Quantum Theory for Mesoscopic Electronic Circuits and Its Applications [1]

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Abstract: This talk contains an overview of the quantum theory for mesoscopic electric circuits and some of its applications. In the theory, the importance of the discreteness of electronic charge in mesoscopic electric circuit is addressed. The mesoscopic LC-design is quantized in accord with the charge discreteness. The uncertainty relation for electric charge and current is obtained. Because the stationary Schrödinger equation is turned to be Mathieu equation in p-representation, the wave function and energy spectrum is formally solved.

As further applications, the persistent current is obtained by considering the mesoscopic ring as a pure L-design. A formula for persistent current arising from magnetic flux is obtained from a new point of view. The Coulomb blockade phenomenon occurs when we applying the theory to the pure C-design. Concerning the time evolution of the state for mesoscopic electric circuit, we are able to study it in terms of the method of characteristics. In order to study the dissipative effect in the circuit, we use density-matrix formulation. In this formulation, several type of "off diagonal" dissipations are expected to be discussed.

Key-Words: Mesoscopic circuit, discreteness of charge, quantization, Coulomb Blockade, persistent current

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1 Introduction

Along with the dramatic achievement in nanotechnology, such as molecular beam epitaxy, atomic scale fabrication or advanced lithography, mesoscopic physics and nanoelectronics are undergoing a rapid development[2, 1]. It has been a strong and definite trend in the miniaturization of integrated circuits and components towards atomic-scale dimensions[3] for the electronic device community. When transport dimension reaches a characteristic dimension, namely, the charge carrier inelastic coherence length, one must address not only quantum mechanical property but also the discreteness of electron charge. Thus a correct quantum theory is indispensable for the device physics in integrated circuits of nanoelectronics. The quantization of the circuit was carried out [4] just likes that of a harmonic oscillator. This only results energy quantization. In fact, a different kind of fluctuation in mesoscopic system is due to the quantization of electronic charge. We studied the quantization of electric circuit of LC-design under the consideration of the discreteness of electric charge[5].

In this talk, we demonstrate the quantum theory for mesoscopic electric circuits and it applications. After recalling the Kirchoff's law in classical LC-design in next section, we quantize the LC-design by considering the fact of charge discreteness in section 3, where a finite-difference Schrödinger equation for the mesoscopic electric circuit is proposed. In section 4, the uncertainty relation for charge and current is discussed. In section 5, the finite-difference Schrödinger equation for a mesoscopic circuit of LC-design is turned to Mathieu equation in 'p-representation' and solved exactly. In section 6, A gauge field is introduced and a formula for persistent current which is a periodic function of the magnetic flux is obtained. In section 7, The pure C-design is studied and the Coulomb blockade is formulated. In section 8, we study the time evolution of the system, particularly the L-design in the presence of time-dependent source. In section 9, we suggest an approach to include the dissipative effects in the circuit. In section 10, we summarize the main results and give some discussions.

2 The classical LC-design

A classical non-dissipative electric circuit of LC-design fulfills the Kirchoff's law, *i.e.*

$$\dot{q} = \frac{\partial H}{\partial p}, \ \dot{p} = -\frac{\partial H}{\partial q}$$

with $H(t) = \frac{1}{2L}p^2 + \frac{1}{2C}q^2 + \varepsilon(t)q$ as the Hamiltonian. The variable q stands for the electric charge instead of the conventional 'coordinate', while its conjugation $p(t) = Ldq/dt$ represents (apart from a factor L) the electric current instead of the conventional 'momentum'.

