $nl_c/\nu$.  

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In this letter various new and general formulas for the evaluation of fundamental quantities like the resonant energies, bound states, energy eigenvalues and eigenfunctions of finite periodic systems, have been reported. Specific and illustrative examples and results, for both scattering and bounded one-dimensional systems, have been also presented.

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FIGURES

FIG. 1. Potential profiles, along the direction $z$, for open, bounded and quasi-bounded $n$-cell systems.

FIG. 2. Level density in the first band of finite and infinite (Kronig-Penney) $GaAs(Al_{0.3}Ga_{0.7}As/GaAs)^n$ superlattice with $a = 100\text{nm}$, $b = 30\text{nm}$ and $V_o = 0.23\text{eV}$. Some eigenvalues $E_{1,\nu}$ (in $\text{eV}$) for $n = 8$ are also indicated.

FIG. 3. Squared wave functions for a system like in Fig. 1a) but with square barrier potential and parameters as in Fig. 2. In a) extended $|\Psi_{\mu}(z, E)|^2$ with $E \neq E_{\mu,\nu}$ and $\mu = 2$ is shown; In b), and c) the indicated resonant states; In d) a localized wave function in the second gap is shown.

FIG. 4. Eigenfunctions $|\Psi_{\mu,\nu}(z)|^2$ for a system like in Fig. 1b) and parameters as in Fig. 2. The oscillations frequency and enveloping minima depend on the band and excitation energy indices $\mu, \nu$. All functions vanish at the surface. In a) and b) the particle density beneath the surface is relatively high.

FIG. 5. Eigenfunctions in the lower bands for a system like in Figs. 1c) but with square barriers and parameters as in Fig. 2), flanked by finite walls.
a) \[ \begin{array}{ccc}
& \rightarrow & 1 & \rightarrow & 2 & \cdots & \rightarrow & j+1 & \rightarrow & n \\
\downarrow & & & & & & & & & \\
z_0 & \vdots & z_j & \vdots & \end{array} \]

\[ j \delta z \]

\[ j l_c \]

\[ \delta z \]

b) \[ \begin{array}{ccc}
& \rightarrow & a & \rightarrow & l_c & \rightarrow & b \\
\downarrow & & & & & & & & \\
z_0 & \vdots & z_1 & \vdots & z_j & \vdots & z_{n-1} & \vdots & z_n \\
\end{array} \]

\[ V_0 \]

c) \[ \begin{array}{ccc}
& \rightarrow & \cdots & \rightarrow & \cdots & \rightarrow & \uparrow \\
\downarrow & & \vdots & & \vdots & & \downarrow \\
& & & & & & V_w \\
\end{array} \]
\[ \rho(E) = \frac{E}{\rho(E_1, \nu)} = 8 \]
\[ \rho(E) = 50 \]

Kronig–Penney
$|\psi_2(z,E)|^2$

$|\psi_{2,2}(z)|^2$

$|\psi_{4,3}(z)|^2$

$|\psi_5(z)|^2$

\[ n = 12 \]
\[ l_c = 130 \text{ nm} \]
\[ |\psi_{2,2}(z)|^2 \] a)

\[ |\psi_{2,3}(z)|^2 \] b)
\[
|\psi_{2,1}(z)|^2
\]

\[
|\psi_{3,2}(z)|^2
\]

\[
|\psi_{4,2}(z)|^2
\]