

# On Fourier Components in Modulation Spectroscopy

*S. K. Abdelraheem*

*Physics Department, Faculty of Sciences, El-Minia University, Egypt*

*A theoretical analysis of the output current of a tunneling experiment involving both square root and logarithmic singularities in the density of states have been discussed. The analysis has been done by calculating Fourier coefficients involved in the experiment.*

## 1. Introduction:

Quantum mechanical tunneling has a wide range of practical applications [1]. One of these is the normal metal-insulator –superconductor (MIS)[2]. The normal metal and superconductor may take density of states of a two-dimensional character [3] having the usual three singularities [4], which are the minimum, the maximum and the saddle point. Both maximum and minimum are of step like form and the saddle point is of logarithmic –like form. Practically the step singularity is weakened to the square root one [5]. In recent years remarkable applications in optoelectronic devices using nanostructure materials utilize the two-dimensional character of the density of states. The current voltage characteristics in MIS or other kinds of multi-layers are often desired to fine or weak the current by using modulation spectroscopy, which can be divided into three kinds which are amplitude, frequency, phase modulations [6].

## 2. Fourier Components in Modulation Spectroscopy:

Let the out put current be a function of voltage such that

$$I = F(V) \quad (1)$$

and for the sake of simplicity both the capacity and inductive are omitted. to weak or fine the current by amplitude modulation we write the potential  $v$  in the form

$$V = u_0 + u \cos(\omega t) ,$$

where  $u_0$  is a d.c. potential difference,  $\omega$  is the frequency and  $u$  is the amplitude modulation, then Eqn. (1) becomes

$$I = F[u_0 + u \cos(\omega t)] \quad (2)$$

Fourier components of Eqn. (2) are in the form

$$A_0 = \omega / \pi \int_0^{\pi/\omega} F[u_0 + u \cos(\omega t)] dt \quad (3)$$

$$A_n = \omega / \pi \int_0^{\pi/\omega} F[u_0 + u \cos(\omega t)] \cos(n\omega t) dt \quad (4)$$

where  $n = 1, 2, 3, \dots$ , and the sine components are zero because the function  $F$  is even. The coefficients  $A$ 's depend on the form of the function  $F$ . For non-smooth function the singularities are connected with the density of states of elementary excitations such as electrons and phonons. The function  $F$  can have two possible forms either

$$F(x) = (x - c)\theta(x - c) \quad (5)$$

where,

$$\begin{aligned} \theta(x - c) &= 1 && x=c \\ &= 0 && \text{otherwise} \end{aligned} \quad (6)$$

or

$$F(x) = \log(1/x) \quad (7)$$

Let us now deal with these two forms of singularities in detail.

### 2.1. Square Root Singularity

The density of states  $D(E)$  can be expressed as [8],

$$\begin{aligned} D(E) &= 1/\sqrt{E - \Delta} && |E| > \Delta \\ &= 0 && |E| < \Delta \end{aligned} \quad (8)$$

where  $E = 0$  at the Fermi level which lies in the middle of the superconductor energy gap and  $2 \Delta$  is energy gap width in the super conductor. In connection with Eqn. (5) appears in normal metal-insulator-superconductor and near the singularity at  $E = \Delta$ , the density of states can be written approximately as:

$$D(E) = (1/\sqrt{E - \Delta}) \theta(E - \Delta) \tag{9}$$

The current density  $j$  can be related to the density of states by

$$\frac{dj}{dV} = D(E)$$

so that the direct integration of Eqn. (9) gives

$$j = \sqrt{E - \Delta} \theta(E - \Delta) \tag{10}$$

This means that the function to be inserted in Eqn. (3) and (4) is

$$F(V) = \sqrt{V} \theta(V) \tag{11}$$

Defining the dimensionless quantities

$$p = \cos(\omega t), \quad B_n = A_n / \sqrt{u} \quad \text{and} \quad q = u_0 / u,$$

one can then rewrite the first three cosine components  $B_0, B_1$  and  $B_2$  as

$$B_0 = 2/\pi \int_{-1}^1 (\sqrt{(q+p)} \theta(q+P) / \sqrt{1-p^2}) dp \tag{12}$$

$$B_1 = 2/\pi \int_{-1}^1 (\sqrt{(q+p)} \theta(q+P) / \sqrt{1-p^2}) p dp \tag{13}$$

$$B_2 = 2/\pi \int_{-1}^1 (\sqrt{(q+p)} \theta(q+P) / \sqrt{1-p^2}) (2p^2 - 1) dp \tag{14}$$

