Wave-front solution in extended quantum circuits with charge discreteness

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We study the capacitively coupled, quantum transmission line with charge discreteness, discussed in an earlier paper [Flores, Phys. Rev. B **64**, 235309 (2001)]. Due to the difficulties of dealing with a highly nonlinear system, only a low-lying propagating wave solution was obtained then, the so-called *cirquiton*. In this work, we obtain a wave-front solution, valid for the long-wavelengh approximation. The propagation velocity v of the wave front depends on the (pseudo) flux parameter f; the physical requirement that v should be real implies the existence of allowed and forbidden regions (gaps) in the space of the parameter f. A study of the stability of the solutions is presented. We remark that it is possible to make a connection between our system and the (quantum) Toda lattice.

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I. INTRODUCTION

The broad field of nanostructures, and particularly so-called double-barrier resonant tunneling,[1] is at the heart of many new technological devices.[2–6] Naturally, at this scale and for low temperatures, quantum mechanics plays a fundamental role.[5] Recently, much effort has been devoted to studying nanostructures, using as a model that of quantum circuits with charge discreteness.[7–13] For example, works have been published on subjects such as persistent currents,[7,8] coupled quantum circuits,[9,10] the electronic resonator,[11] quantum point contacts,[12] and others.[3] In this Brief Report, we are interested in spatially extended quantum circuits (transmission lines) with charge discreteness. So this is an interesting theoretical subject with broad potential applications, since nanodevices could be put together forming chains, and then be viewed as electric transmission lines. For instance, electric transport properties in DNA have been measured recently.[14–16] Some degree of disagreement related to conducting properties exists; nevertheless, it is clear that the DNA molecule could be viewed and modeled as a quantum transmission line. Moreover, molecular electronic circuits[17] are actively studied theoretically and experimentally; in such systems, chains of individual molecules form a line of circuits. Therefore, this area of quantum circuits is a broad field involving future applications from the perspective of nanodevices, electric transmission in macromolecules, left-handed materials, Toda lattice, and others.

In this work we consider a wave-front solution for an extended quantum circuit, the quantum version of the classical LC transmission line. We proposed the quantum Hamiltonian for this system in 2001.[9] The propagation velocity of the wave-front solution, v, is found to possess a rich structure of allowed and forbidden regions, a structure that relates directly to charge discreteness. This finding gives us hope that it will allow us to apply these methods to the description of more complex extended systems, such as dual transmission lines, transmission lines with complex bases, etc.

In Sec. II we introduce the Hamiltonian for coupled circuits, and the equations of motion for the spatially continuous systems. In Sec. III, the wave-front solution is obtained and the band-gap structure is characterized; in Sec. IV the stability question is considered. In Sec. V the connection with the Toda lattice is presented. Finally, we state our conclusions (Sec. VI).

II. QUANTUM TRANSMISSION LINES WITH DISCRETE CHARGE

It is known that for a chain of quantum-capacitively-coupled quantum circuits with charge discreteness (q_e), the Hamiltonian may be written as[9]

$$\hat{H}=\sum_{l=-\infty}^{\infty}\left[\frac{2\hbar^2}{Lq_e^2}\sin^2\!\left(\frac{q_e}{2\hbar}\hat{\phi}_l\right)+\frac{1}{2C}(\hat{Q}_l-\hat{Q}_{l-1})^2\right], \qquad (1)$$

where the index l describes the cell (circuit) at position l, containing an inductance L and capacitance C. The conjugate operators, charge $\hat{Q}$ and pseudoflux $\hat{\phi}$, satisfy the usual commutation rule $[\hat{Q}_l,\hat{\phi}_{l'}]=i\hbar\delta_{l,l'}$. Any spatially extended solution of Eq. (1) will be called a *cirquitonlike solution*, corresponding to the quantization of the classical electric transmission line with discrete charge (i.e., elementary charge q_e). Note that, in the formal limit $q_e\to 0$, the above Hamiltonian gives the well-known dynamics related to the one-band quantum transmission line, similar to the phonon case. The system described by Eq. (1) is very cumbersome since the equations of motion for the operators are highly nonlinear due to charge discreteness. However, this system is invariant under the transformation $Q_l\to(Q_l+\alpha)$, that is, the total pseudoflux operator $\hat{\phi}_T=\Sigma\hat{\phi}_l$ commutes with the Hamiltonian; in turn, the use of this symmetry helps us in simplifying the study of this system.

