Quantum LC - circuits with diffusive modification of the continuity equation

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Proofs are given that the quantum-mechanical description of the LC-circuit with a time dependent external source can be readily established by starting from a general discretization rule of the electric charge. For this purpose one resorts to an arbitrary but integer-dependent real function \( F(n) \) instead of \( n \). This results in a nontrivial generalization of the discrete time dependent Schrödinger-equation established before via \( F(n) = n \). Such generalization leads to site-dependent hopping amplitudes as well as to diffusive modification of the continuity equation. One shows, in particular, that there are firm supports concerning rational multiples of the elementary electric charge.

**Keywords:** Quantum LC-circuits; Charge discretization; Discrete Schrödinger-equations

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I. INTRODUCTION

Quantum transport of carriers in nanoscale systems has received much interest during the last two decades. It has been realized that fluctuations of the electric current are able to be implemented by virtue of the discretness of electric charge \( Q \). Such issues opened the way to the quantum-mechanical description of RLC-circuits. Accordingly, current fluctuations have to be understood as typical manifestations of appropriate quantum-mechanical Hamiltonians incorporating complementary charge and magnetic flux observables. Studies in this field look promising, as they provide ideas for further technological developments. The discretized charge referred to above means that the application of the discrete calculus looks rather suitable. The understanding is that discrete tight binding models rely naturally on semiconductor quantum wells and nano-electronic devices. The aim of this short paper is to discuss in more detail the quantum-mechanical description of the mesoscopic LC-circuit with a time dependent voltage source \( V(t) \). So far the discrete Schrödinger equation characterizing the LC-circuit has been established by starting from the charge eigenvalue equation

\[
Q_q |n\rangle = n_q e |n\rangle \tag{1}
\]

where \( n \) is an integer playing the role of the discrete coordinate. This shows that the electric charge gets quantized in units of the elementary electric charge \( q_e \equiv e \), as indicated by (2.2) in [9], or by (1) in [12–15]. One could also say that \( q_e = 2e \) when dealing with Cooper-pairs. However, more general charge quantization rules can also be proposed. For this purpose we shall resort to an arbitrary \( n \)-dependent function \( F(n) \) instead of \( n \). This results in a generalized counterpart of the discrete Schrödinger-equation relying on [11] as well as in non-trivial modification of the charge conservation law. Such modifications indicate that we have to account for diffusion effects. One starts from an appropriate implementation of the canonically conjugated observable, i.e. of suitable magnetic flux operators. For this purpose the charge discreteness will be handled by applying left- and right-hand discrete derivatives, i.e \( \nabla \) and \( \Delta \), to charge eigenfunctions one deals with. This provides a pair of non-Hermitian but conjugated magnetic flux operators. The product of such operators is then responsible for the Hermitian operator of the square magnetic flux. Of course, the Hermitian magnetic flux operator, which plays the role of the momentum, can also be readily established in terms of a subsequent symmetrization.

II. PRELIMINARIES AND NOTATIONS

We have to recall that the classical RLC-circuit is described by the balance equation:

\[
L \frac{dI}{dt} + IR + \frac{Q}{C} = V_s(t) \tag{2}
\]

in accord with Kirchhoff’s law, where the current is given by \( I = dQ/dt \), as usual. Inserting \( R = 0 \), leads to the Hamiltonian

\[
\mathcal{H}_c(Q, \Phi/c) = \frac{\Phi^2}{2Lc^2} + \frac{Q^2}{2C} - QV_s(t) \tag{3}
\]

where \( \Phi = ILc \) and \( L \) stand for the magnetic flux and the inductance, respectively. Indeed, (2) is produced by Hamiltonian equations of motion characterizing (4):

\[
I = \frac{dQ}{dt} = \frac{\partial \mathcal{H}}{\partial (\Phi/c)} = \frac{\Phi}{Lc} \tag{4}
\]

and

\[
\frac{d}{dt} \left( \frac{\Phi}{c} \right) = - \frac{\partial \mathcal{H}}{\partial Q} = - \frac{Q}{C} + V_s(t) \tag{5}
\]

as usual. This also means that the electric charge \( Q \) and \( \Phi/c \) are canonically conjugated variables. This result suggest that the quantization of the LC-circuit could be done in terms of the canonical commutation relation

\[
[Q, \Phi] = i\hbar c \tag{6}
\]
in which case one gets faced with the flux-operator\(^\text{10}\)
\[ \Phi = -i\hbar c \frac{\partial}{\partial Q} . \]  