**2.2. Logarithmic Singularity**

The form of singularity of Eqn. (7) appears in the experiments such as hetrostructures (8&9) and in connection with the density of states and their

changes. Recently, the change in the density of states has been dealt with in resonant tunneling structures as if it was a transmission coefficient. Now  $F$  can be obtained by the direct integration of Eqn. (7) and then one gets

$$F(x) = -x \log |x| + x \quad (15)$$

and for the non-vanishing Fourier components we have

$$A_0 = 1/\pi \int_0^\pi -(q + \cos x) \{\log |q + \cos x| - 1\} dx \quad (16)$$

$$A_n = 1/\pi \int_0^\pi -(q + \cos x) \{\log |q + \cos x| - 1\} \cos(nx) dx \quad (17)$$

where

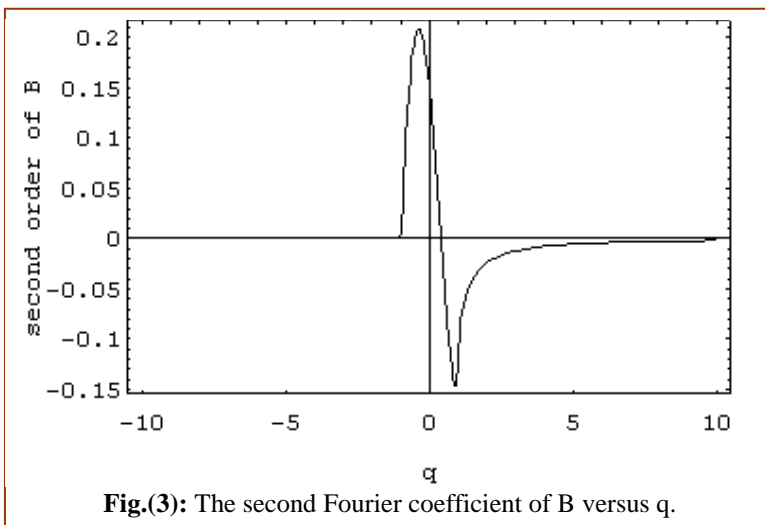
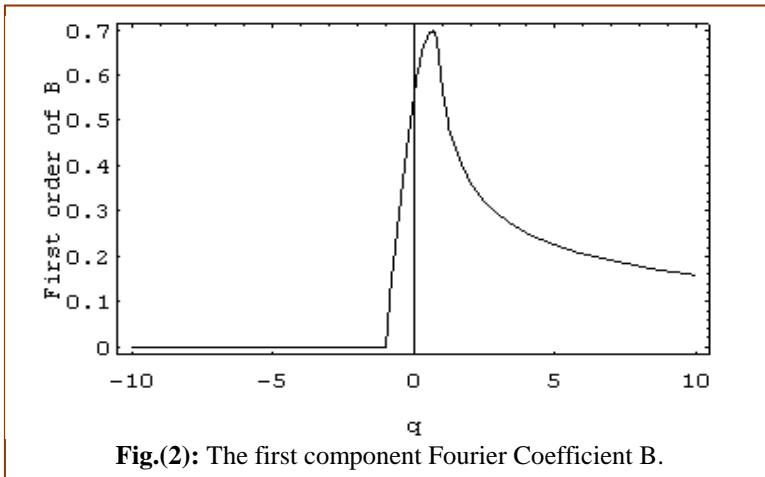
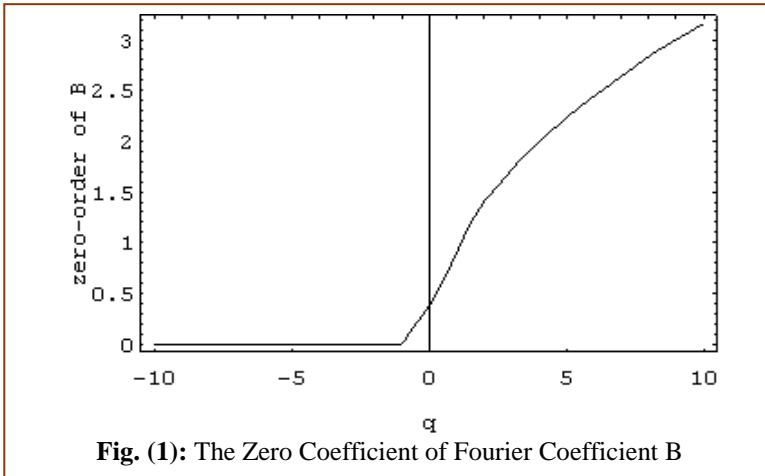
$$x = \omega t \quad n = 1, 2.$$