The equation of motion (Heisenberg) related to the Hamiltonian (1) are

$$\frac{\partial}{\partial t}\hat{\phi}_l=\frac{1}{C}(\hat{Q}_{l+1}+\hat{Q}_{l-1}-2\hat{Q}_l), \qquad (2)$$

$$\frac{\partial}{\partial t}\hat{Q}_l = \frac{\hbar}{Lq_e}\sin\frac{q_e}{\hbar}\hat{\phi}_l. \tag{3}$$

To handle the above nonlinear equations, we will assume a continuous approximation[18] (infrared limit); that is to say, we will use the standard technique suggested in Remoissenet's book[19] (p. 26). Let a be the size of the unitary cell in the chain (i. e., the size of an LC cell) and define the spatial variable $y=al$. Consider the Taylor expansion[19] $\hat{Q}_{l\pm1}-\hat{Q}_l \approx \pm a\partial\hat{Q}/\partial y + a^2\partial^2\hat{Q}/2\partial y^2 \pm \cdots$, and the substitutions $\hat{\phi}_l \to \hat{\phi}(y)$ and $\hat{Q}_l \to \hat{Q}(y)$. Now, making the formal changes $\Phi_0=\hbar/q_e a$, defining the pseudoflux density $\hat{\Phi}=\hat{\phi}/a$, taking the limit $a\to 0$ (with $q_e a$ equal to a constant) the above pair of equations could be rewritten as

$$\frac{\partial}{\partial t}\hat{\Phi} = \frac{1}{\mathcal{C}}\frac{\partial^2}{\partial y^2}\hat{Q}, \tag{4}$$

$$\frac{\partial}{\partial t}\hat{Q} = \frac{\Phi_0}{\mathcal{L}}\sin\left(\frac{\hat{\Phi}}{\Phi_0}\right). \tag{5}$$

Here the new parameters $\mathcal{L}$ and $\mathcal{C}$ are, respectively, the inductance and capacitance per unit of length. We note that, with the above definitions, the commutator between the charge and density pseudoflux operators becomes Dirac's δ function, as is usual in a field theory. In the next section, a wave-front-like solution of the above system will be obtained. To end this section, we notice that some candidates for physical applications of our studies could be chains of double-barrier resonant-tunneling[1] among other nanosystems.[6]

III. WAVE-FRONT SOLUTIONS

As stated previously, we are interested in wave-front-like solutions of the system of Eqs. (4) and (5). We proceed in the standard way,[19] by assuming traveling wave solutions for our operators, i.e., we define a new variable $z=y-vt$, and assume

$$\hat{Q}(y,t) = \hat{Q}(z), \tag{6}$$

$$\hat{\Phi}(y,t) = \hat{\Phi}(z), \tag{7}$$

where v stands for the unknown propagation velocity. Therefore, from the Heisenberg equations of motion (4) and (5), the wave-front equations in the new variable z become

$$-v\frac{d}{dz}\hat{\Phi} = \frac{1}{\mathcal{C}}\frac{d^2}{dz^2}\hat{Q}, \tag{8}$$

$$-v\frac{d}{dz}\hat{Q} = \frac{\Phi_0}{\mathcal{L}}\sin\frac{\hat{\Phi}}{\Phi_0}. \tag{9}$$