3 Quantization

In order to take account of the discreteness of electronic charge. we must impose that the eigenvalues of the self-adjoint operator $\hat{q}$ take discrete values[5], i.e.

$$\hat{q}|q>= nq_e|q> \tag{1}$$

where $n \in \mathbf{Z}$ (set of integers) and $q_e = 1.602 \times 10^{-19}$ coulomb, the elementary electric charge. Obviously, any eigenstate of $\hat{q}$ can be specified by an integer. This allows us to introduce a minimum 'shift operator' $\hat{Q} := \exp[iq_e\hat{p}/\hbar]$, which satisfies

$$[\hat{q}, \hat{Q}] = -q_e\hat{Q}, \quad [\hat{q}, \hat{Q}^+] = q_e\hat{Q}^+,$$
$$\hat{Q}^+\hat{Q} = \hat{Q}\hat{Q}^+ = 1. \tag{2}$$

In ref.[5] we obtained the following finite-difference Schrödinger equation,

$$\left[-\frac{\hbar^2}{2q_eL}(\nabla_{q_e} - \bar{\nabla}_{q_e}) + V(\hat{q})\right]|\psi>= E|\psi> . \tag{3}$$

This is the stationary equation, the time evolution will be studied in section 8.

4 Uncertainty relation

We have shown [5] that the uncertainty relation for electric charge and electric current, becomes

$$\Delta\hat{q} \cdot \Delta\hat{P} \geq \frac{\hbar}{2}(1 + \frac{q_e^2}{\hbar^2} < \hat{H}_0 >). \tag{4}$$

Obviously, this uncertainty relation recovers the usual Heisenberg uncertainty relation if q_e goes to zero, i.e. the case that the discreteness of electric charge vanishes. Moreover, the uncertainty relation (4) has shown us further knowledge than the traditional Heisenberg uncertainty relation.

5 The quantum LC-design

We only consider the adiabatic approximation here so that $\varepsilon(t)$ is considered as a constant ε, *i.e.*, $V(\hat{q}) = C^{-1}\hat{q}^2/2 + \varepsilon\hat{q}$. Let us consider a representation in which the operator $\hat{p}$ is diagonal and called it as p-representation. The transformation of wave functions between charge representation and p-representation is given by

$$< n|\psi >= (\frac{q_e}{2\pi\hbar})\int_{-\hbar(\frac{\pi}{q_e})}^{\hbar(\frac{\pi}{q_e})} dp < p|\psi > e^{-inq_e p/\hbar} \tag{5}$$

In the 'p-representation', the finite-difference Schrödinger equation becomes a differential equation for $\tilde{\psi}(p) :=< p|\psi >$,

$$\left[-\frac{\hbar^2}{2C}\frac{\partial^2}{\partial p^2} - \frac{\hbar^2}{q_e^2 L}(\cos(\frac{q_e}{\hbar}p) - 1)\right]\tilde{\psi}(p) = E\tilde{\psi}(p). \tag{6}$$

which is the well known Mathieu equation [7, 8]. This equation was ever appeared in [9] on the discussion of Padé approximates.

In terms of the conventional notations [7, 8], the wave functions in p-representation can be solved as follows

$$\tilde{\psi}_l^{+}(p) = \mathrm{ce}_l(\frac{\pi}{2} - \frac{q_e}{2\hbar}p,\, \xi)$$

or

$$\tilde{\psi}_{l+1}^{-}(p) = \mathrm{se}_{l+1}(\frac{\pi}{2} - \frac{q_e}{2\hbar}p,\, \xi) \tag{7}$$

where the superscripts '+' and '-' specify the even and odd parity solutions respectively; $l = 0, 1, 2, \cdots$; $\xi = (2\hbar/q_e^2)^2 C/L$; $\mathrm{ce}(z,\xi)$ and $\mathrm{se}(z,\xi)$ are periodic Mathieu functions. In this case, there exist infinitely many eigenvalues $\{a_l\}$ and $\{b_{l+1}\}$ which are not identically equal to zero. Then the energy spectrum is expressed in terms of the eigenvalues a_l, b_l of Mathieu equation

$$E_l^{+} = \frac{q_e^2}{8C}a_l(\xi) + \frac{\hbar^2}{q_e^2 L},$$
$$E_{l+1}^{-} = \frac{q_e^2}{8C}b_{l+1}(\xi) + \frac{\hbar^2}{q_e^2 L}. \tag{8}$$

