Quantum capacitance: a microscopic derivation

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We start from microscopic approach to many body physics and show the analytical steps and approximations required to arrive at the concept of quantum capacitance. These approximations are valid only in the semi-classical limit and the quantum capacitance in that case is determined by Lindhard function. The effective capacitance is the geometrical capacitance and the quantum capacitance in series, and this too is established starting from a microscopic theory.

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I. INTRODUCTION

Several new concepts and ideas have developed in last few decades on nano-electronics and they are often questioned [1]. AC response of quantum dots in the coherent regime has been measured in recent experiments [2]. A good understanding and control over such phenomenon can lead to many novel devices, specially in metrology [2]. The experimental results are analyzed in a series of works using effective variables like quantum capacitance [3–12]. Capacitance of mesoscopic systems are very different from geometric capacitance. In mesoscopic systems one can differentiate between electrostatic capacitance and electro-chemical capacitance. Although, in principle one can also define a magnetic field induced capacitance, in practice one defines a field dependent electrostatic or electrochemical capacitance [3]. Ref [14] gives a detailed analysis of electrochemical capacitance which gives corrections to the geometrical capacitance due to field penetration into the conductor which occurs over a finite length scale comparable to the dimensions of the sample and ignored in large systems. Electrochemical capacitance is a property of open systems (systems connected to leads and electron reservoirs). In such open systems, electron-electron interaction cannot be treated exactly and characteristic potentials were introduced to account for Coulomb interaction approximately. The correction term appear as another capacitance in series with the geometric capacitance. Both, open and closed systems can have an electro-static voltage induced capacitance. A closed system of a finite wire (referred as a stub) connected to a closed ring was analyzed in Ref. [13]. The system was reduced to a two level system, wherein there is a hybridization of a single level coming from the stub and another single level coming from the ring. Coulomb interaction was again treated approximately with the help of characteristic potentials and single particle level approximations. Quantum corrections was again shown to appear as a capacitance that appear in series with the geometric capacitance. The quantum capacitance is given by the Lindhard function [13]. Subsequently, several authors have tried to interpret experimental data and numerical calculations in terms of quantum capacitance [13–15]. A microscopic analysis stating under what circumstances and assumptions one can use such a parameter is not done so far.

Capacitance of a system is self consistently determined by Coulomb interactions and this is no exception for quantum capacitance as well. However, quantum mechanically electrons can also interact via Fermi statistics and so even when Coulomb interaction is ignored, a system can have a quantum capacitance. While geometric or classical capacitance is determined by the volume, shape and dielectric constant of the system, charge in quantum mechanics can reside in orbitals that do not have a space-time description. The existence of an effective variable of quantum capacitance, can simplify the complexity of many body physics.

Unlike that in open systems, electron-electron interaction and statistics can be treated exactly in closed systems. In this work we deal with closed systems so that an analytical proof can be given and exact numerical diagonalization is possible for verification. We would like to analyze the assumptions and concepts required to arrive at a statistical mechanical variable of electrostatic quantum capacitance. When a system is weakly coupled to a reservoir, making it an open system, one can describe the system in terms of the eigenenergies of the system and Fermi-Dirac distribution function [17]. So our results are also valid for weakly coupled open systems. Electro-chemical potential also works by affecting the electrostatic potential inside the system [14]. So if electrostatic quantum capacitance cannot be proved then electro-chemical quantum capacitance may also not hold.

Our analysis is independent of model and valid for any arbitrary geometry in any dimension. However, we will use some models and systems for numerical verification, that are described in section II. Analytical derivation of quantum capacitance is given in section III. Conclusions are given in section IV.
II. MODELS FOR NUMERICAL VERIFICATION AND ILLUSTRATION

We have given in Fig. 1, schematic diagrams of a ring (Fig. 1a), a stub connected to a ring (Fig. 1b), and a 2D square geometry (Fig. 1c). Although our analysis is not restricted to these geometries, we will use them as reference and examples. Figs. (1a), (1b) and (1c) represent discrete versions of the same systems as that in (1a), (1b) and (1c), respectively. Discrete models are useful for numerical analysis. The vector potential due to a magnetic field can non-trivially change the electronic states of a system (due to quantum interference) while having very little effect on the bound positive charges. As a result, the potential will drastically change the states of the system due to interference effects. For numerical verification, we use the generalized Hubbard Hamiltonian describing a discrete system consisting of sites.

