

The Friedel sum rule at Fano resonances

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2009 J. Phys.: Condens. Matter 21 285303

(<http://iopscience.iop.org/0953-8984/21/28/285303>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 29/05/2010 at 20:35

Please note that [terms and conditions apply](#).

The Friedel sum rule at Fano resonances

P Singha Deo

Unit for Nano Science and Technology, S N Bose National Centre for Basic Sciences,
JD Block, Sector III, Salt Lake City, Kolkata 98, India

Received 18 March 2009

Published 18 June 2009

Online at stacks.iop.org/JPhysCM/21/285303

Abstract

If a mesoscopic system is non-chaotic or non-ergodic then the thermodynamic and transport properties do not depend on the impurity averaged density of states. We show that the partial density of states as well as the density of states of a given system with a given impurity configuration can be determined exactly from the asymptotic wavefunction (or scattering matrix) at the resonances. The asymptotic wavefunction can be determined experimentally without any knowledge about the quantum mechanical potential (including electron–electron interaction) or wavefunction in the interior of the system. Some counterintuitive relations derived here allow this.

For bulk samples, ensemble averaging makes it unnecessary to know the exact impurity configuration and the exact Hamiltonian of the sample. This is because experiments can only observe ensemble averaged physical properties. Ensemble averaging works because of the well known ergodicity hypothesis and the fact that sample to sample fluctuations are not very large [1]. For mesoscopic systems, even when dealing with an ensemble, sample to sample fluctuations are often so large that we cannot talk of any averaged physical quantity [2]. If disorder averaging cannot be done, then it becomes necessary to know the exact impurity configuration of a system, a seemingly impossible task for an experimentalist. Also sometimes for mesoscopic systems ergodicity itself does not hold for a single sample, a fact which is further illustrated later. Assumption of equal *a priori* probability also breaks down. In this work we derive some exact relations. These relations are not only counterintuitive but can also provide a way for experimentalists to bypass the requirement of knowledge of the exact Hamiltonian of the system to arrive at thermodynamic and transport properties of a mesoscopic system.

Consider an arbitrary potential $V(x, y)$ in the shaded region Ω of figure 1. The z degree of freedom is usually frozen due to strong confinement in the z direction. This potential defines a mesoscopic system that could be a quantum dot or a quantum ring or anything else [3]. Typically such a system is coupled to leads or measuring probes. The leads connect the system to reservoirs that are at fixed chemical potentials. The reservoirs inject (or absorb) electrons to (or from) the system through the leads. We consider quasi-one-dimensional (Q1D) single-channel leads as in most experiments. When leads are multichannel, we do not have enough control over the properties of the system to make it of practical use [2]. By

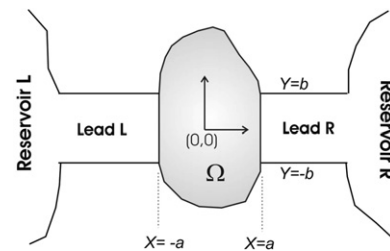


Figure 1. A mesoscopic system (shaded region) coupled to reservoirs through leads. The origin of the coordinates is shown. The figure is drawn in the most general way. Normally, if $F(x)$ and $G(x)$ are smooth functions and the potential in the shaded region has some symmetries, then the system can be non-ergodic. Also if $F(x)$ and $G(x)$ are extremely rough then there can be localized states, surface localized states and scarred states which again can make the system non-ergodic. Our mathematical analysis is for any arbitrary $F(x)$ and $G(x)$. Equations (2)–(6) define the quasi-one-dimensional nature of the system and the leads.

