Eur. Phys. J. B **36**, 137–140 (2003)
DOI: 10.1140/epjb/e2003-00326-9

THE EUROPEAN PHYSICAL JOURNAL B

Surface plasmons on a quasiperiodic grating

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Received 24 June 2003
Published online 19 November 2003 –

Abstract. A method is presented for calculating the frequencies of non-retarded surface plasmons propagating on a semi-infinite medium with a surface profile described by a one-dimension quasiperiodic function. The profiles are generated, in analogy with previous work on quasiperiodic superlattices, by repeating unitary cells constructed according to an inflation rule. Dispersion relations are obtained for a semi-infinite free-electron metal as the active medium, with surface profiles obeying the Fibonacci and Thue-Morse sequences.

PACS. 73.20.Mf Collective excitations (including excitons, polarons, plasmons and other charge-density excitations) – 71.45.Gm Exchange, correlation, dielectric and magnetic response functions, plasmons

1 Introduction

Extensive experimental and theoretical work on quasiperiodic systems has revealed interesting new properties which are not found in either periodic or in disordered systems. Examples of quasiperiodic systems are artificial structures such as surfaces with quasiperiodic tilling patterns [1], as well as multilayers constructed by juxtaposing different building blocks following quasiperiodic inflation rules [2]. These structures are generally considered as intermediate states between ordered and disordered systems. It has been found that the energy spectra of elementary excitations (e.g. polaritons, phonons, spin waves) of such structures are highly fragmented, with a self-similar pattern (for a comprehensive review, see Ref. [2] and references therein). In fact, this property is now accepted as a signature of a quasiperiodic system.

Another topic that has attracted considerable attention is the study of the propagation of surface modes on disordered media. Among these excitations, surface plasmons, which are electronic collective modes bound to a dielectric-metal interface, have been some of the most intensively studied. Due to their surface nature, these modes are strongly influenced by the shape of the interface along which they propagate. In fact, the excitation of surface plasmon modes on randomly rough surfaces can lead to localization effects [3], and is also associated with surface phenomena such as the enhanced second harmonic generation [4]. Recent studies [5,6] of surface plasmons on periodically corrugated surfaces have indicated the presence of absolute band gaps in the frequency spectrum, which in turn show a dependence on the geometry of the surface.

The aim of this work is to present a method for calculating the spectrum of excitations of a metal-dielectric interface with a quasiperiodic grid of parallel ridges. In this case, since the quasiperiodic elements are restricted to the surface of the medium, they may exert a significant influence on its spectrum of surface excitations. Specifically, we calculate the surface plasmon spectrum of surfaces with one-dimensional profiles described by functions created by substitutional sequences. We use these functions to construct a series of periodic profiles, with each consisting of a unitary cell obtained from a quasiperiodic sequence, repeated along the x_1 direction. For each generation of the sequence, the period length a increases, and the quasiperiodic case is obtained in the limit $a \to \infty$.

2 Model

The theory is based on the Rayleigh hypothesis formalism described in reference [7], which has been shown to give exact results for surfaces with small corrugations (i.e. with height to width ratios < 0.072) defined by analytic functions. In this formalism, solutions of Laplace's equation are found that vanish as the distance ($|x_3|$) to the interface increases. For a semi-infinite medium with a surface described by a one-dimensional periodic profile, the potentials associated with modes propagating along the

