

GREEN FUNCTIONS FOR ATOMIC WIRES

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Abstract. The relevance of vibrations for the drops in atomic wires conductivity is discussed. The Green function of an atomic wire with pyramidal connection is calculated.

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During the last decade, a traditionally idealized textbook example, the atomic chain, has become a system intensively explored experimentally [1]. A string of gold atoms adsorbed on a silicon surface has been obtained by Segovia *et al.* [2]. When an atomic chain is used to bridge two contacts, an *atomic wire* is formed. It can be considered as ultimate conductors of future nanoelectronics.

The investigation of conduction properties of atomic wires has put into evidence drops of the conductance at a critical voltage [3]. This effect has been interpreted as a sign of the excitation of vibrational modes in the wire [4]. The highest-frequency longitudinal modes couple most strongly [4, 5]. In fact, it is clear that the longitudinal vibrations should have the strongest influence on conduction – a “longitudinal” process as well. The electron-vibration coupling constant is proportional to $\omega_{vibr}^{1/2}$ [4]. In spite of the sophistication of the theoretical tools used in the investigation of the properties of atomic wires, the vibrational characteristics seem not to be always fully explored. Some authors apply to atomic wires results obtained for long chains with periodic boundary condition. “Using the self-contained methods of optimizing the geometry, we obtain vibrational frequencies which are of the correct order of magnitude, usually to within a factor of 2.” [4] It seems that this precision could be improved.

Another sensitive aspect is the geometry of the leads which are bridged by the atomic wire. It may connect small cluster of atoms, or “pyramids”, on the two surfaces of the junction, or it may connect the plane surfaces of two semi-infinite crystals (see for instance [4], Fig. 1 and 2, or [6], Fig. 1).

A prerequisite of a correct understanding of the behavior of an atomic wire is the calculation of its vibrational properties. In this paper, we shall calculate the Green function of an atomic wire for “pyramidal” geometry.

The Green functions for atomic chains with various boundary conditions has been evaluated by Wallis and Maradudin [7], Bass [8] and Akjouj and coworkers [9]. In [7] the Green function of a finite harmonic chain with cyclic boundary conditions is obtained using a contour integration method. In [8] the Green function of the same chain, but satisfying various boundary conditions (cyclic, free ends, fixed ends, an end fixed and the other free) is computed using the connection between these response functions and the Cebyshev polynomials. Akjouj and coworkers [9] have developed a powerful method, of “cleavage operators”, to obtain Green’s functions for very general boundary conditions. In [9], the Green function for a chain with free ends is computed explicitly. Garcia Moliner and Velasco obtain the same results, using a more sophisticated approach [10].

In this paper, we shall propose a direct method for calculating the Green function of an atomic wire, starting from its definition [11]:

$$G(j, j'; \omega^2) = \sum_{r=1}^N \frac{a_r(j)a_r(j')}{\omega^2 - \omega_r^2}. \quad (1)$$

and using a summation formula obtained by one of the present authors (SC) [12]. This formula has already shown its efficiency in the theory of ferromagnets and orbitons [13]. In this context, it is useful to recall the classical paper of Louck on harmonic chains [14]. Louck examines the vibrations of a chain of N identical masses m , $m_1 = m_2 = \dots = m_n = \dots = m_N$, coupled with identical strings γ . The first ($n = 1$) and the last ($n = N$) mass are connected to a rigid wall with a string K , respectively K' . Various values of the ratios

$$\frac{K}{k} = s + 1, \quad \frac{K'}{k} = s' + 1. \quad (2)$$

simulate various boundary conditions. A recent discussion of Louck’s work, with applications in the theory of conduction in nanowires, may be found in [15].

It is possible to simulate the behavior of an atomic wire in any geometry, *i.e.* in any configuration of the leads, by tuning the values of s and s' in (2). For instance, an atomic wire between semi-infinite crystals corresponds, at least qualitatively, to $s = s' = 1$, and one with “pyramidal” connections – to $s = s' = 1$. For some particular values of s , s' ($= 0, -1$ or $+1$), Louck’s method gives exact expressions for all normal modes. However, for small values of N , relevant in many experimental situations involving atomic wires, Louck’s method gives exact results for arbitrary values of s , s' . So, in these cases, it is possible to obtain exact values of vibrational frequencies for any geometry.