taking specific forms of $V(x, y)$ we can control the strength of the coupling between the system and the leads. This is explained in more detail later. For a fully chaotic (or ergodic) system (such that equal *a priori* probability is expected), electrons will access all the states in the system especially when the coupling to the leads is very weak and the electron spends sufficient time in the system. However, for a non-chaotic (or non-ergodic) system, all the states will not be accessed (breakdown of equal *a priori* probability). Only part of the states will be accessed which depends on the position and details of the leads and the system, that will constitute the partial density of states (PDOS). For mesoscopic systems, even a chaotic system may not exhibit equal *a priori* probability [4]. So the contribution of these electrons to

thermodynamic observables like the quantum capacitance and heat capacity of the system, as well as the linear response non-equilibrium effects, will be determined by this PDOS [5]. This PDOS cannot be determined from the Hamiltonian of the isolated system as the PDOS depends on initial conditions (that is, through which lead the electrons enter the system and through which lead they leave, as well as the characteristics of the leads and that of the system). However, the scattering matrix depends on these factors. So the scattering matrix has more information than the Hamiltonian of the isolated system and the scattering matrix formulation is very important for mesoscopic systems [6]. For a recent review on mesoscopic transport we refer the reader to [7].

The many-body Hamiltonian for an N -particle system is a function of $3N$ coordinates. It has been proved that the motion of one of these N particles is governed by an effective potential that is just a one-body potential and a function of three coordinates [8]. This is known as the Hohenberg–Kohn theorem and it is exact. So in the preceding paragraph, when we refer to the confining potential $V(x, y)$ of the system, we are referring to this one-body effective potential V_{eff} , that includes electron–electron interaction exactly. The determination of this one-body potential is however very difficult and has until now not been obtained exactly [9]. Approximate schemes like local density approximations are used. For bulk systems these are fairly good, although approximate methods are used for obtaining the effective potential, but the same need not be the case for finite systems. So for mesoscopic systems, if we can bypass the determination of the internal details, the exact Hamiltonian and the effective potential of the system, by using the S -matrix then the S -matrix includes the effect of electron–electron interaction exactly. However, we would like to mention that electron–electron interaction can in principle be obtained for finite systems but the impurity configuration, in principle, cannot be known. This makes the single-particle scattering problem more formidable than many-body effects.

The approach proposed in this paper is due to some recent experiments [10, 11] that are motivated by the possibility of obtaining important information from the scattering phase shift. So the present work is an effort to identify information that can be obtained from such experiments. A series of experiments [12, 13] also tell us that resonances in such a system as that schematically shown in figure 1 are Fano resonances. Recently it has been shown for a delta function potential in a quantum wire that at the Fano resonance the density of states (DOS) and partial density of states (PDOS) can be determined exactly from semi-classical formulae involving the energy derivative of scattering phase shift (the Friedel sum rule or FSR), although the Fano resonance is a purely quantum phenomenon [14]. Hence earlier works [14] are for a specific potential $V(x, y) = \gamma\delta(x - x_i)\delta(y - y_i)$ and hence of academic interest. In the first of these works the DOS was explicitly calculated from the integration of the wavefunction for the δ function potential and it was shown graphically as well as mathematically that FSR becomes exact at the Fano resonance. In the second of these works the quantum regime and semi-classical regime of the above

mentioned δ function potential were identified and it was shown that FSR becomes exact in a quantum regime. A physical picture was provided, based on the dispersion of wavepackets, showing why FSR becomes exact in the quantum regime of the above mentioned potential. In this work we show that FSR becomes exact at a Fano resonance for any general potential $V(x, y)$ that can define a real disordered (or clean) ring or dot. Thus the results can be practically used as described earlier.

We shall use the following identity to arrive at our conclusions. It can be rigorously derived for one dimension (1D) and is naturally also true for the quasi-one-dimensional (Q1D) case [15] that involves tracing over the sub-band index. In simpler form [16], for any such system schematically shown in figure 1,

$$-\int_{\Omega'} d^3r \Lambda_{mn}^* \frac{\delta \Lambda_{mn}}{\delta V(r)} = \Lambda_{mn}^* \frac{d\Lambda_{mn}}{dE_m} + \frac{1}{4E_m} (\Lambda_{mn} - \Lambda_{mn}^*). \quad (1)$$

Here Λ denotes the scattering matrix and E_m denotes the kinetic energy in the m th channel which is further defined below. Ω' is the volume of the region where the wavefunction is different from the asymptotic wavefunctions and it may or may not coincide with Ω , depending on the scattering potential.