However, a such realization is questionable because the electric charge, such as defined by (11) is not a continuous observable. This means that the introduction of a discretized version of (7) like
\[ \Phi_q = -i\hbar c \frac{\Delta}{q_e} \]  
for which \( \Phi_q^\dagger = -i\hbar c \nabla /q_e \) is in order. The Hermitian time-dependent Hamiltonian of the quantum \( LC \)-circuit can then be established as
\[ \mathcal{H}_q = \frac{\Phi_q^\dagger \Phi_q}{2Lc^2} + \frac{q_e^2}{2C} Q_q V_s(t) . \]  
in which \( \mathcal{H}_q^{(0)} = \Phi_q^\dagger \Phi_q /2Lc^2 \) has the meaning of the kinetic energy. The Hermitian momentum operator can also be readily introduced as \( P_q = (\Phi_q^\dagger + \Phi_q) /2 \). Note that right- and left-hand discrete derivatives referred to above proceed as\(^\text{16}\)
\[ \Delta f(n) = f(n+1) - f(n) , \]  
and
\[ \nabla f(n) = f(n) - f(n-1) , \]  
so that \( \Delta^+ = - \nabla \) and
\[ \nabla \Delta = \Delta - \nabla . \]  

In addition, one has the product rule
\[ \nabla (f(n)g(n)) = g(n) \nabla f(n) + f(n-1) \nabla g(n) \]  
and similarly for \( \Delta \).

III. GENERALIZED VERSION OF THE ELECTRIC CHARGE QUANTIZATION

Looking for generalizations let us replace (1) by the charge eigenvalue equation
\[ \tilde{Q}_q |\tilde{n}\rangle = q_e F(n) |\tilde{n}\rangle , \]  
in which \( F(n) \) is an arbitrary integer-dependent real function. We have to assume that, in general, \(|\tilde{n}\rangle \) is different from \(|n\rangle \). Working within the subspace spanned by \(|\tilde{n}\rangle \), one finds
\[ \tilde{Q}_q \Delta = q_e F(n+1) \Delta + q_e \Delta F(n) , \]  
and
\[ \nabla \tilde{Q}_q = q_e F(n-1) \nabla + q_e \nabla F(n) . \]  

Performing the Hermitian conjugation gives\( \nabla \tilde{Q}_q = q_e F(n) \nabla \) and \( \Delta \tilde{Q}_q = q_e F(n) \Delta \), where \( \tilde{Q}_q^\dagger = \tilde{Q}_q \). Accordingly
\[ [\tilde{Q}_q, \Delta] = q_e \Delta F(n) (1 + \Delta) , \]  
and
\[ [\tilde{Q}_q, \nabla] = q_e \nabla F(n) (1 - \nabla) . \]  

Now we are ready to introduce rescaled magnetic flux operators like
\[ \tilde{\Phi}_q = -i\hbar c \left( \frac{1}{\Delta F(n)} \nabla \right) , \]  
which can be viewed as the generalized counterparts of (8) and
\[ \tilde{\Phi}_q^\dagger = -i\hbar c \left( \frac{1}{\nabla F(n)} \nabla + \frac{1}{\Delta F(n)} - \frac{1}{\nabla F(n)} \right) . \]  

Accordingly, the interaction-free Hamiltonian is given by
\[ \mathcal{H}_q^{(0)} \rightarrow \tilde{\mathcal{H}}_q^{(0)} = \frac{\tilde{\Phi}_q^\dagger \tilde{\Phi}_q}{2Lc^2} \]  
which can be rewritten equivalently as
\[ \tilde{\mathcal{H}}_q^{(0)} = - \frac{\hbar^2}{2L(n) q_e^2} (\tilde{\Delta} - \nabla) . \]  

This time the inductance gets rescaled as
\[ L \rightarrow \tilde{L}(n) = L (\nabla F(n))^2 \]  
whereas the discrete right hand derivative \( \Delta \) is replaced by
\[ \tilde{\Delta} = (1 - G(n)) \Delta . \]  
One has
\[ G(n) = 1 - \left( \frac{\nabla F(n)}{\Delta F(n)} \right)^2 . \]  
which leads to sensible effects for non-linear realizations of \( F(n) \). Under such conditions the discrete Schrödinger equation implemented by the generalized charge quantization condition (11) is given by
\[ \frac{\hbar^2}{2L(n) q_e^2} C_{n+1}(t) + i\hbar \frac{\partial}{\partial t} C_n(t) + \frac{\hbar^2}{2L(n) q_e^2} C_{n-1}(t) = \]  
\[ = \left[ \frac{\hbar^2}{L(n) q_e^2} \left( 1 - \frac{G(n)}{2} \right) + \frac{q_e^2}{2C} F^2(n) - q_e F(n) V_s(t) \right] C_n(t) \]  
which leads to the usual result\(^\text{9}\)
\[ - \frac{\hbar^2}{2Lq_e^2} (C_{n+1} + C_{n-1}) + A = i\hbar \frac{\partial}{\partial t} C_n(t) \]  
with \( A = \left[ \frac{q_e^2}{2C} n^2 - q_e n V_s(t) + \frac{\hbar^2}{Lq_e^2} \right] C_n(t) \) via \( F(n) \rightarrow n \).
IV. MODIFIED CHARGE CONSERVATION LAWS