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x_1 direction can be assumed to obey the Bloch property

$$\phi(x_1 + a, \omega) = \phi(x_1, \omega)e^{ika}, \tag{1}$$

where a is the period of the surface. Thus, the potential associated with a surface mode can be expressed as,

$$\phi(x_1, x_3) = \sum_n^{\infty} C_n \exp(ik_n x_1 - \alpha_n x_3) \tag{2}$$

where $\alpha_n = |k+2\pi n/a|$, $k_n = k+2\pi n/a$, k is the wavevector, x_3 is the direction normal to the surface of the active medium and the C_n factors are the Fourier amplitudes of the potential. By applying the interface boundary conditions, the frequencies of the non-retarded surface plasmons can be obtained by solving the eigenvalue equation

$$\sum_{p=-\infty}^{\infty} M_{rp}(k)C_p = \frac{\epsilon(\omega)+1}{\epsilon(\omega)-1}C_r, \tag{3}$$

with the elements of the matrix $M_{rp}(k)$ being given by

$$M_{rp}(k) = \frac{\alpha_r\alpha_p - k_r k_p}{\alpha_r(\alpha_r - \alpha_p)}K(\alpha_r - \alpha_p, k_r - k_p) \tag{4}$$

for $r \neq p$ and $M_{rp}(k) = 0$ otherwise. The function $K(\alpha_r - \alpha_p, k_r - k_p)$ is obtained from the integral

$$K(\alpha, k_l) = \frac{1}{a}\int_{-a/2}^{a/2} e^{\alpha\zeta(x)}e^{-ik_l x}dx, \tag{5}$$

where we used $\alpha \equiv \alpha_r - \alpha_p$ and $k_l \equiv k_r - k_p$. The function $\zeta(x)$ describes the surface profile.

In the following calculations, we employ a surface model designed in a similar fashion to the structures used in the multilayer calculations. The goal is to construct a profile that approximates a quasiperiodic surface by using a known function, taken in finite intervals, in order to define a *periodic* function. Thus a series of periodic surfaces can be described, each consisting of unitary cells made of building blocks arranged in a finite quasiperiodic sequence, repeated along the x_1 direction. The overall periodic nature of the surface allows us to use the formalism of Glass et al. However, for each successive generation of the sequence, the period length a increases, and an actual quasiperiodic surface is obtained as the length of the unitary cell grows to infinity. In the present case, the building blocks are chosen to be sinusoidal functions. These functions are defined in intervals such that each block corresponds to a ridge on the surface of the metal. This approach to the definition of the profile is similar to the one used in reference [8] for isolated ridges on a flat surface. The ridges can be of two types, with different heights or widths, which we henceforth refer to as blocks 'A' and 'B' (see Fig. 1). These sinusoidal blocks are described by the functions

$$\zeta_a(x_1) = 2A_a\cos^2(\pi x_1/L_a) \tag{6}$$

in intervals $s_aL_a + s_bL_b - L_a/2 < x < s_aL_a + s_bL_b + L_a/2$, for 'A' ridges, and

$$\zeta_b(x_1) = 2A_b\cos^2(\pi x_1/L_b), \tag{7}$$

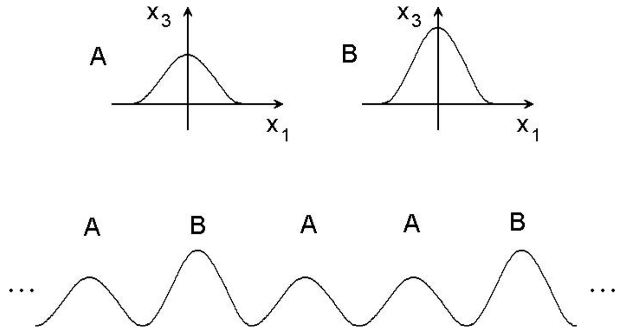

Fig. 1. Schematic representation of the surface profile used. Ridges, labeled A and B are arranged periodically on a flat surface. The unitary cell is constructed according to an inflation rule. The lower image represents a unitary cell corresponding to the 5th term in the Fibonacci sequence.

in intervals $s_aL_a + s_bL_b - L_b/2 < x < s_aL_a + s_bL_b + L_b/2$, for the 'B' ridges, with $s_{a,b} = 0, 1, 2, ...$ In order to construct the unitary cell, one has only to specify the intervals corresponding to each block.