The Schrödinger equation describing the system is

$$-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi(x, y) + V(x, y)\psi(x, y) = E\psi(x, y). \quad (2)$$

For $|x| < a$, $V(x, y)$ has to be such that it can create at least one bound state (otherwise there will be no Fano resonance). For $|x| \geq a$, $V(x, y) = V_c(y)$, where $V_c(y)$ is the confinement potential in the leads. The most general solution to equation (2) in the different regions of figure 1 is

$$\psi^{(L)}(x, y) = \frac{e^{ik_m x}}{\sqrt{k_m}} \theta_m(y) + \sum_{n=1}^{\infty} \frac{e^{-ik_n x}}{\sqrt{k_n}} r_{nm} \theta_n(y) \quad (x \leq -a) \quad (3)$$

$$\psi^{(R)}(x, y) = \sum_{n=1}^{\infty} \frac{e^{ik_n x}}{\sqrt{k_n}} t_{nm} \theta_n(y) \quad (x \geq a). \quad (4)$$

Here $\theta_n(y)$ is the solution to the following equation that holds for $|x| \geq a$:

$$\left[-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial y^2} + V_c(y) \right] \theta_n(y) = \epsilon_n \theta_n(y). \quad (5)$$

Therefore,

$$E = \epsilon_n + \frac{\hbar^2 k_n^2}{2\mu} = \epsilon_n + E_n. \quad (6)$$

If $\epsilon_n > E$, then one can see from equation (6) that k_n is imaginary (the mode is evanescent). The electron is incident along the m th channel which implies $\epsilon_m < E$. For all $n \leq m$, $\epsilon_n < E$ and such channels are propagating. For $n > m$, $\epsilon_n > E$, implying that these channels are evanescent. For $n \leq m$, r_{nm} and t_{nm} give the reflection and transmission amplitudes, respectively. They also constitute the elements of the scattering matrix Λ . For $n > m$, t_{nm} and r_{nm} give the amplitude of transition from the propagating mode to the n th

evanescent mode in the right lead and left lead, respectively. However, they are not scattering matrix elements.

We can now define two functions $\psi^{(ev)}(x, y)$ and $\psi^{(od)}(x, y)$ such that $\psi^{(ev)}(x, y) = \psi^{(ev)}(-x, y)$ and $\psi^{(od)}(x, y) = -\psi^{(od)}(-x, y)$:

$$\psi^{(ev)}(x, y) = \sum_{n=1}^{\infty} (\delta_{nm} e^{-ik_n x} - S_{nm}^{(ev)} e^{ik_n x}) \frac{\theta_n(y)}{\sqrt{k_n}} \quad (7)$$

$$\psi^{(od)}(x, y) = \sum_{n=1}^{\infty} (\delta_{nm} e^{-ik_n x} - S_{nm}^{(od)} e^{ik_n x}) \frac{\theta_n(y)}{\sqrt{k_n}}. \quad (8)$$

Then one can see that $\psi^{(L)}$ as well as $\psi^{(R)}$ is given by

$$\frac{1}{2}(\psi^{(ev)} - \psi^{(od)}) \quad (9)$$

where

$$r_{nm} = -(S_{nm}^{(od)} + S_{nm}^{(ev)})/2 \quad (10)$$

$$t_{nm} = (S_{nm}^{(od)} - S_{nm}^{(ev)})/2. \quad (11)$$

This works because any function can be written as a sum of an even function and an odd function. And any square matrix can be written as a sum of a symmetric matrix and an antisymmetric matrix.

Due to the same principle, the wavefunction in the scattering region can be written as a sum of an even function and an odd function. We denote them as $\phi_n^{(ev)}(x, y)$ and $\phi_n^{(od)}(x, y)$:

$$\phi_n^{(ev)}(x, y) = \sum_{m=1}^{\infty} c_m \chi_m^{(ev)}(x, y) \quad (12)$$

$$\phi_n^{(od)}(x, y) = \sum_{m=1}^{\infty} c_m \chi_m^{(od)}(x, y) \quad (13)$$

where $\chi^{(ev)}$ and $\chi^{(od)}$ satisfy the Schrödinger equation (2) with $V(x, y) = 0$ in the region Ω . Therefore $\chi^{(ev)}$ and $\chi^{(od)}$ will satisfy the following equations:

$$\chi_m^{(eo)}(a, y) = \theta_m(y) \quad \text{for } |y| \leq b \quad (14)$$

$$\chi_m^{(eo)}(x, y) = 0 \quad \text{for } y = F(x) \text{ or } G(x) \quad (15)$$

$$\chi_m^{(ev)}(x, y) = \chi_m^{(ev)}(-x, y) \quad (16)$$

$$\chi_m^{(od)}(x, y) = -\chi_m^{(od)}(-x, y). \quad (17)$$

$F(x)$ and $G(x)$ define the two curves at the upper and lower boundaries of the region Ω . Here ‘eo’ stands for ‘ev’ or ‘od’. One can define the following matrix elements:

$$F_{n,m}^{(eo)} = \frac{1}{b(k_m k_n)^{\frac{1}{2}}} \int_{-b}^b \theta_n(y) \left(\frac{\partial \chi_m^{(eo)}}{\partial x} \right)_{x=a} dy. \quad (18)$$

Now we require $\phi_n^{(eo)}$ and $\frac{\partial \phi_n^{(eo)}}{\partial x}$ to be continuous at $x = a$ for all $|y| \leq b$. Thus we get

$$\sum_{m=1}^{\infty} (\delta_{n,m} e^{-ik_m a} - S_{m,n}^{(eo)} e^{ik_m a}) \frac{\theta_m(y)}{\sqrt{k_m}} = \sum_{m=1}^{\infty} c_m \theta_m(y) \quad (19)$$

$$\begin{aligned} & - \sum_{n=1}^{\infty} i\sqrt{k_m} (\delta_{n,m} e^{-ik_m a} + S_{m,n}^{(eo)} e^{ik_m a}) \theta_m(y) \\ & = \sum_{m=1}^{\infty} c_m \left(\frac{\partial \chi_m^{(eo)}}{\partial x} \right)_{x=a}. \end{aligned} \quad (20)$$

Multiplying equations (19) and (20) with $\frac{1}{b}\theta_n(y)$ and integrating from $y = -b$ to b and then combining them we get a single matrix equation:

$$\sum_{m=1}^{\infty} (F_{qm}^{(eo)} - i\delta_{qm}) e^{ik_m a} S_{mn}^{(eo)} = (F_{qn}^{(eo)} + i\delta_{qn}) e^{-ik_n a} \quad (21)$$

or

$$S_{mn}^{(eo)} = e^{-ik_m a} [1 + 2i(F^{(eo)} - i1)^{-1}]_{mn} e^{-ik_n a}. \quad (22)$$

It is known in scattering theory that the bound states of the potential $V(x, y)$ can also be obtained from equations (7) and (8) by omitting the terms $\delta_{nm} e^{ik_n x}$. Without this term equations (7) and (8) are solutions to the equation (2) with correct boundary condition wherein there is no incident wave. Analysis identical to that leading to equation (21) in this case gives

$$\sum_{m=mt}^{\infty} [F_{qm}^{(eo)} - i\delta_{qm}] e^{-\kappa_m a} S_{mn}^{(eo)} = 0. \quad (23)$$

Here mt is the threshold value of m for which bound states exist. And $\kappa_m = ik_m$. For $m < mt$ states will be scattering states. Supposing that only the first channel is propagating, then $mt = 2$. This will be further illustrated soon. Solutions to equation (23) or solutions to the following equation will give bound states:

$$\det[F_{cc}^{eo} - i1] = 0. \quad (24)$$

Here ‘cc’ means closed channel (i.e., channels for which $m \geq mt$). Let us partition $F^{(eo)}$ into propagating and evanescent (or closed) channels:

$$F^{(eo)} = \begin{pmatrix} F_{pp}^{(eo)} & F_{pc}^{(eo)} \\ F_{cp}^{(eo)} & F_{cc}^{(eo)} \end{pmatrix}. \quad (25)$$