6 Quantum L-design and persistent currents

Introducing an operator $\hat{G} := \exp(-i\beta\hat{q}/\hbar)$, we can find that $\hat{G}|p >= |p - \beta >$ and $\hat{G}^{+}|p >= |p + \beta >$. For a unitary transformation to the eigenstates of Schrödinger operator given by

$$|\psi > \rightarrow |\psi' >= \hat{G}|\psi >,$$

we find that the Schrödinger equation (3) is not covariant. This requests that we introduce a gauge field and define a reasonable covariant discrete derivative. By making the definitions:

$$D_{q_e} := e^{-i(q_e/\hbar)\phi}\frac{\hat{Q} - e^{i(q_e/\hbar)\phi}}{q_e},$$
$$\bar{D}_{q_e} := e^{i(q_e/\hbar)\phi}\frac{e^{-i(q_e/\hbar)\phi} - \hat{Q}^{+}}{q_e}, \tag{9}$$

we can verify that they are covariant under a gauge transformation. The gauge transformations are expressed as

$$\hat{G}D_{q_e}\hat{G}^{-1} = D'_{q_e},$$
$$\hat{G}\bar{D}_{q_e}\hat{G}^{-1} = \bar{D}'_{q_e}, \tag{10}$$

as long as the gauge field ϕ transforms in the following way

$$\phi \rightarrow \phi' = \phi - \beta.$$

Either the transformation law or the dimension of the field ϕ indicates that ϕ plays the role of the magnetic flux threading the circuit. Then the Schrödinger equation for a pure L-design in the presence of magnetic flux is given by,

$$-\frac{\hbar^2}{2q_e L}(D_{q_e} - \bar{D}_{q_e})|\psi >= E|\psi > . \tag{11}$$

The energy spectrum is easily solved

$$E(p,\phi)=\frac{2\hbar}{q_e^2}\sin^2\left[\frac{q_e}{2\hbar}(p-\phi)\right], \qquad (12)$$

which has oscillatory property with respect to ϕ or p. Differing from the usual classical pure L-design, the energy of a mesoscopic quantum pure L-design can not be large than $2\hbar/q_e^2$. Clearly, the lowest energy states are such states that $p=\phi+nh/q_e$. Thus the eigenvalues of the electric current of ground state are calculated

$$I(\phi)=\frac{\hbar}{q_e L}\sin(\frac{q_e}{\hbar}\phi). \qquad (13)$$

Obviously, the electric current on a mesoscopic circuit of pure L-design is not null in the presence of a magnetic flux except $\phi=n(h/q_e)$. Clearly, this is a pure quantum characteristic. (13) exhibits that the persistent current in a mesoscopic L-design is an observable quantity periodically depending on the flux ϕ. Because a mesoscopic metal ring is a natural pure L-design, the formula (13) is valid for persistent current on a single mesoscopic ring[10]. One can easily calculate the inductance of mesoscopic metal ring and obtain the formula for persistent currents

$$I(\phi)=\frac{\hbar}{8\pi r(\frac{1}{2}\ln(8r/a)-1)q_e}\sin(\frac{q_e}{\hbar}\phi), \qquad (14)$$

where r is the radius of the ring and a is the radius of the metal wire. Differing from the conventional formulation of the persistent current on the basis of quantum dynamics for electrons, our formulation presented a method from a new point of view. Formally, the $I(\phi)$ we obtained is a sine function with periodicity of $\phi_0=h/q_e$, But either the model that the electrons move freely in an ideal ring[11], or the model that the electrons have hard-core interactions between them[12] can only give the sawtooth-type periodicity.