One sees that (24), which differs in a sensible manner from (23), has a rather complex structure such as involved by the $n$-dependence of coefficients and especially of hopping amplitudes. However, (24) as it stands provides useful insights for a more general description of quantum mechanical circuits. Indeed, (26) produces a modified continuity equation like

$$\frac{\partial}{\partial t}\rho_n(t) + \Delta J_n(t) = g_n(t)$$  \hspace{1cm} (28)

where

$$\rho_n(t) = |C_n(t)|^2$$  \hspace{1cm} (29)

denotes the usual charge density, whereas

$$\Delta J_n(t) = \frac{\hbar}{L(n)q_e} \text{Im} \left[ C_n(t)C_{n-1}^\ast(t) \right]$$  \hspace{1cm} (30)

stands for the related current density. The additional term in the continuity equation is

$$g_n(t) = G(n)\frac{\tilde{L}(n+1)}{L(n)}J_{n+1}(t)$$  \hspace{1cm} (31)

which shows that there are additional effects, say diffusion processes, which are able to affect the time dependence of the charge density. This results in the onset of an extra charge density like

$$\rho_n^{\text{diff}}(t) = -G(n)\frac{\tilde{L}(n+1)}{L(n)} \int_{-\infty}^{t} J_{n+1}(t')dt'$$  \hspace{1cm} (32)

relying typically on the nonlinear attributes of the generalized charge discretization function. The total charge density is then given by

$$\rho_n^{\text{tot}}(t) = \rho_n(t) + \rho_n^{\text{diff}}(t)$$  \hspace{1cm} (33)

in which it has been assumed that $\rho_n^{\text{diff}}(t) \to 0$ when $t \to \infty$.

V. OTHER DETAILS

After having been arrived at this stage, a systematic study of charge discretization function would be in order, but such tasks go beyond the immediate scope of this short paper. Choosing, however, a rational generalization of (14) like

$$F(n) = \frac{P}{Q}n$$  \hspace{1cm} (34)

where $P$ and $Q$ are mutually prime integers, one finds immediately that (27) reproduces (26) just in terms of substitution

$$q_e \to \tilde{q}_e = \frac{P}{Q}q_e$$  \hspace{1cm} (35)

This shows that $q_e$ and $Pq_e/Q$ can be placed on the same footing. Accordingly, we are in a firm position to replace the elementary electric charge $q_e$ by a rational multiple like $Pq_e/Q$, which represents, strictly speaking, a non-trivial result. In addition, (34) leads this time to $G(n) = 0$, so that the usual form of the charge conservation law gets restored. We have to recognize that nonlinear realizations of the charge discretization function $F(n)$, although interesting from the mathematical point of view, are not easily tractable. Indeed, they lead, in general, to position dependent hopping amplitudes, to anharmonic effects as well as to complex valued energy dispersion laws. Moreover, in such cases the equivalence between the L-ring circuit and the electron on the 1D lattice under the influence of the induced time dependent electric field is lost and the same concerns interrelated dynamic localization conditions. In other words, quantum LC-circuits may be rather complex, but this is the point where (26) looks promising for applications concerning diffusive motion of electrons or of other carriers. Unusual commutation relations like

$$[\tilde{Q}_q, \Phi_q] = -i\hbar c \left( 1 + \frac{q_e}{\hbar c} \Delta F(n)\tilde{\Phi}_q \right)$$  \hspace{1cm} (36)

and

$$[\tilde{Q}_q, \Phi_q^+] = -i\hbar c \left( 1 - \frac{q_e}{\hbar c} \nabla F(n)\tilde{\Phi}_q^+ + \frac{\nabla F(n)}{\Delta F(n)} - 1 \right)$$  \hspace{1cm} (37)

have also to be mentioned. Such relationships can be viewed as non-Hermitian versions of generalized canonical commutation relations acting on non-commutative spaces, which looks rather challenging. Going back to (31) yields, however, a closed algebra encompassing the kinetic energy, the momentum and the charge, as indicated before.

VI. CONCLUSIONS

In this paper we succeed to establish the quantum-mechanical description of LC-circuits by starting from a rather general discretization rule for the electric charge. To this aim one resorts to a real, but integer dependent function $F(n)$ instead of $n$. This leads to the generalized discrete Schrödinger-equation (26), which reproduces the usual result as soon as $F(n) = n$. A such generalized equation is able to incorporate additional diffusion effects, as indicated by (28) and (32). It is understood that such effects go beyond the charge conservation proceeding usually in terms of ingoing and outgoing electron flows. Equation (35) shows that we are in a firm position to replace the elementary electric charge $q_e$ by a
rational multiple like $Pq_e/Q$. It is clear that proceeding via $C \to \infty$ leads to more general descriptions of L-ring circuits, too. Selected realization of such generalized descriptions deserve further attention, which looks promising fur further applications.

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