Therefore,

$$\begin{aligned} & \begin{pmatrix} F_{pp}^{(eo)} - i1 & F_{pc}^{(eo)} \\ F_{cp}^{(eo)} & F_{cc}^{(eo)} - i1 \end{pmatrix} \begin{pmatrix} F_{pp}^{(eo)} - i1 & F_{pc}^{(eo)} \\ F_{cp}^{(eo)} & F_{cc}^{(eo)} - i1 \end{pmatrix}^{-1} \\ & = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned} \quad (26)$$

From this one can show that

$$[(F^{(eo)} - i1)^{-1}]_{pp} = [F_{pp}^{(eo)} - i1 - F_{pc}^{(eo)}(F_{cc}^{(eo)} - i1)^{-1}F_{cp}^{(eo)}]^{-1}. \quad (27)$$

So from equations (22) and (27) (for m and n being propagating channels)

$$\begin{aligned} S_{mn}^{(eo)} & = e^{-ik_m a} [1 + 2i[F_{pp}^{(eo)} \\ & - F_{pc}^{(eo)}(F_{cc}^{(eo)} - i1)^{-1}F_{cp}^{(eo)} - i1]_{mn}^{-1}]_{mn} e^{-ik_n a} \\ & = e^{-ik_m a} [(G^{(eo)} - i1)^{-1}(G^{(eo)} + i1)]_{mn} e^{-ik_n a} \end{aligned} \quad (28)$$

where

$$G_{mn}^{(eo)} = [F_{pp}^{(eo)} - F_{pc}^{(eo)}(F_{cc}^{(eo)} - i1)^{-1}F_{cp}^{(eo)}]_{mn}. \quad (29)$$

If there is only one propagating channel, then $m = n = 1$. Also for one propagating channel, $p = 1$. Hence $G^{(eo)}$ becomes a number. Therefore, from equation (28)

$$S_{11}^{(eo)} = e^{-2ik_1 a} \frac{G^{(eo)} + i}{G^{(eo)} - i} = e^{2i(\text{arccot}[G^{(eo)}] - k_1 a)} = e^{2i\delta^{(eo)}} \quad (30)$$

where

$$G^{(eo)} = F_{11}^{(eo)} - \sum_{m=2, n=2} F_{1m}^{(eo)} [(F_{cc}^{(eo)} - i1)^{-1}]_{mn} F_{n1}^{(eo)} \quad (31)$$

and

$$\delta^{(eo)} = \text{arccot}[G^{(eo)}]. \quad (32)$$

Note that for equation (1), the definition of the scattering phase shift requires us to absorb the term $k_1 a$ in $\delta^{(eo)}$. All of the infinite S_{mn} appear in S_{11} through F_{cc} , which carries information for the entire Hilbert space accessed by the incident wave. For non-ergodic systems there can be many more states not accessed by the incident wave, i.e., the transition amplitude between these states and the incident wave being 0. These states are not populated. So they contribute neither to the DOS and PDOS nor to the scattering matrix. Trivial examples are cases like that when the incident wave has a certain symmetry that is incompatible with the symmetry of these states. More generally, there can be localized and scarred states that are known to occupy a subset of the Hilbert space and do not connect to the rest. Once again the position and characteristics of the leads will determine which states will be accessed and which not. Due to ergodicity, bulk samples are isotropic, wherein the correlation function between two points depends on the separation between the points and not on the position of the points. For such ergodic bulk samples the PDOS is an ill-defined quantity. If equal *a priori* probability holds, then by definition the PDOS cannot exist.

Threshold energy E for the second channel is given by $\frac{2\mu}{\hbar^2}(E - \epsilon_2) > 0$. Below this energy the second channel can have bound states. Such bound states will occur at energies given by the solution to equation (24). At these energies the first channel will be propagating as its threshold is given by $\frac{2\mu}{\hbar^2}(E - \epsilon_1) > 0$ and S_{11} is given by equation (30). But at these energies $G^{(eo)}$ will diverge as it includes matrix elements of $[F_{cc}^{(eo)} - i1]^{-1}$ as can be seen from equations (31) and (24). That in turn implies that at a Fano resonance (as can be seen from equation (32))