7 Quantum C-design and Coulomb blockade

We observe the Schrödinger equation for a LC-design. The mesoscopic capacity may be relatively very small (about $10^{-8}F$) but the inductance of a macroscopic circuit connecting to an adiabatic voltage source is relatively large because the inductance of a circuit is proportional to the area which the circuit span. Thus we may neglect the term reversely proportional to L in the Schrödinger equation and study the equation for a pure C-design:

$$\left(\frac{1}{2C}\hat{q}^2-\varepsilon\hat{q}\right)|\psi>=E|\psi>. \qquad (15)$$

Apparently, the Hamiltonian operator commutes with the charge operator, so they have simultaneous eigenstates. The energy for the eigenstate $|n>$ is

$$E=\frac{1}{2C}(nq_e-C\varepsilon)^2-\frac{C}{2}\varepsilon^2, \qquad (16)$$

which involves both the charge quantum number and the voltage source. After some analysis, we can find the relations between charge q and the voltage ε for the ground state,

$$q=\sum_{m=0}^{\infty}\left\{\theta[\varepsilon-(m+\frac{1}{2})\frac{q_e}{C}] -\theta[-\varepsilon-(m+\frac{1}{2})\frac{q_e}{C}]\right\}q_e. \qquad (17)$$

where $\theta(x)$ denotes the step function. The corresponding eigenstates are

$$|\psi(\varepsilon)>_{ground}=\sum_{m=-\infty}^{\infty}\left\{\theta[\varepsilon-(m-\frac{1}{2})\frac{q_e}{C}] -\theta[-\varepsilon-(m+\frac{1}{2})\frac{q_e}{C}]\right\}|m> \qquad (18)$$

The dependence of the currents on the time is obtained by taking derivative of (17),

$$\frac{dq}{dt}=\sum_{m=0}^{\infty}q_e\left\{\delta[\varepsilon-(m+\frac{1}{2})\frac{q_e}{C}] +\delta[\varepsilon+(m+\frac{1}{2})\frac{q_e}{C}]\right\}\frac{d\varepsilon}{dt}. \qquad (19)$$

Clearly, the currents are of the form of sharp pulses which occurs periodically according to the changes of voltage. The voltage difference between two pulses are q_e/C. This is the called Coulomb blockade phenomena caused by the charge discreteness.

8 Time evolution with time dependent source

We consider a L-design in the presence of time dependent source. The time dependent Schrödinger equation for the circuit in charge representation is given by

$$i\hbar\frac{d}{dt}|\psi(t)>= \left[-\frac{\hbar^2}{2q_eL}(\nabla_{q_e}-\bar{\nabla}_{q_e})+\varepsilon(t)\hat{q}\right]|\psi(t)>. \qquad (20)$$

Expanding the state vector in terms of the orthonormal set of charge eigenstates

$$|\psi(t)>=\sum_{n=-\infty}^{\infty}u_n(t)|n>, \qquad (21)$$

we obtain the evolution equation for the amplitudes $u_n(t)$, namely

$$i\frac{d}{dt}u_n(t)=[n\frac{q_e}{\hbar}\epsilon(t)+\frac{\hbar}{q_eL}]u_n(t) -\frac{\hbar}{2q_eL}(u_{n+1}(t)+u_{n-1}). \qquad (22)$$

Obviously, $du_n/dt=-i\omega u_n$ corresponds to the stationary case which was discussed in section 6.

Multiplying eq.(5) with $\exp(inq_ep'/\hbar)$ and summing over the index n, we obtain

$$<p|\psi>=\sum_{n=-\infty}^{\infty}<n|\psi>e^{inq_ep/\hbar}. \qquad (23)$$

Then eq. (20) can be written in a convenient form in p-representation, namely,

$$\left\{-\frac{\hbar}{q_eL}[\cos(\frac{q_e}{\hbar}p)-1]-i\frac{\hbar}{q_e}\varepsilon(t)\frac{\partial}{\partial p}\right\}\tilde{\psi}=i\frac{d}{dt}\tilde{\psi}, \qquad (24)$$

where

$$\tilde{\psi}(p)=<p|\psi>=\sum_{n=-\infty}^{\infty}u_n(t)e^{inq_ep/\hbar}. \qquad (25)$$