In order to exemplify how important the boundary conditions can be for the evaluation of the vibration frequencies of a short atomic chain, let us mention here the formulae giving the normal mode frequency for a chain with cyclic boundary conditions, with fixed ends, and with “pyramidal” ($s = s' = 1$) connections:

$$\begin{aligned}\omega_k^{(c)} &= \omega_L \sin \frac{\pi k}{N}, & k = 1, 2, \dots, N. \\ \omega_k^{(f)} &= \omega_L \sin \frac{\pi k}{2(N+1)}, & k = 1, 2, \dots, N. \\ \omega_k^{(p)} &= \omega_L \sin \frac{\pi k}{2N}, & k = 1, 2, \dots, N.\end{aligned}\quad (3)$$

where ω_L is, as usual [16], the largest frequency of vibration:

$$\omega_L = \frac{4\gamma}{m}. \quad (4)$$

The normalized frequencies

$$f_k = \frac{\omega_k}{\omega_L}. \quad (5)$$

for the aforementioned boundary conditions, for a chain with $N = 4$ atoms, are:

$$\begin{aligned}f^{(c)} &= (0, 0.71, 0.71, 1). \\ f^{(f)} &= (0.31, 0.59, 0.81, 0.91). \\ f^{(p)} &= (0.38, 0.71, 0.92, 1).\end{aligned}$$

It is clear that, for short wires, the boundary conditions are crucial when computing the vibration modes.

Let us address now the main issue of our short note, the calculation of the Green function for a finite atomic wire for “pyramidal” connections. The orthonormalized amplitudes of atomic oscillations are

$$a_r(j) = \sqrt{\frac{2}{N}} \sin\left(j - \frac{1}{2}\right) \frac{r\pi}{N}. \quad (6)$$

Here, j refers to the atom, and r – to the vibration mode. It is easy to check that the amplitudes (6) satisfy the orthogonality condition:

$$\sum_{j=1}^N a_r(j) a_{r'}(j) = \delta_{rr'}. \quad (7)$$

So, using (1), the expression of the Green function is:

$$G(j, j'; \omega^2) = \frac{2}{N} \sum_{r=1}^N \frac{\sin\left(j - \frac{1}{2}\right) \frac{r\pi}{N} \sin\left(j' - \frac{1}{2}\right) \frac{r\pi}{N}}{\omega^2 - \omega_r^2}, \quad (8)$$

or

$$G(j, j'; \omega^2) = \frac{2}{\omega_L^2 N} \left\{ \sum_{r=1}^N \frac{\cos\left(j + j' - 1\right) \frac{r\pi}{N}}{p - \cos \frac{r\pi}{N}} - \sum_{r=1}^N \frac{\cos\left(j + j'\right) \frac{r\pi}{N}}{p - \cos \frac{r\pi}{N}} \right\}, \quad (9)$$

where

$$p = 1 - 2f^2 = 1 - 2\left(\frac{\omega}{\omega_L}\right)^2. \quad (10)$$

The summation formula proposed by Cojocaru [12]:

$$\frac{1}{N} \sum_{m=0}^{N-1} \frac{\cos\left(2\pi \frac{m}{N} M\right)}{p - \cos\left(2\pi \frac{m}{N}\right)} = \frac{1}{\sinh v} \left(\coth \frac{Nv}{2} \cosh Mv - \sinh Mv \right), \quad p = \cosh v \quad (11)$$

gives, after simple manipulations:

$$\begin{aligned} \sigma_N(M) &\equiv \frac{1}{N} \sum_{r=0}^{N-1} \frac{\cos \frac{rm}{N} \mu}{p - \cos \frac{r\pi}{N}} = -\frac{1}{2N} \left(\frac{1}{p-1} + \frac{\cos M\pi}{p+1} \right) + \\ &+ \frac{1}{\sinh v} (\coth Nv \cos Mv - \sinh Mv). \end{aligned} \quad (12)$$

and

$$G(j, j'; \omega^2) = \frac{2}{\omega_L^2} \{ \sigma_N(j + j' - 1) - \sigma_N(j - j') \}. \quad (13)$$

Equation (13) is the main result of our short note. The Green function has an explicit dependence on N , and an implicit one, through (10) and (3).

Let us recall here the expression of the Green function for a harmonic chain with fixed ends, according to Bass [8]:

$$G^{(f)}(j, j'; \omega^2) = \frac{2}{\omega_L^2} \{ \sigma_{2N}(j + j') - \sigma_{2N}(j - j') \}. \quad (14)$$

Here, σ_N corresponds to the function G_N used by Bass (up to a constant factor). These formulae are written for a limited frequency range, corresponding to $p > 0$, according to eq. (10), (11), but that can be easily analytically continued to any p (see for instance [9]).

So, these Green's functions ((13), (14)) describe the vibrations of an atomic wire with two geometries of the wire-lead interface. As already mentioned, tuning

the values of s , s' (see eq. (1)), similar Green's functions could be found, in principle, according to other specific boundary conditions. Using simple transformations, eq. (13) – as well as eq. (14) – may generate the Green functions for diatomic or more complex chains [16]. The knowledge of this Green function allows the calculation of the densities of states per site, the vibrational contribution to the thermodynamic functions, the influence of isolated defects, etc. [16]. Taking into account the similarities between harmonic chains, tight binding Hamiltonians, and spin waves in 1D ferromagnets, these results may be relevant also in these fields.

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