By following the prescriptions above, one can then obtain the kernel in equation (3), by applying suitable changes of variables in equation (5), as

$$K(\alpha, k_l) = f_a(k_l)K_a(\alpha, k_l) + f_b(k_l)K_b(\alpha, k_l), \tag{8}$$

where

$$K_c(\alpha, k_l) = \frac{1}{a}\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}\int_{-L_c/2}^{L_c/2}\zeta_c^n(x_1)e^{-ik_l x_1}dx_1, \tag{9}$$

with $c = a, b$. The functions $f_a(k_l)$ and $f_b(k_l)$ contain the information concerning the positions of the ridges in the unitary cell, and therefore depend on the sequence generation. In this paper we consider the case where $A_a \neq A_b$ and $L_a = L_b$.

Let us first consider the Fibonacci sequence. In this case, we assume $S_0 = B$, $S_1 = A$ as the first two terms in the sequence. The other terms are generated by an operation that consists of juxtaposing the two previous terms in the sequence, following the rule

$$S_{n+1} = S_n\, S_{n-1}. \tag{10}$$

Thus, the next three terms are $S_2 = AB$, $S_3 = ABA$, $S_4 = ABAAB$ etc. Therefore, for the S_3 generation we obtain an unitary cell of length $a = 3L$. This cell can be defined as

$$\zeta(x_1) = \begin{cases} \zeta_a(x_1), & -3L/2 < x < -L/2, \\ \zeta_b(x_1), & -L/2 < x < L/2, \\ \zeta_a(x_1), & L/2 < x < 3L/2. \end{cases} \tag{11}$$

In this particular case, there is a B ridge centered at the origin, a A ridge shifted L units to the left of the origin, and another A ridge shifted by L units to the right. That translates as

$$f_b(k_l) = 1, \qquad f_a(k_l) = 2\cos(k_l L). \tag{12}$$

For the sinusoidal profiles considered here, it can be shown that,

$$K_c(\alpha, k_l) = \sum_{n=0}^{\infty} \frac{\xi^n}{n!} \left(\frac{A_c}{L}\right)^n F^{-n}$$

$$\times \sum_{m=0}^{2n} \binom{2n}{m} \frac{\sin\left[\pi(n-m) - \pi(r-p)/F\right]}{\pi\left[F(n-m) - (r-p)\right]}, \quad (13)$$

where F is the total number of ridges in the unitary cell.

This formalism can be extended to profiles generated by other sequences in a straightforward way. In the case of the Thue-Morse sequence, one applies the following substitution rules:

$$S_n = S_{n-1}\, S_{n-1}^{+} \quad (14)$$

and

$$S_n^{+} = S_{n-1}^{+}\, S_{n-1} \quad (15)$$

for $n \geq 1$, with $S_0 = A$ and $S_0^{+} = B$. Thus, the next three generations of this sequence are: $S_1 = AB$, $S_2 = ABBA$ and $S_3 = ABBABAAB$. Thus, the number of blocks in a unitary cell corresponding to a sequence generation S_n is 2^n.

3 Numerical results

We now present numerical results for gratings ruled on a free-electron metal, with the dielectric constant

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}, \quad (16)$$

where ω_p is the plasma frequency of the conduction electrons in the metal. The surface plasmon spectra for sinusoidal gratings are known to display an infinite set of dispersion branches distributed symmetrically around the flat-surface-plasmons frequency $\omega_{fsp} = \omega_p/\sqrt{2}$ [7]. This behaviour is also found in the present results. The graphs in Figure 2 show a comparison of the dispersion relations of surface plasmons for gratings constructed with the Fibonacci sequence, for increasing generation numbers, using $A_a/L = 0.04$ and $A_b/L = 0.07$. Only higher frequency branches are shown. The frequencies are normalized by ω_{fsp} and the wavevectors are normalized by $2\pi/a$. As the number of blocks in the unitary cells increases, the convergence of the results becomes slower, and more terms must be added to the summation in equation (3). However, even for S$_8$, a good convergence can be obtained for $N < 100$ terms. Graph (a) shows the periodic case, which corresponds to a sinusoidal grating with $A/L = 0.07$. Graphs (b) to (d) show the results for sequence generations S$_4$($F = 5$), S$_6$ ($F = 13$) and S$_8$ ($F = 34$), respectively. In contrast with the periodic case, in which most of the branches are found in close proximity to ω_{fsp}, as the generation number increases, several high-frequency branches are found and one can observe a tendency to the formation of frequency bands for large generation numbers. The results also indicate the presence of several frequency gaps arising in the plasmon spectrum. This result is consistent with what has been previously observed for excitations in multilayer systems. Nevertheless, in the present case the width of the gaps is directly related to the height to width ratios of the different blocks, a parameter that can, in principle, be varied continuously, whereas in multilayer systems the gaps depend on the different properties of each block, which cannot be as easily controlled.