The partial differential equation (24) can be reduced to a first order ordinary differential equation by means of the method of characteristics [13]. Although this reduction involves complicated mathematical formulations, the solution of the above equation can be given in terms of Bessel functions[14]. Using Graf's addition theorem for Bessel functions [8], one is able to obtain

$$|u_n(t)|^2=J_n^2(-\frac{\hbar}{q_eL}\sqrt{a^2(t)+b^2(t)}\,), \qquad (26)$$

where

$$\begin{aligned} a(t) &= \int_0^t\cos[f(t')]dt', \\ b(t) &= -\int_0^t\sin[f(t')]dt' \\ f(t) &= \int_0^t\varepsilon(t')dt'. \end{aligned}$$

The mean-square charge is obtained with the help of the identity $\sum_n J_n^2(z)=z^2/2$,

$$<\hat{q}^2>=\frac{\hbar^2}{2L}[a^2(t)+b^2(t)]. \qquad (27)$$

Some interesting physics phenomena, such as dynamic localization etc are expected to be studied furthermore.

9 About the dissipatives

In order to take account of the effects of dissipatives in the circuit, we introduce the density matrix $\rho_{m,n}(t)=u_m^*(t)u_n(t)$. The evolution equation for the density matrix is obtained from the equation (22) for the amplitudes $u_n(t)$,

$$i\frac{\partial}{\partial t}\rho_{m,n}=-\varepsilon(t)\frac{q_e}{\hbar}(m-n)\rho_{m,n} +\frac{\hbar}{2q_e^2L}(\rho_{m+1,n}+\rho_{m-1,n}-\rho_{m,n+1}-\rho_{m,n-1}). \qquad (28)$$

Putting a term describing some kind of dissipatives in the circuit, we should write the evolution equation for the density matrix as

$$i\frac{\partial}{\partial t}\rho_{m,n}=-\varepsilon(t)\frac{q_e}{\hbar}(m-n)\rho_{m,n} +\frac{\hbar}{2q_e^2L}(\rho_{m+1,n}+\rho_{m-1,n}-\rho_{m,n+1}-\rho_{m,n-1}) +i\sum_{m',n'}\gamma_{mn}^{m'n'}\rho_{m'n'}, \qquad (29)$$

which is the stochastic Liouville equation. Eq.(29) is a good start point to study the dissipative effects in the mesoscopic L-design. The one-parameter off-diagonal dissipative is particularly interesting, *i.e.*, $\gamma^{mn}_{m'n'} = \gamma(1-\delta_{m,n})\delta_{m,m'}\delta_{n,n'}$ Further discussions are in progress.

10 Conclusions

In the above, we studied the quantization of mesoscopic electric circuit. Differing from the literature in which it is simply treated as the quantization of a harmonic oscillator, we addressed the importance of the discreteness of electric charge. Taking the discreteness into account, we proposed a quantum theory for mesoscopic electric circuit and give a finite-difference Schrödinger equation for mesoscopic electric circuit. We used the charge representation and p-representation. Due to the discreteness of electric charge, $\hat{p}$ is no longer a current operator.

As the Schrödinger equation for LC-design in p-representation becomes the well known Mathieu equation, it is solvable. We obtain the wave functions in terms of Mathieu functions and the energy spectrum in terms of the eigenvalues of Mathieu equation. The discussion on uncertainty relation for the charge and current shed some new light on the knowledge of transitional Heisenberg uncertainty relation. As further applications of our theory, Introducing a gauge field and gauge transformation, we obtained a formula for the persistent current on the mesoscopic pure L-design in the presence of the magnetic flux. As the mesoscopic metal ring is a natural pure L-design, the formula is certainly valid for the persistent current on mesoscopic rings. In our formula, the mass of electrons, the carriers for electric current, is not involved. It is worthwhile to check that property by experiments. The theory is applied to explain the Coulomb blockade. By considering a quantum C-design, the Coulomb blockade phenomenon was formulated as an immediate consequence. The time evolution of quantum L-design is solved formally, and the dissipative is introduced with the help of density matrix formulation.

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