\[ H = \sum_{i, \sigma} \epsilon_i C_{i, \sigma}^\dagger C_{i, \sigma} + \sum_{\langle ij \rangle, \sigma} (\epsilon J_{i,j} C_{j, \sigma}^\dagger C_{i, \sigma} + H C) + \sum_{i} U_1 n_{i, \uparrow} n_{i, \downarrow} \]

\[ + \sum_{\langle ij \rangle, \sigma, \sigma'} U_2 n_{i, \sigma} n_{j, \sigma'} \]

where \( \epsilon_i \) is the site energy of the \( i \)th site, \( t \) is the hopping parameter (in presence of magnetic field it becomes complex, i.e., \( t \rightarrow t e^{i \phi} \)), \( U_1 \) and \( U_2 \) are respectively, the on site and nearest neighbor Coulomb interaction. In Fig. 2 we show a three dimensional ring (shaded region) with a flux \( \phi \) through the center of the ring that can cause polarization. At a particular point \( r \) on the ring we can bring an STM tip at a voltage \( V \) to cause further polarization at that position \( r \) (or \( i \)) while another STM tip can measure the local potential \( V(r) \) (or \( V_i \)) at \( r \) (or \( i \)). The polarization charge in a segment of the ring can be measured by a cylinder around the ring by looking at the induced charge on this cylinder (unshaded contour in Fig. 2).

III. ANALYTICAL DERIVATION

We will outline here all the mathematical steps required to describe the polarization of a quantum system in terms of electrostatic quantum capacitance. When assumptions are used, we will give numerical verification and also cite appropriate earlier works. Suppose the potential \( V(r) \) at a point \( r \) is changed infinitesimally giving rise to a delta potential term in the Hamiltonian, of the form \( dV^{ext} = \sum_n \kappa \delta (r - r_n) \), where \( r_n \) is the coordinate of the \( n \)th electron. The Kohn-Hohenberg theorem states that the energy is an unique functional of the local potential. But we just use first order perturbation correction to the energy which is in terms of the applied potential only and no self consistency is required. So the increase in energy of the system can be expanded as

\[ \Delta E = \sum_n \int d^3 r_1 d^3 r_2 \ldots d^3 r_M \psi^* (r_1, r_2, \ldots r_M) \kappa \delta (r - r_n) \]

\[ \psi (r_1, r_2, \ldots r_M) + O(\kappa^2) + O(\kappa^3) + \ldots \]  (2)

As \( \kappa \rightarrow 0 \), then

\[ \frac{\partial E}{\partial V(r)} = Q(r) \]  (3)

where

\[ Q(r) = M \int d^3 r_2 \ldots d^3 r_M \psi^* (r, r_2, \ldots r_M) \psi (r, r_2, \ldots r_M) \]  (4)

is the charge at \( r \). We verify this numerically for all the geometries shown in Fig. 1. A plot is shown in Fig. 3 for a disordered ring whose site energies \( \epsilon_i \) vary from \(-0.5t\) to \(0.5t\). Other parameters are explained in figure caption. We have used a single disorder configuration as the agreement is equally same for all other configurations. The figure shows the correctness of Eq. 3. We stress that we use exact diagonalization using Lanczos algorithm to determine \( E \) and \( Q_i \) and hence this is a numerical verification of Eq. 3.

Therefore, we can define a Lindhard function \( \eta(r) \).

\[ \eta(r) = -\frac{\partial Q(r)}{\partial V(r)} = -\frac{\partial^2 E}{\partial V(r)^2} \]

(5)

The last step follows from Eq. 3. For the geometry in Fig. 1(a) or 1(b) or 1(d) or 1(e), we can change the magnetic flux \( \phi \) through the center. This will immediately cause a redistribution of electronic charge in every site of the system. This is shown in Fig. 4 for the site numbered 8 in a 11 site ring. There is no qualitative difference between Fig. 1(d) and 1(e) even when the stub is weakly coupled to the ring. Also consider a case when an external voltage \( dV_i^{ext} \) is applied at site \( i \) (in the discrete model one can change \( \epsilon_i \) infinitesimally as \( V_i \) and \( \epsilon_i \) are linearly related). Obviously one can change both, \( \phi \) and \( V_i^{ext} \) simultaneously. Charge at site \( i \), \( Q_i \), will change. Due to electron-electron interaction the local potential \( V_i \), will change. Such a potential change will in turn have a feedback effect on charge displacement to determine \( dV_i \). This feedback effect is a purely quantum effect as this feedback occurs because the initial charge displacement (in this case induced by externally changed flux or potential) can change the quantum states or eigenenergies of the system. The externally applied flux and
potential also work indirectly by affecting the quantum states of the system. In other words external changes give rise to electron displacements for which potential at site \( i \) (or \( j \)) change, and this in turn gives rise to further charge displacements that is self consistently determined by Coulomb interactions and Fermi statistics. \( dV_i \) (or \( dV_j \)) is this self consistently determined increment in potential at site \( i \) (or site \( j \)) and \( dQ_i \) is the self consistently determined charge at site \( i \). We can begin by writing for the discrete system