$$\delta^{(ev)} = m\pi \quad \text{and} \quad \delta^{(od)} = n\pi. \quad (33)$$

This is consistent with the fact that at the Fano resonance $t_{11} = 0$ (which is a necessary requirement for a Fano resonance) as can be seen from equations (11), (30) and (33). Therefore $t_{11} - t_{11}^* = 0$ at the Fano resonance. Also from equations (10) and (33) at the Fano resonance $r_{11} = -\frac{\cos(2\delta^{(ev)}) + \cos(2\delta^{(od)})}{2}$ and hence

$$r_{11} - r_{11}^* = 0. \quad (34)$$

Transmission zero ($t_{11} = 0$) does not guarantee that the right-hand side (RHS) of the above equation becomes 0, because one can see from equations (11) and (30) that $t_{11} = \frac{e^{2i\delta^{(od)}} - e^{2i\delta^{(ev)}}}{2}$. Hence $t_{11} = 0$ can be due, at some energies, to $\delta^{(od)} = \delta^{(ev)}$, none of them being an integer times π . Only equation (33) obtained from a Fano resonance makes the RHS of equation (34) be 0. Therefore, at the Fano resonance

$$\Lambda - \Lambda^\dagger = \begin{pmatrix} r_{11} - r_{11}^* & t_{11} - t_{11}^* \\ t_{11} - t_{11}^* & r_{11}^* - r_{11} \end{pmatrix} = 0. \quad (35)$$

Therefore at the Fano resonance, from equations (1) and (35),

$$\begin{aligned} -\frac{1}{4\pi i} \int_{\Omega'} d^3r \Lambda_{mn}^* \frac{\delta \Lambda_{mn}}{\delta V(r)} - HC &= \frac{1}{4\pi i} \left(\Lambda_{mn}^* \frac{d\Lambda_{mn}}{dE} - HC \right) \\ &= \frac{1}{2\pi} |\Lambda_{mn}|^2 \frac{d[\text{Arg}(\Lambda_{mn})]}{dE}. \end{aligned} \quad (36)$$

Here $\text{Arg}(\Lambda_{mn}) = \text{Arctan} \frac{\text{Im} \Lambda_{mn}}{\text{Re} \Lambda_{mn}}$. The complicated integral involving the local potential on left-hand side (LHS) is the PDOS for an electron incident in channel n and scattered to channel m . So at the Fano resonance the PDOS can be determined exactly from the scattering phase shift $\frac{d[\text{Arg}(\Lambda_{mn})]}{dE}$ and $|\Lambda_{mn}|^2$. If $m = 1$ and $n = 2$ then the RHS of (36) is $\frac{1}{2\pi} |t_{11}|^2 \frac{d\text{Arg}(t_{11})}{dE}$. Both these quantities ($|t_{11}|^2$ and $\text{Arg}(t_{11})$) i.e., transmission probability and transmission phase) were measured in [10, 12, 13]. So the LHS which is the PDOS for a transmitted particle in the above mentioned experiments can be obtained from the experimental data at the Fano resonance. Summing over m and n we get at the Fano resonance

$$\begin{aligned} -\frac{1}{4\pi i} \sum_{mn} \int_{\Omega'} d^3r \Lambda_{mn}^* \frac{\delta \Lambda_{mn}}{\delta V(r)} - HC &= \frac{d[\frac{1}{2\pi} \log \text{Det}[\Lambda]]}{dE} \\ &= \left[|r_{11}|^2 \frac{d\text{Arg}(r_{11})}{dE} + |t_{11}|^2 \frac{d\text{Arg}(t_{11})}{dE} \right] / \pi \end{aligned} \quad (37)$$

which is the Friedel sum rule. Here again $|r_{11}|^2$ is reflection probability and $\text{Arg}(r_{11})$ is reflection phase. The LHS is the DOS and the RHS is same as the RHS of equation (36) summed over m and n and simplified. So in this case apart from the data of [10, 12, 13] one needs similar data for the reflected electrons. This was done in [17].