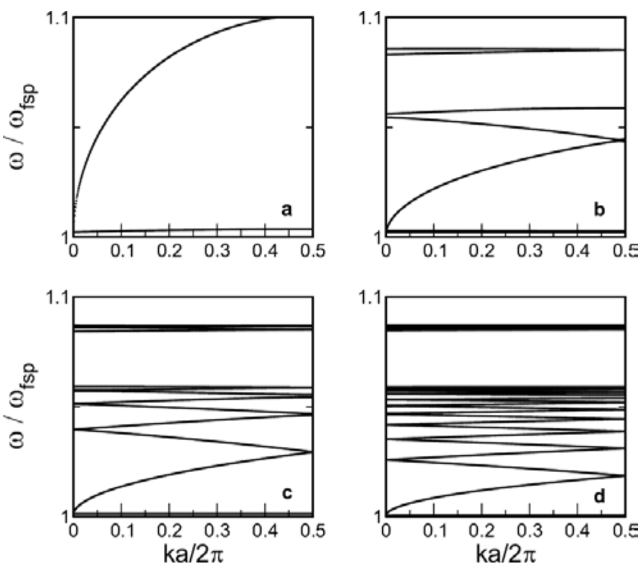

Fig. 2. Surface plasmon frequencies as a function of wavevector for a sinusoidal grating (a), with $A/L = 0.07$, and gratings with unitary cells obtained from the Fibonacci rule: (b) S$_4$, (c) S$_6$ and (d) S$_9$, for $A_a/L = 0.04$ and $A_b/L = 0.07$.

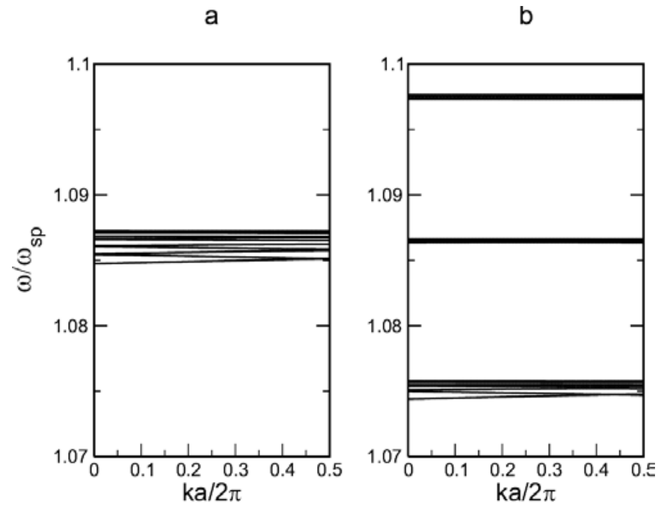

Fig. 3. High-frequency surface plasmon dispersion branches for gratings with a unitary cell corresponding to the 9th generation of the Fibonacci sequence, for (a) $A_a/L = 0.04$, $A_b/L = 0.07$ and (b) $A_a/L = 0.07$, $A_b/L = 0.04$.