From the above pair of equations we obtain a closed equation for the pseudoflux density operator resulting in the "eigenvalue" problem:

$$\frac{\Phi_0}{\mathcal{LC}}\sin\frac{\hat{\Phi}}{\Phi_0} = v^2\hat{\Phi}, \tag{10}$$

where the integration constant has been chosen as zero for simplicity [however, see Eq. (15)]. Equation (10) corresponds to an eigenvalue problem for the nonlinear superoperator $\mathcal{O}(\hat{\phi})=\sin(\hat{\phi})$ and there are at least two kinds of solutions: a projection operator $\hat{\Phi}=\hat{P}$, satisfying $\hat{P}^2=\hat{P}$, and $\hat{\Phi}=\hat{\sigma}$ satisfying $\hat{\sigma}^2=1$. For simplicity, we will consider only the first case (a projector). Consider the pseudoflux operator only in one LC cell of the chain, and its spectral decomposition in the Schrödinger picture $\hat{\phi}_{cell}=\int\phi|\phi\rangle\langle\phi|d\phi$. Now, pick up only one term from there (call it ϕ_0, say), consider now the well-defined operator

$$\hat{\Phi} = f\hat{P}_0 \quad \text{where } \hat{P}_0 = |\phi_0\rangle\langle\phi_0|, \tag{11}$$

where f is an arbitrary density pseudoflux parameter, and replace it in Eq. (10).

Now, since $\hat{P}_0$ is a projector, then from Eq. (10) the equation for the pseudoflux density f becomes related to the velocity by

$$v^2 = \frac{1}{\mathcal{LC}}\frac{\sin(f/\Phi_0)}{(f/\Phi_0)}. \tag{12}$$

Since both signs ($\pm f$) are possible, then we can construct the wave-front solution (step $2f$) of the equations of motion (4) and (5):

$$\hat{\Phi}_{sol}(z) = \begin{cases} +f\hat{P}_0, & z>0, \\ -f\hat{P}_0, & z<0, \end{cases} \tag{13}$$

corresponding to a solution with zero total flux (Sec. I). Concerning the matching condition at $z=0$, the solution (13) satisfies the matching implied by Eqs. (8) and (9).

The condition $v^2 \geqslant 0$ on the wave-front velocity gives the band-gap conditions on the system. In fact, from (12) the restriction

$$\frac{\sin(f/\Phi_0)}{(f/\Phi_0)} \geqslant 0 \tag{14}$$

means that there exists a sequence of bands and gaps. As is well known, the existence of this kind of sequence is closely related to transport, thermodynamical, and optical properties. For instance, in Refs. 14–16 the existence of gaps is directly related to the constant value of electrical current (*plateau*) for the increasing external voltage. Figure 1 shows a plot of the wave-front velocity (12) for different values of the pseudoflux density f, in which one observes an alternating sequence of bands and gaps, corresponding to propagating and forbidden modes. Note that the main allowed band ($-\pi\Phi_0<f<\pi\Phi_0$) is twice as wide as the other allowed bands.

Recall that the integration constant was set equal to zero to obtain (10). Now consider the nonzero case, i.e., let $\hat{C}$ be the integration constant; then the wave-front velocity becomes formally

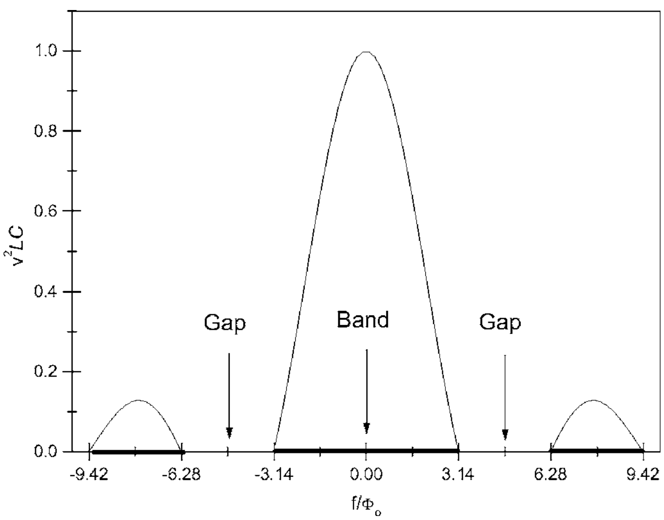

FIG. 1. Plot of the velocity of the wave front, as a function of the flux parameter f. As specified by Eq. (12) there is a structure of bands and gaps. The main allowed velocity band is twice as wide as the other allowed bands. This structure is a direct consequence of charge discreteness, an effect that disappears in the limit $q_e \to 0$.

