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QUANTUM LC-CIRCUITS WITH A TIME DEPENDENT EXTERNAL SOURCE

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Abstract
Starting from the discretization of the electric charge in terms of integer multiples of an elementary charge leads to the onset of non-Hermitian but conjugated flux operators. Such operators get established in terms of left- and right-hand discrete derivatives. The Hermitian kinetic energy term can then be readily established by resorting to the product of flux operators just referred to above. Dealing with the LC-circuit amounts to consider the influence of quadratic and linear terms in a time dependent discrete Schrödinger-equation. Such terms are responsible for the magnetic flux and the time-dependent electric field, respectively. One shows that the electric charge discretization can also be readily described by accounting, in general, for integer dependent functions instead of the integer referred to above.
Keywords: Quantum LC-circuits, Charge discretization, Discrete Schrödinger –equation.

1. Introduction

Quantum transport of carriers in nanoscale systems has received much interest during the last two decades [1-5]. It has been realized that fluctuations of the electric current are able to be implemented by virtue of the discreteness of electric charge Q [6-10]. 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 Hamiltonians incorporating the charge and magnetic flux observables. Studies in this field look promising, as they provide ideas for further technological developments. To this aim we have to resort to advanced theoretical methods [11]. In this context we shall discuss in some more detail the mesoscopic LC-circuit with a time dependent voltage source $V_s(t)$. The starting point is the charge eigenvalue equation [9, 12]

$$Q_q|n\rangle = nq_e|n\rangle , \qquad (1)$$

where n is an integer. This shows that the electric charge gets quantized in units of q_e. In general, q_e can be identified with the electron charge, but $q_e = 2e$ when dealing with Cooperpairs [13]. However, more general alternatives to (1) can also be proposed. Next we have to account for the discreteness implied in this manner, by resorting to left- and right-hand discrete derivatives. This results in a discrete Schrödinger-equation for the quantum LC-circuit which is similar to the one derived before [12]. However, in the present case one deals basically with 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.

2. 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 $I=dQ/dt$, whereas $V_s(t)$ stands for the external voltage. Inserting $R=0$, leads to the Hamiltonian

$$\mathrm{H}_c\left(Q,\frac{\Phi}{c}\right)=\frac{\Phi^2}{2Lc^2}+\frac{Q^2}{2C}-QV_s(t)\,, \tag{3}$$

where $\Phi=ILc$ and L denote the magnetic flux and the inductance, respectively. Indeed, (2) is produced by the equations of motion characterizing (3) via

$$I=\frac{dQ}{dt}=\frac{\partial \mathrm{H}}{\partial(\Phi/c)}=\frac{\Phi}{Lc}, \tag{4}$$

and

$$\frac{d}{dt}\left(\frac{\Phi}{c}\right)=-\frac{\partial \mathrm{H}}{\partial Q}=-\frac{Q}{C}+V_s(t)\,, \tag{5}$$

as usual. We can then say that the electric charge Q and Φ/c are canonically conjugated variables. The quantization of the LC-circuit could then 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

$$\Phi = -i\hbar c \frac{\partial}{\partial Q} . \qquad (7)$$

However, a such realization is questionable because the electric charge, such as defined by (1) is not a continuous observable. This means that the derivation of discretized versions of (7) is in order. For this purpose we have to account for right- and left-hand discrete derivatives like

$$\Delta f(n) = f(n+1) - f(n) , \qquad (8)$$

and

$$\nabla f(n) = f(n) - f(n-1) , \qquad (9)$$

in which case $\Delta^+ = -\nabla$ and

$$\nabla\Delta = \Delta - \nabla . \qquad (10)$$

In addition one has the product rule

$$\nabla(f(n)g(n)) = g(n)\nabla f(n) + f(n-1)\nabla g(n) , \qquad (11)$$

and similarly for Δ .

3. The derivation of the tight binding Hamiltonian

Let us apply the discrete derivatives just mentioned above to the eigenvalue equation (1). This yields the relationships

$$Q_q\Delta = q_e(n+1)\Delta + q_e , \qquad (12)$$

and

$$Q_q\nabla = q_e(n-1)\nabla + q_e , \qquad (13)$$

by accounting for $\Delta|n\rangle = |n+1\rangle - |n\rangle$ and $\nabla|n\rangle = |n\rangle - |n-1\rangle$. Accordingly, there is

$$\Delta Q_q = q_e n\Delta , \qquad (14)$$

and $$\nabla Q_q = q_e n\nabla , \qquad (15)$$

by virtue of the Hermitian conjugation, where $Q_q^+ = Q_q$. Commutation relations such as given

by $$[Q_q, \Delta] = q_e(1+\Delta) \qquad (16)$$

and $$[Q_q, \nabla] = q_e(1-\nabla) \qquad (17)$$

can then be readily established.