\[
dQ_i = \frac{\partial Q}{\partial \phi} d\phi + \frac{\partial Q}{\partial V_i} dV_i + \sum_{j \neq i} \frac{\partial Q}{\partial V_j} dV_j \quad (6)
\]

Although \( Q_i \) is a functional of \( V_i \), one can change the potential infinitesimally at a particular point without changing the potential at any other point to define a partial derivative and this is in fact done to arrive at the concept of functional derivative [19]. Not to mention, that in the standard definition for total derivatives, \( \frac{dQ}{dV} \) is change in \( Q_i \) due to an infinitesimal test change in \( V_i \) (i.e., \( V_i^{ext} \)), but \( dQ_i \) on the LHS and \( dV_i \) and \( dV_j \) on the RHS are actual changes which in these systems are determined self consistently. By the virtue of the fact that we are considering a sum over \( j \) makes our treatment valid for any geometry and any dimension, where the sum over \( j \) will run over all the sites making the system. For the continuous system Eq. 6 becomes, where the sum is replaced by an integration,

\[
dQ(r) = \frac{\partial Q(r)}{\partial \phi} d\phi + \frac{\partial Q(r)}{\partial V(r)} dV(r) + \int_{r' \neq r} \frac{\partial Q(r')}{\partial V(r')} dV(r') d^3r' \quad (7)
\]

Here partial derivative with respect to \( V(r) \) means we are changing the potential in the region \( r \) to \( r + dr \) infinitesimally [19]. In the following we will argue analytically and numerically that

\[
-\sum_{j \neq i} \frac{\partial Q_j}{\partial V_j} \approx -\sum_{j \neq i} \frac{\delta Q_j}{\delta V_j} \quad (8)
\]

Or by replacing the sum by integration,

\[
\int_{r' \neq r} \frac{\partial}{\partial V(r')} d^3r' \approx \int_{r' \neq r} \frac{\delta}{\delta V(r')} d^3r' \quad (9)
\]

While LHS is a sum of partial derivatives, the RHS is a functional derivative. Integration or sum of all (but one point) partial derivatives on the LHS is approximately a total derivative. Had this one point \( (r = r') \) been included it would have been an exact total derivative with respect to energy (electronic charge times potential being energy) [20]. So in the above approximation an energy derivative is being replaced by a functional derivative with respect to local potential. This approximation is known in other context like deriving the semi-classical limit of Friedel sum rule [20]. That means this approximation is valid in the semi classical regime. Numerical verification of the approximate equality in Eq. 8 above is shown in Fig. 5. By doing exact numerical diagonalization it is difficult to go to a truly semi-classical limit as that will require us to take a large ring. However, the approximation in Eqs. 8 and 9 are known in context of deriving the semi-classical limit of Friedel sum rule [20]. If this approximation holds then one can relate induced voltage and polarization charge through quantum capacitance as shown below. Therefore, from Eq. 6 and 8,

\[
dQ_i \approx \frac{\partial Q_i}{\partial \phi} d\phi + \frac{\partial Q_i}{\partial V_i} dV_i + \sum_{j \neq i} \frac{\delta Q_j}{\delta V_j} dV_j \quad (10)
\]

Similarly, from Eq. 7 and 9,

\[
dQ(r) \approx \frac{\partial Q(r)}{\partial \phi} d\phi + \frac{\partial Q(r)}{\partial V(r)} dV(r) + \int_{r' \neq r} \frac{\delta Q(r')}{\delta V(r')} dV(r') d^3r' \quad (11)
\]

We have to assume that \( dV_j \) is independent of \( j \) as further explained below. Now it follows from charge conservation that

\[
-\eta = \frac{\partial Q_i}{\partial V_i} = -\sum_{j \neq i} \frac{\delta Q_i}{\delta V_j} \quad (12)
\]

The RHS is the net change in \( Q_i \), due to an infinitesimal functional increase (or decrease) in the potential at all points except at \( i \). That is equivalent to not changing the potential anywhere but decreasing (or increasing) the potential at \( i \) infinitesimally. Due to charge conservation the change in charge at \( i \) will be the same in both cases.