$$v^2(\hat{\Phi} - \hat{C}) = \frac{\Phi_0}{\mathcal{LC}}\left(\sin\frac{\hat{\Phi}}{\Phi_0} - \sin\frac{\hat{C}}{\Phi_0}\right). \tag{15}$$

To end this section let us briefly mention the dual transmission line. It is well known that the direct classical LC transmission line [related to Eq. (1)] has associated with it a so-called dual transmission line. In the direct line the interaction between cells is through capacitances, while in the dual line it is through mutual inductances. The dual line is closely related to the so-called *left-handed* materials, which render its quantization physically relevant; moreover, the role of charge discreteness must also be considered. This two-step process (quantization and charge discreteness) could be performed in analogy with the direct line (Sec. I), but in this case long-range interactions between cells appear in the Hamiltonian. The expression for the Hamiltonian is cumbersome.[20] Nevertheless, the equation of motion for the charge and pseudoflux variables may be obtained after some algebra. We will not continue the description of the dual line, but only mention here that the expressions are quite involved and, so far, no explicit solution has been found.

IV. STABILITY

In this section we present briefly our results concerning the stability of the solution (11). We use the standard method of linear analysis. Consider now the perturbed solutions

$$\hat{\Phi} = \hat{\Phi}_{sol} + \hat{\varepsilon},$$

$$\hat{Q} = \hat{Q}_{sol} + \hat{\eta}, \tag{16}$$

where the operators $\hat{\varepsilon}$ and $\hat{\eta}$ are the perturbation. We assume that these operators possess small eigenvalues. Moreover, consider the well-known perturbation expansion[21]

$$\sin(\hat{\Phi} + \hat{\varepsilon}) = \sin(\hat{\Phi}) + \mathrm{Re}\left(e^{i\hat{\Phi}}\int_0^1 d\theta\, e^{-i\hat{\Phi}\theta}\hat{\varepsilon}e^{i\hat{\Phi}\theta}\right). \tag{17}$$

Since $\hat{\Phi}_{sol} = \pm f\hat{P}_0$, and $\hat{P}_0$ is a projector, then from the above equation [and Eqs. (4) and (5)] we obtain the linear evolution equation for the pseudoflux perturbation $\hat{\varepsilon}$, namely,

$$\mathcal{LC}\frac{\partial^2}{\partial t^2}\hat{\varepsilon} = \mathrm{Re}\,\frac{\partial^2}{\partial y^2}\left(e^{i(f/\Phi_0)\hat{P}_0}\int_0^1 d\theta e^{-i(f/\Phi_0)\hat{P}_0\theta}\hat{\varepsilon}e^{+i(f/\Phi_0)\hat{P}_0\theta}\right). \tag{18}$$

We have three cases, the first when the perturbation exists in the same subspace spanned by $\hat{P}_0$ [case (a)] and the others [cases (b) and (c)], in orthogonal subspaces.

(a) In the first case we consider $\hat{\varepsilon} = \varepsilon_{00}(y,t)|\phi_0\rangle\langle\phi_0|$, and we obtain the linear wave equation

$$\mathcal{LC}\frac{\partial^2}{\partial t^2}\varepsilon_{00} = (\cos f/\Phi_0)\frac{\partial^2}{\partial y^2}\varepsilon_{00}.$$

This type of perturbation is unstable in the range where the pseudoflux satisfies $\cos(f/\Phi_0) < 0$.