FSR is expected to hold only for bulk samples that are in the semi-classical limit. For finite systems that are in a quantum regime there is always a correction term arising from $\frac{1}{4E_m}(\Lambda_{mn} - \Lambda_{mn}^*)$. For semi-classical systems this term is small. For details one can see [16] and references therein. Semi-classical behaviour occurs when the energy E_m is large compared to the potential because then the de Broglie wavelength is much smaller than the scales determining the potential. $(\Lambda_{mn} - \Lambda_{mn}^*)$ depends on the characteristics and scales of the potential. Essentially at high energies nothing is reflected, typically like the case for a classical particle. Fano resonances are different. These can occur at high energies and can also occur at low energies. Around a Fano resonance, quantum mechanical reflection is very high, phase fluctuations are very strong; and it is due to pure quantum interference effects. In Q1D, although the Fano resonance is a purely quantum interference phenomenon, the correction terms are exactly 0 making the Friedel sum rule exact. The correction terms are extremely non-universal (resonances are generally characterized by the line shape, i.e., $|\Lambda_{mn}|^2$, and scattering phase shifts, $\text{Arg}(\Lambda_{mn})$), and also depend on sample specific parameters (e.g., E_m depends on $V_c(y)$ as well as material parameters like the bottom of the conduction band, effective mass μ , etc).

In regimes where the single-particle picture is valid (it is always valid when Coulomb interaction can be ignored and sometimes valid even in the presence of Coulomb interactions through an effective potential V_{eff}), most mesoscopic systems

coupled to leads can be described using a Schrödinger equation of the form given in equation (2). For example, if $F(x) = \sqrt{R^2 - x^2}$, $G(x) = -\sqrt{R^2 - x^2}$ and $V(x, y) = -V_0 + \text{ran}(x, y) + V_{\text{eff}}$, where $\text{ran}(x, y)$ is a random function of x and y and V_0 is a positive constant, then we get a disordered circular dot coupled to leads. If we set $V(x, y) = -V_0 + V_{\text{eff}}$ then we get a clean circular dot. Dropping the interaction term, if we set $V(x, y) = \text{per}(x, y) + \text{ran}(x, y) - V_0$ where $\text{per}(x, y)$ is a periodic potential, then it can account for the underlying lattice structure. If we take $V(x, y) = V_L$ for $(a - \epsilon) < |x| < a$ and $V(x, y) = \text{ran}(x, y) - V_0$ in the rest of the shaded region in figure 1, then we get a disordered circular dot weakly coupled to leads. Here V_L is a large potential and ϵ is a small number. Alternatively, we can make $F(x) = \infty$, $G(x) = -\infty$ and $V(x, y) = A(x^2 + y^2) + \text{ran}(x, y)$; then we get a disordered parabolic dot (the potential in the leads has to be suitably chosen). Likewise one can choose various forms of $V_c(y)$ to account for different kinds of leads. Our results are independent of all the details, which means that equations (36) and (37) will be exact at the resonances.

Nevertheless there can be excitations that are not described by density functional theory like single-particle theory cases, for which systems our work is not relevant. Examples include excitonic and polaronic excitations. There is also some debate regarding whether single-particle theories can be applied to quantum dots [18–20]. In [21], Yannouleas and Landman discuss the applicability of single-particle models with reference to the Wigner parameter R_W and the formation of Wigner molecules when $R_W > 1$. R_W is the ratio of the strength of the Coulomb interaction over that of the kinetic energy. Single-particle descriptions are applicable for $R_W < 1$, that is the regime of weak to moderate many-body correlations. We would like to point that firstly there exists a proof that FSR (equation (37)) is valid for interacting electrons where the proof is not restricted to single-particle theories for interactions but rather uses some theorems from number theory. And secondly our proof does not require the nature of the wavefunction inside the dot (single particle or many body) but only requires the structure of the wavefunction far away from the dot, given by equations (3) and (4), which has been at least confirmed in the experiments of Kobayashi *et al* [12, 13]. Thirdly our result is more useful for non-interacting small systems where we cannot know the impurity configuration inside the system, that can be a ring or a wire.