Coulomb repulsion tends to distribute charge uniformly in a system. On the other hand quantum interference effect tends to give rise to un-even distribution of charge. Assuming that in the semi-classical regime, Coulomb interactions dominate over quantum interference effects and distributes the charge uniformly, \( dV_j \) becomes independent of \( j \) and we denote it as \( dV_{rest} \). Numerical calculations for small size quantum systems show that for a wide range of parameter space the charge distribution is uniform [21, 22]. Only in very low density regime, quantum interference effects dominate and the charge density breaks up into crests and troughs [21, 22]. Any measurement process may not be able to resolve these crests and troughs and may show an average value for the local potential implying \( dV_j \) can be taken to be independent of \( j \). Transverse variation can be mapped to an effective variation in the longitudinal direction [22]. So one can write to a linear order,

\[
dQ_i = C(dV_i - dV_{rest}) \quad (13)
\]

where \( C \) is the definition of geometric or classical capacitance. We know that when we ignore quantum interference effects (i.e., large systems without boundary and impurity effects averaged out or treated in random phase approximation) we can always get such a linear regime. Substituting Eq. 12 and Eq. 13 in Eq. 10 and simplifying one gets that.
\[(C + \eta)\left(\frac{dV_i - dV_{rest}}{d\phi}\right) = \frac{\partial Q_i}{\partial \phi} = \frac{\partial Q_i}{\partial V_{rest}} \frac{\partial V_{rest}}{\partial \phi}\] (14)

Now since \(V_{rest}\) can be changed by changing \(V_i\) or \(\phi\), one can write \(V_{rest}(\phi, V_i)\). Therefore,

\[dV_{rest} = \frac{\partial V_{rest}}{\partial \phi} d\phi + \frac{\partial V_{rest}}{\partial V_i} dV_i\]

Since, the region indexed \(i\) is very small compared to the rest of the system, \(\frac{\partial V_{rest}}{\partial \phi} \rightarrow 0\) Therefore,

\[
\frac{dV_{rest}}{d\phi} = \frac{\partial V_{rest}}{\partial \phi}.
\] (15)

From Eq. (14) it follows that

\[(C + \eta)\left(\frac{dV_i - dV_{rest}}{d\phi}\right) = \eta \frac{\partial V_{rest}}{\partial \phi} = \eta \frac{dV_{rest}}{d\phi}\]

Multiplying both sides of the above equation by \(C\) we get,

\[C\left(\frac{dV_i - dV_{rest}}{d\phi}\right) = C\eta \frac{dV_{rest}}{d\phi}\]

or on using Eq. 13

\[dQ_i = \frac{C\eta}{C + \eta} dV_{rest}\] (16)

or

\[dQ_i = -dQ_{rest} = C_{eff} dV_{rest}\] (17)

where, \(C_{eff} = \frac{C\eta}{C + \eta}\). That is

\[
\frac{1}{C_{eff}} = \frac{1}{C} + \frac{1}{\eta}\] (18)

When we define capacitance we do not consider the sign of the charge. Normally one plate of the capacitor has charge \(+Q\) and the other has charge \(-Q\), wherein we write \(Q = CV\). Hence if we want to include quantum effects then only in the semi-classical regime we find it possible to describe polarization in terms of capacitance.

A quantum capacitor of capacitance \(\eta\) in series with the classical capacitance determines the effective capacitance of the system. The characteristic potential (or the potential difference between two parts of the ring) is determined by this effective variable. The AC response of the ring is also determined by this effective variable along with the inductance. For a purely capacitive response, \(I(t) = dQ_1/dt\) or \(dL_\omega = -i\omega C_{eff} dV_\omega\) [13]. Such an effective variable will exist only if assumptions given in Eq. 3, Eq. 8, and Eq. 15 are valid. Although quantum capacitance was introduced first by Serge Luryi [24], he introduced it on very general grounds and the above relation was not obtained. The above relation was obtained for a closed system only in the framework of single particle two level system [13]. We have derived it generally for arbitrary system including many body effects and outlined the assumptions so that such an effective variable will exist.