(b) In the second case, we assume a perturbation of the form $\hat{\varepsilon} = \varepsilon_{\phi\phi'}(y,t)|\phi\rangle\langle\phi'|$, where $\phi \neq \phi_0$ and $\phi' \neq \phi_0$. In this case the wave equation becomes

$$\mathcal{LC}\frac{\partial^2}{\partial t^2}\varepsilon_{\phi\phi'} = \frac{\partial^2}{\partial y^2}\varepsilon_{\phi\phi'},$$

and the perturbation is always stable.

(c) In the last case, the perturbation has the form $\hat{\varepsilon} = \varepsilon_{\phi 0}(y,t)|\phi\rangle\langle\phi_0|$, with $\phi \neq \phi_0$, and the wave equation for the perturbation becomes

$$\mathcal{LC}\frac{\partial^2}{\partial t^2}\varepsilon_{\phi 0} = \frac{\sin(f/\Phi_0)}{(f/\Phi_0)}\frac{\partial^2}{\partial y^2}\varepsilon_{\phi 0}.$$

This perturbation is stable when $\sin(f/\Phi_0)/(f/\Phi_0) < 0$; namely, the bands are marginally stable with respect to this kind of perturbation.

V. TODA LATTICE AND CIRQUITONS

The cirquiton Hamiltonian (1) gives the equations of motion for charge and pseudoflux in the cell l along the discrete transmission line, namely, Eqs. (2) and (3), while, as explained before, Eqs. (4) and (5) in Sec. I are the spatially continuous version of the above pair of equations. The first-order system for the variables $\hat{Q}_l$ and $\hat{\phi}_l$ may be written as a second-order system for the pseudoflux operator, namely,

$$LC\frac{\partial^2}{\partial t^2}\hat{\phi}_l = \frac{\hbar}{q_e}\left(\sin\frac{q_e}{\hbar}\hat{\phi}_{l+1} + \sin\frac{q_e}{\hbar}\hat{\phi}_{l-1} - 2\sin\frac{q_e}{\hbar}\hat{\phi}_l\right), \tag{19}$$

which, in the formal limit $q_e \to 0$, gives the usual single-band system with frequency spectrum $\omega(k) = (2/\sqrt{LC})|\sin(k/2)|$, as expected. Consider now the equation

$$LC\frac{\partial^2}{\partial t^2}\hat{\phi}_l = \frac{\hbar}{iq_e}(e^{(iq_e/\hbar)\hat{\phi}_{l+1}} + e^{(iq_e/\hbar)\hat{\phi}_{l-1}} - 2e^{(iq_e/\hbar)\hat{\phi}_l}); \quad (20)$$

then any Hermitian solution of this last equation is also a solution of the cirquiton equation (19) (observe that the reverse is not necessarily true). To show this, it suffices to conjugate Eq. (20) and subtract the result from the first version.

On the other hand, there is a broad field of research related to the Toda lattice, with results and spplications in a variety of branches in physics and engineering,[19] including nonlinear physics, statistical mechanics, classical electric circuits, etc. The classical evolution equation for the Toda lattice has the generic form

$$M\frac{\partial^2}{\partial t^2}\phi_l = -A(e^{-B\phi_{l+1}} + e^{-B\phi_{l-1}} - 2e^{-B\phi_l}) \quad (21)$$

where M, A, and B are real constants. A simple observation of the above equation shows one important result: the formal replacement $q_e \rightarrow iq_e$ transforms (20) into the (quantum) Toda lattice equation. This provides a direct connection between Toda lattice and cirquiton theory, which will be considered elsewhere.

VI. CONCLUSIONS

For the quantum electric transmission line with charge discreteness described by the Hamiltonian Eq. (1), and equations of motion (4) and (5), a one-parameter (f) wave-front solution was found [Eqs. (12) and (13)]. The condition Eq. (12) on the velocity generates a band-gap structure dependent on the pseudoflux density parameter f (see Fig. 1), namely, there exist regions (values of f) for which a solitary wave front propagates with constant speed. The existence of the band-gap structure described, very closely related to transport properties, is the main result of this work.

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