### 3. Calculation and Discussion:

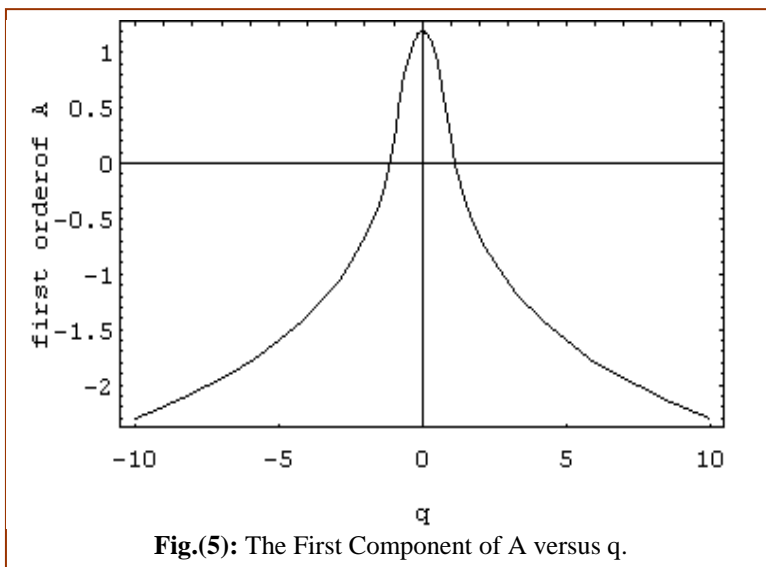
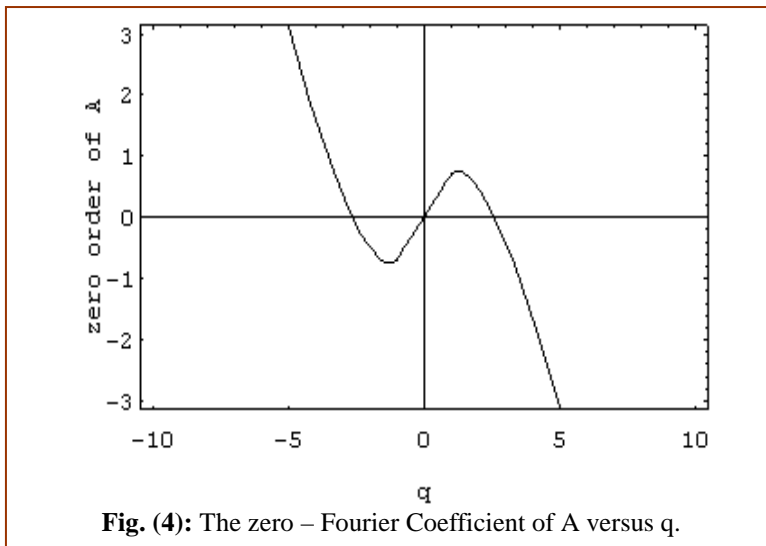
The importance of Fourier components can be realized when we look at Eqn. (1) in which  $dI/dV$  gives the conductance of the device where the current pass through. Also the second derivative of current has its importance.

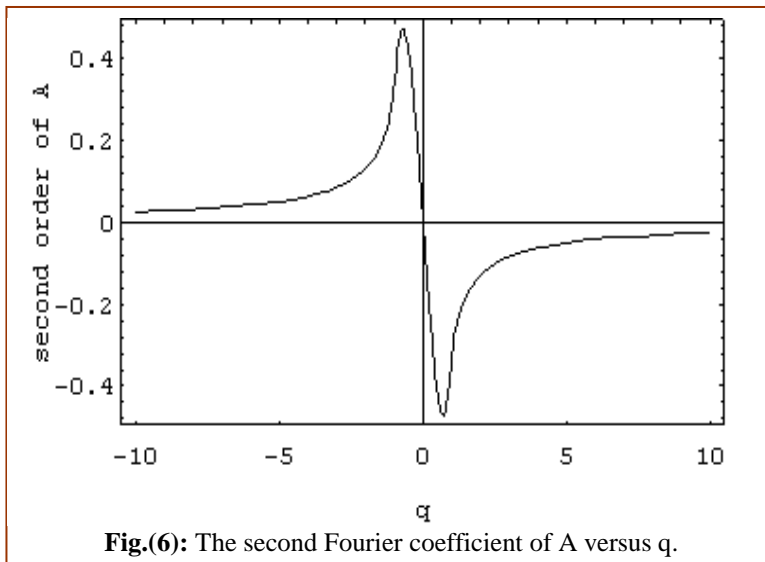
Calculation of Fourier components for NIS system where the second root singularity is important starts by numerical integration of equation 11-13 to get the Fourier coefficients  $B_n$  where  $n=0, 1, 2$ . These coefficients are plotted versus  $q$  as shown in Figs. (1), (2) and (3) for  $B_0$ ,  $B_1$  and  $B_2$ , respectively. From Fig (1), it can be noticed that the relation between the modulation amplitude and the coefficient  $B_0$  (zero order) is singular when the biasing voltage is comparable with the modulation amplitude and there is an inflection point when  $q = \pm 1$ . The coefficient  $B_1$  (the first order) is exactly straight line near  $q = -1$  and has also inflection point near  $q = 1$  and as  $q$  gets larger the first order coefficient takes the form of a negative square root of  $q$ . When I-V curves are non smooth the differential conductivity shows clearly the signature of singularity on the I-V curves or at the same footing density of states  $D(E)$  curves. This is clarified by Fig. (3).

Concerning the logarithmic singularity, we see from Eqn. (16) that  $(q + \cos x)$  might be negative, so we always take the modulus of that value due to the fact that a negative value is not allowed for a logarithmic function.



The values  $A_0$ ,  $A_1$  and  $A_2$  given by Eqn. (16) and (7) are plotted in Figs.(4), (5) and (6), respectively. From these figures the differential conductivity and its derivative give more structures to analyze the results of an experiment involving the logarithmic singularity with high resolution.





#### 4. Conclusion:

From the calculation of Fourier coefficients, one can control the structure in the out put current for the square root and logarithmic singularities in terms of the biasing voltage used in the amplitude modulation.

#### 5. References:

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