In Figs. 6 and 7 we have made a comparison of quantum capacitance at site 8, i.e., \(\eta_8\) in the non-interacting system and the interacting system to show that \(\eta\) is a good parameter to effectively capture the effect of Coulomb repulsion. Here again we are considering the 11 site disordered ring considered in Figs. 3 and 4. We have applied a small external potential at the 8th site to evaluate \(dQ_8/dV_8 = \eta_8\). Fig. 6 is for the non-interacting case i.e., \(U_1 = 0\) and \(U_2 = 0\) although the electrons still interact through Fermi statistics. In Fig 7 we have made \(U_1 = 2\) with all other parameters remaining the same. There is a large qualitative as well as quantitative difference between the two figures which shows the importance of including Coulomb interaction and many body effects in defining capacitance. \(dQ_i = -dQ_{rest}\) can be measured as outlined in Fig. 2. \(\frac{\partial Q_i}{\partial V_i} = -\eta\) can also be measured as outlined in Fig. 2. Geometrical capacitance \(C\) is independent of finite size or quantum interference effects and is known for a given sample from its bulk properties.

So one can determine \(C_{eff}\). Thus \(dV_i\) and \(dV_{rest}\) can be known for any applied external potentials as \(C_{eff}\) is the single parameter that determines this.

**IV. CONCLUSION**

In conclusion, in the semi-classical regime we prove polarization charge and induced potential of a mesoscopic isolated sample are related by an effective capacitance \(C_{eff}\). Effective capacitance can be decoupled as a linear combination of classical capacitance and quantum capacitance. The quantum capacitance is given by the Lindhard function. In this regime, we can design quantum circuits in terms of this parameter \(C_{eff}\) just as classical circuits are built in terms of parameters like resistance, capacitance and inductance. While in earlier works, Eq. 18 was derived for single particle theory for a two level system, we have started from the principles of many body physics and derived Eq. 18 for any arbitrary geometry in any dimension. We have shown the approximations necessary to get this in the framework of fully interacting fermions. All these approximations are justified in the semi-classical limit. So Eq. 18 can provide a simple way to understand DC and AC response of quantum finite sized many body electronic systems in the semi-classical limit, in terms of an effective variable.

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M. Buttiker, Pramana Journal of Physics, 58 (2007).

See for example Eq. 5 in M. Buttiker, "Time in quantum mechanics", edited by J.G. Muga, R. Sala Mayato and M. Mottelson, Phys. Rev. Lett. 102, 236801 (2009).

S. E. Nigg, R. Lopez and M. Buttiker, Phys. Rev. Lett. 97, 206804 (2006).

M. Buttiker and S. E. Nigg, Nanotechnology 18, 044029 (2007).

M. Buttiker, Physica Scripta T54, 104 (1994).

M. Buttiker, J. Phys.: Condens. Matter. 5, 9361 (1993).

A. A. Shylau, J. W. Klos, and I. V. Zozoulenko, Phys. Rev. B 80, 205402 (2009).

M. Buttiker and M. L. Polianski, J. Phys. A 38, 10559 (2005).

M. Buttiker, Phys. Rev. B 32, 1846-1849 (1985).

P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).

See for example Eq. 5 in M. Buttiker, "Time in quantum mechanics", edited by J.G. Muga, R. Sala Mayato and I.L. Egusquiza, Lecture note in Physics (Springer, Berlin, 2002).

M. Buttiker, Pramana Journal of Physics, 58, 241 (2002).

S. M. Reimann, M. Koskinen, M. Manninen and B. R. Mottelson, Phys. Rev. Lett. 83, 3270 (1999).

T. Chakraborty and P. Pietilainen, Phys. Rev. B 52, 1932 (1995).

H. Wu, D. W. L. Sprung and J. Martorell, Phys. Rev. B 45, 11960 (1992); F. Guinea and J. A. Verges, Phys. Rev. B 35, 979 (1987).

S. Luryi, Appl. Phys. Lett. 52, 501 (1988).

Fig. 1. Schematic diagrams of some mesoscopic geometries used in this work as examples and also for numerical verifications. Fig. 1(a) represents a one-dimensional ring pierced by a magnetic flux $\phi$. Fig. 1(b) represents a one-dimensional ring to which a quantum wire or stub is attached. The ring is again pierced by a magnetic flux $\phi$. Fig. 1(c) represents a two-dimensional square geometry. Once again a magnetic field can be applied perpendicular to the plane of the geometry. Figs. 1(d), 1(e) and 1(f) are discrete versions of those in 1(a), 1(b) and 1(c) respectively, that can be described by a generalized Hubbard Hamiltonian and useful for numerical verifications. The dots represent sites. Nearest neighbor sites are marked $i$ and $j$.