On the other hand the magnetic flux operators should rely on the discrete alternatives of (7). This yields the non-Hermitian realization

$$\Phi_q = -\frac{i\hbar c}{q_e}\Delta \tag{18}$$

in accord with the discretization rule $Q \rightarrow nq_e$ of the electric charge. So the square magnetic flux is described by the Hermitian operator

$$\Phi_h^2 = \left(\Phi_h^2\right)^+ = \Phi_q^+\Phi_q = \Phi_q\Phi_q^+ \ , \tag{19}$$

where

$$\Phi_q^+ = -\frac{i\hbar c}{q_e}\Delta . \tag{20}$$

Keeping in mind (3), we are ready to establish the general form of the Hermitian time-dependent Hamiltonian of the quantum LC-circuit as follows

$$\mathrm{H}_q = \frac{\Phi_q^+\Phi_q}{2Lc^2} + \frac{Q_q^2}{2C} - Q_q V_s(t) \tag{21}$$

So far one has the quantization rule

$$[\Phi_q, Q_q] = i\hbar c\left(1 + \frac{iq_e}{\hbar c}\Phi_q\right) \tag{22}$$

in accord with (16), but further realizations can be done in terms of generalized versions of (1).

We shall then have to look for solutions of the discrete Schrödinger-equation

$$\mathrm{H}_q\left|\Psi(t)\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle \tag{23}$$

by resorting to expansions over Wannier like states relying on (1). Using the amplitude

$$C_n(t) = \left\langle n \,||\, \Psi(t)\right\rangle \tag{24}$$

produces the second-order discrete equation

$$-\frac{\hbar^2}{2Lq_e^2}\left(C_{n+1}+C_{n-1}\right)+\left(\frac{q_e^2}{2C}n^2-q_e nV_s(t)+\frac{\hbar^2}{2Lq_e^2}\right)C_n(t)= \\ =i\hbar\frac{\partial}{\partial t}C_n(t) \tag{25}$$

which has been written down before [12]. However, this time one proceeds rigorously in terms of discrete derivatives needed.

The present description is characterized by the commutation relations

$$[Q_q, \mathrm{H}_q^{(0)}L]=-\frac{i\hbar}{c}P_q, \tag{26}$$

$$\left[Q_q, \frac{P_q}{c}\right]=i\hbar\left(1-\frac{q_e^2}{\hbar^2}\mathrm{H}_q^{(0)}L\right), \tag{27}$$

and $$\left[\mathrm{H}_q^{(0)}, P_q\right]=0, \tag{28}$$

working in accord with (1). It should be specified that

$$P_q=-\frac{i\hbar c}{2q_e}(\Delta+\nabla)=\frac{1}{2}\left(\Phi_q+\Phi_q^+\right) \tag{29}$$

denotes the Hermitian flux-operator, while

$$\mathrm{H}_q^{(0)}=\frac{\Phi_q^+\Phi_q}{2Lc^2}=-\frac{\hbar^2}{2q_e^2 L}(\Delta-\nabla) \tag{30}$$

is the Hermitian interaction-free Hamiltonian.

4. Generalized versions of the electric charge quantization

Looking for generalizations let us replace (1) the charge eigenvalue equation

$$\tilde{Q}_q\left|\tilde{n}\right\rangle=q_e F(n)\left|\tilde{n}\right\rangle, \tag{31}$$

in which $F(n)$ is an arbitrary real function. We shall also assume that, in general $\left|\tilde{n}\right\rangle$ is different from $\left|n\right\rangle$. Working within the subspace spanned by $\left|\tilde{n}\right\rangle$, one finds

$$\tilde{Q}_q\Delta=q_e F(n+1)\Delta+q_e\Delta F(n), \tag{32}$$

and

$$\tilde{Q}_q \nabla = q_e F(n-1)\nabla + q_e \nabla F(n). \tag{33}$$

Performing the Hermitian conjugation gives $\nabla \tilde{Q}_q = q_e F(n)\nabla$ and $\Delta \tilde{Q}_q = q_e F(n)\Delta$, so that

$$\left[\tilde{Q}_q, \Delta\right] = q_e \Delta F(n)(1+\Delta), \tag{34}$$

and

$$\left[\tilde{Q}_q, \nabla\right] = q_e \nabla F(n)(1-\nabla). \tag{35}$$

One sees that (34) and (35) reproduce precisely (16) and (17) as soon as $F(n) = n$.