Two results for gratings following the Fibonacci sequence are displayed in Figure 3. Both graphs show some of the high-frequency dispersion branches of surface

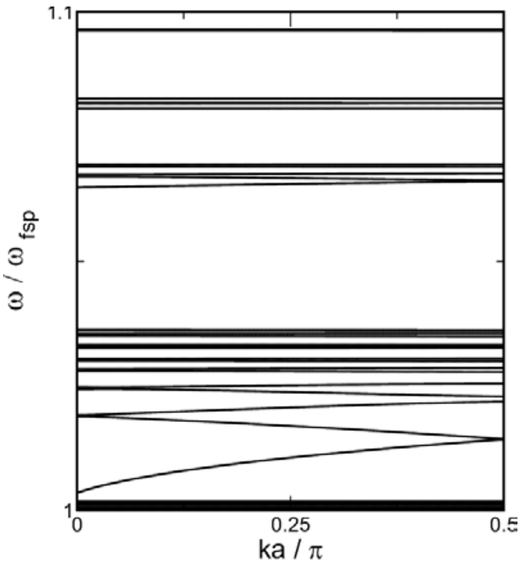

Fig. 4. Surface plasmon dispersion branches for a grating with a unitary cell obtained from the Thue-Morse sequence (S_5), for $A_a/L = 0.02$, $A_b/L = 0.07$.

plasmons on gratings with unitary cells corresponding to the S_9 term in the sequence ($F = 34$). However, for the graph labeled (a), the values $A_a/L = 0.04, A_b/L = 0.07$ were used, whereas for graph (b) the parameters were $A_a/L = 0.07, A_b/L = 0.04$. One can see from the graphs that, in contrast with the three high-frequency bands that arise in the $A_a > A_b$ case, the results for $A_a < A_b$ show the appearance of a single high-frequency band. These results illustrate the inherent asymmetry of the Fibonacci sequence, which is a consequence of the fact that, in that sequence, the number of B blocks is found to be always smaller than the number of A blocks (for large generation numbers, the ratio of the number of B blocks and the number A blocks approaches the number $\phi \approx 0.618$). In addition, in the Fibonacci sequence, the B blocks are always located between A blocks. This asymmetry does not occur in the Thue-Morse sequence, in which the number of A and B blocks is always the same.

Figure 4 shows the upper dispersion branches for surface plasmons propagating on a grating with a unitary cell corresponding to the 5th generation of the Thue-Morse sequence, for $A_a/L = 0.02$ and $A_b/L = 0.07$. As in the previous cases, the graph shows several gaps in the spectrum, with three groups of high-frequency branches separated by large gaps, with several small gaps located in the high-frequency regions. This behavior points to a fractal nature of the spectrum as the generation number increases.

4 Conclusions

In summary, we calculated the frequencies of surface plasmons propagating on gratings with one-dimensional surface profiles that follow quasiperiodic sequences. The surface morphology is described by a model that allows us to employ methods previously developed for the study of surfaces with ordered profiles, and at the same time to explore a topography that displays deterministic disorder. The results were obtained for gratings constructed with Fibonacci and Thue-Morse sequences and can be easily extended to other sequences. The surface plasmon dispersions show a large number of gaps that are related to the sequence generation and to the aspect ratio of the ridges that form the grating. The spectra have a fractal character that is similar to what has been previously observed for other excitations in quasiperiodic structures. The method presented here allows the calculation of the frequencies of *propagating* modes. However, one cannot rule out the possibility of existence of *non-propagating* plasmon modes in such structures. In fact, such localized modes are often found in quasiperiodic superlattice structures, with frequencies located in the gaps of the spectrum. Surfaces with periodic features have been constructed by photolithography, and such a technique could in principle be applied in order to create the quasiperiodic structures described here. Currently we are developing a method to study other surface excitations, such as surface polaritons, and to investigate the light scattering properties of quasiperiodic surfaces.

The authors would like to acknowledge the financial support of the Brazilian council for research (CNPq).

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