Fig. 2. A three-dimensional mesoscopic ring pierced by a magnetic flux $\phi$. The ring can be polarized by a voltage probe (without making a contact) at site $r$ at a given voltage $V$. The flux can also polarize the ring. Another voltage probe (without making contact) whose voltage is allowed to vary can measure the voltage at the site $r$. A solenoid around the ring, as shown in the figure, can measure the induced charge in a segment of the ring due to polarization. The idea of quantum capacitance is valid only when the polarized charge is uniformly distributed in the rest of the ring, apart from the region at $r$.

Fig. 3. The figure shows that for the geometries shown in Fig. 1, Eq. 3 is valid. In this figure we have used the geometry in Fig. 1(d). It consists of 11 sites ($N = 11$), with 4 spin up electrons and 4 spin down electrons. The on-site Hubbard $U_1 = 2$, the nearest neighbor Hubbard $U_2 = 1$. The hopping parameter $t = 1$. The solid line is the charge on the 6th site as a function of the flux in units of $Z_0$ which is electronic charge taken to be 1. The dashed line is $\partial E / \partial \phi$ in units of $Z_0$ = electronic charge taken as 1. $E$ is the ground state eigen-energy of the many body system found by exact diagonalization using Lanczos algorithm. The dimension of the matrix being of the order $10^5 \times 10^5$. Here $\phi_0 = hc/e$. We have also verified Eq. 3 for the geometries in Fig. 1(e) and 1(f).

Fig. 4. The fig shows that a disordered mesoscopic ring can be polarized by an Aharonov-Bohm flux alone. We have used the geometry of Fig 1(d) here. Parameters used are shown in the inset. We have used only one disorder configuration for this figure with site energies varying from $-5t$ to $5t$. But we have also checked for other disorder configurations. The graphs for other geometries is qualitatively similar and so not shown here. $Q_8$ is the charge density at the 8th site, in units of $Z_0$ which is electronic charge. At zero flux we expect the system to be neutral. As the flux changes, strong dispersion of energy levels is seen. The graphs for other geometries is qualitatively similar and so not shown here. $Q_8$ is the charge density at the 8th site, in units of $Z_0$ which is electronic charge. At zero flux we expect the system to be neutral. As the flux changes, strong dispersion of $Q_8$ suggests polarization of the system wherein the positive charge in the system can be taken to be uniform and independent of flux. Here $\phi_0 = hc/e$.

Fig. 5. Here we are considering a ring in the semi classical limit. That is the potential in the ring varies very slowly compared to de-Broglie wavelength. In particular we have taken a 11 site ring with a single defect, $\epsilon_1 = 0.3$ and rest of the site energies are 0. The solid line is $\partial Q / \partial V$ and the dashed line is $-\sum_{j \neq i} \partial Q / \partial V_i$. Both quantities are in units of electronic charge taken as 1. Here $U_1 = 2$ and $U_2 = 1$ with 4 spin up and 4 spin down electrons in the ring. Here $\phi_0 = hc/e$.

Fig. 6. The figure shows a plot of $\eta_8 = \partial Q_8 / \partial V_8$ as a function of flux. Here $\eta_8^0 = e/t$ where $e$ is electronic charge. $\phi_0 = hc/e$. This is for an eleven site disordered ring with site energies varying from $-5t$ to $5t$. In this case $U_1 = 0$ and $U_2 = 0$. Which means electrons are interacting only through Fermi statistics. Here $\phi_0 = hc/e$.

Fig. 7. The figure shows a plot of $\eta_8 = \partial Q_8 / \partial V_8$ as a function of flux. Here $\eta_8^0 = e/t$ where $e$ is electronic charge. $\phi_0 = hc/e$. This is for an eleven site disordered ring with site energies varying from $-5t$ to $5t$. In this case $U_1 = 0$ and $U_2 = 0$. Which means electrons are interacting only through Fermi statistics. Here $\phi_0 = hc/e$. And rest of the site energies are 0.
case $U_1 = 2$ and $U_2 = 0$. Here $\phi_0 = \hbar c/e$. 
Fig. 1
Fig. 3
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