In conclusion, the Friedel sum rule and similar semi-classical formulae (equations (36) and (37)) become exact at resonances for any general potential in a single-channel Q1D case that can support a resonance. This is very counterintuitive as the Fano resonance is a purely quantum phenomenon. We do not know of any other situation where semi-classical formulae can become exact, as the mesoscopic world is always quantum. A semi-classical formula can at most be a good approximation. Thereby, the experimental data of [10, 12, 13] carry important information. Using such data, experimentalists can bypass the requirement of knowledge of the microscopic Hamiltonian to find the DOS and PDOS and hence thermodynamic and transport properties at Fano

resonance. Given a sample, for example a quantum dot, a theoretician would like to know the Hamiltonian and hence the exact impurity configuration inside the dot. This is in principle impossible to know for a single sample. Supposing it is known, a theoretician can proceed by solving equations like the Kohn–Sham equation [8] to find the effective potential V_{eff} . The effective potential is a purely theoretical concept that is of no importance to experimentalists. However, once the effective potential is determined, the density and density of states can be determined theoretically. Experimentally however, one can bypass all this. The quantum dot can be plugged into the experimental set up of [10, 12, 13, 17] and one can directly measure the transmission probability $|t_{11}|^2$, transmission phase $\text{Arg}(t_{11})$, reflection probability $|r_{11}|^2$ and reflection phase $\text{Arg}(r_{11})$. Substituting them in equations (36) and (37), one can get the PDOS and DOS respectively, at Fano resonance. So the determination of the effective potential or impurity configuration is of no consequence. The transport and thermodynamic properties of mesoscopic systems directly depend on DOS and PDOS and this has been reviewed in detail in [22].

Acknowledgment

The author thanks Professor S Sengupta for carefully reading the manuscript.

References

- [1] Huang K 2000 *Statistical Mechanics* 2nd edn (New York: John Wiley)
- [2] Datta S 1995 *Electronic Transport in Mesoscopic Systems* (Cambridge: Cambridge University Press)
- [3] Bayman B F and Mehoke C J 1983 *Am. J. Phys.* **51** 875
- [4] Brouwer P W and Buttiker M 1997 *Europhys. Lett.* **37** 441
- [5] Buttiker M, Thomas H and Pretre A 1994 *Z. Phys. B* **94** 133
- [6] Buttiker M 1986 *Phys. Rev. Lett.* **57** 1761
- [7] Das M P and Green F 2009 *J. Phys.: Condens. Matter* **21** 10
- [8] Hohenberg P and Kohn W 1964 *Phys. Rev.* **136** B864
Kohn W and Sham L J 1965 *Phys. Rev.* **140** A1133
- [9] Reimann S M and Manninen M 2002 *Rev. Mod. Phys.* **74** 1283–342
- [10] Schuster R *et al* 1997 *Nature* **385** 417
- [11] Englman R and Yahalom A 2000 *Phys. Rev. B* **61** 2716
- [12] Kobayashi K, Aikawa H, Katsumoto S and Iye Y 2003 *Phys. Rev. B* **68** 235304
- [13] Kobayashi K, Aikawa H, Sano A, Katsumoto S and Iye Y 2004 *Phys. Rev. B* **70** 035319
- [14] Bandopadhyay S and Singha Deo P 2003 *Phys. Rev. B* **68** 113301
Singha Deo P 2007 *Phys. Rev. B* **75** 235330
- [15] Gasparian V, Ortuno M, Ruiz J, Cuevas E and Pollak M 1995 *Phys. Rev. B* **51** 6743
Aronov A G, Gasparian V and Gummich U 1991 *J. Phys.: Condens. Matter* **3** 3023
- [16] Gramespacher T and Buttiker M 1997 *Phys. Rev. B* **56** 13026
- [17] Buks E *et al* 1996 *Phys. Rev. Lett.* **77** 4664
- [18] Gurvitz G S 2008 *Phys. Rev. B* **77** 201302
- [19] Ihn T *et al* 2007 *New J. Phys.* **9** 111
- [20] Baksmaty L O *et al* 2008 *Phys. Rev. Lett.* **101** 136803
- [21] Yannouleas C and Landman U 2007 *Rep. Prog. Phys.* **70** 2067
- [22] Buttiker M 2002 *Pramana J. Phys.* **58** 241