Now we are ready to introduce rescaled flux operators like

$$\tilde{\Phi}_q = -\frac{i\hbar c}{q_e}\left(\frac{1}{\Delta F(n)}\Delta\right), \tag{36}$$

and

$$\tilde{\Phi}_q^{+} = -\frac{i\hbar c}{q_e}\left(\frac{1}{\nabla F(n)}\nabla + \frac{1}{\Delta F(n)} - \frac{1}{\nabla F(n)}\right), \tag{37}$$

which can be viewed as generalized counterparts of (18) and (20), respectively.

Accordingly, the interaction-free Hamiltonian is given by

$$H_q^{(0)} \to \tilde{H}_q^{(0)} = \frac{\tilde{\Phi}_q^{+}\tilde{\Phi}_q}{2Lc^2}, \tag{38}$$

instead of (30), which can be rewritten equivalently as

$$\tilde{H}_q^{(0)} = -\frac{\hbar^2}{2\tilde{L}(n)q_e^2}\left(\Delta(1-G(n)) - \nabla\right). \tag{39}$$

This time the inductance gets rescaled as

$$L \to \tilde{L}(n) = L(\nabla F(n))^2, \tag{40}$$

whereas

$$G(n) = 1 - \left(\frac{\nabla F(n)}{\Delta F(n)}\right). \tag{41}$$

Under such conditions the discrete Schrödinger-equation implemented by the generalized charge-quantization condition (31) is given by

$$
\begin{aligned}
&-\frac{\hbar^2}{2\tilde{L}(n)q_e^2}C_{n+1}(t)-\frac{\hbar^2(1-G(n-1))}{2\tilde{L}(n-1)q_e^2}C_{n-1}(t)+\\
&+\left[\frac{\hbar^2}{2\tilde{L}(n)q_e^2}\left(1-\frac{G(n)}{2}\right)+\frac{q_e^2}{2C}F^2(n)-q_eF(n)V_s(t)\right]C_n(t)=\\
&=i\hbar\frac{\partial}{\partial t}C_n(t)
\end{aligned}
\tag{42}
$$

which differs in a sensible manner from (25). One recognizes that equation (42) is rather complex. However, it provides useful insights for a better understanding of quantum mechanical circuits. Choosing as an illustrative example the charge-quantization rule

$$F(n)=\frac{P}{Q}n \quad , \tag{43}$$

where P and Q are mutually prime integers, one finds that (25) reproduces (42) just in terms of the substitution

$$q_e \to \frac{P}{Q}q_e . \tag{44}$$

This means that if q_e is elementary charge, the same concerns Pq_e/Q. In other words the selection of the elementary charge is actually a matter of convenience with respect to the very quantum mechanical description of the LC-circuit. Accordingly, nothing prevents us from inserting from the very beginning the modified elementary charge Pq_e/Q instead of q_e, which looks rather unexpected.

5. Conclusions

In this paper we succeed to establish the quantum-mechanical description of an LC-circuit in terms of the discrete Schrödinger-equation (42). This time one starts from a rather general quantization rule for the electric charge. To this aim one resorts to a real, but integer dependent function F (n). One proceeds by keeping invariant the “unit cell” realization of the (Q, P) phase-space, such as displayed by the commutation relation

$$\left[\tilde{P}_q, \tilde{Q}_q\right] = \left[P_q, Q_q\right] = i\hbar c\left(1 + \frac{\Delta - \nabla}{2}\right) \tag{45}$$

in which the flux and charge observables $\tilde{P}_q = \left(\tilde{\Phi}_q + \tilde{\Phi}_q^+\right)/2$ and $\tilde{Q}_q$ (P_q and Q_q) rely on the general usual $F(n) = n$ quantization rule of the electric charge. This results in sensible rescaling of the discrete right-hand derivative and of the inductance. Such rescalings are indicated by (39) and (40), respectively. Other concrete selections of the charge quantizations function $F(n)$ deserve further attention.

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