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A new approach to discrete Schrödinger equations with external field: DC electric field

J C Flores

CEAT, Los Acacios 1755, casilla 39, San Pedro, Concepción, Chile

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Abstract. For continuous Schrödinger equations the discretization process is defined by preserving the Heisenberg equation of motion rather than the Schrödinger equation itself. For instance, strong changes are obtained for one particle in DC electric fields. In the old discretization process, all eigenstates are factorially localized and the spectrum becomes discrete. On the other hand, in our model, we conjectured that the spectrum becomes continuous. We remark that discrete systems play an important role in physics because they are, in many cases, a first approach to real systems. Our goal is to study the equivalence between continuous and discrete Schrödinger equations by preserving the Heisenberg equations of motion.

1. Introduction

Discrete equations are used extensively in physics. For instance in solid state physics, the model of Anderson with static disorder displays localization of eigenstates [1]. In quantum chaos, we have the well known kicked quantum rotator which could be related to discrete Schrödinger-type equations [2]. In classical mechanics, many properties of chaos were found using discrete maps (Poincaré-sections). For particles in magnetic fields, the discrete Hofstadter model has been studied extensively. So, discrete models display properties which are in many cases similar to their continuous counterpart and that could be advantageous from a mathematical point of view.

In this paper we are concerned with such a discrete model. We are concerned with one particle in external fields (eventually DC electric fields). To consider an external field in discrete systems is not as straightforward as in the continuous case. For instance, many authors consider the discrete Schrödinger equation

$$Fl\psi_l - D\{\psi_{l+1} + \psi_{l-1}\} = E\psi_l \tag{1}$$

as a model for one particle in a DC electric field F. Equation (1) has a resemblance with the continuous (1D) Schrödinger equation with DC electric field. The term between brackets must be interpreted as equivalent to the operator ∂_x^2. Nevertheless, that similarity could be deceptive: Heisenberg's equation of motion, related to (1), does not represent one particle with constant acceleration. Moreover, any eigenstate of (1) is factorially localized ($F \neq 0$) and the spectrum becomes discrete [3]. Those results are opposite to others found in the continuous model where any eigenstate is also extended in the presence of bounded periodic potentials [4].

To consider the external field on discrete systems we use, for the moment, the generic Hamiltonian

$$\hat{H} = \sum_l V_l \hat{C}_l^\dagger \hat{C}_l - D_{l+1} \hat{C}_l^\dagger \hat{C}_{l+1} - D_l^* \hat{C}_l^\dagger \hat{C}_{l-1} \tag{2}$$

where the 'potentials' V and D are functions of position l and are calculated by using the corresponding Heisenberg equation related to the particular problem. The $\hat{C}$s are the usual fermion creation and anihilation operators at site l. Explicitly

$$\hat{C}_l^\dagger |s\rangle = \delta_{ls} |\phi\rangle \qquad \hat{C}_l |\phi\rangle = |l\rangle \tag{3}$$

where $|\phi\rangle$ denotes the state without a particle and $|l\rangle$ the state of the particle at the l-position.

The corresponding time-independent Schrödinger equation related to (2) is

$$V_l \psi_l - D_{l+1} \psi_{l+1} - D_l^* \psi_{l-1} = E \psi_l \tag{4}$$

and we want to determine V_l and D_l in such a way that (4) becomes 'equivalent' to the continuous Schrödinger equation

$$V(x)\psi(x) - \partial_x^2 \psi(x) = E\psi(x)\,. \tag{5}$$

Equivalence between (4) and (5) will be assumed when Heisenberg equations of motion are equal. For instance, in the continuous case the acceleration operator $\hat{A}$ related to (5) is given by $\hat{A}(x) = -\partial_x V(x)$. Namely, $\hat{A}$ is diagonal in the space-representation. In our discrete model (4), the acceleration operator becomes diagonal in that representation only if V_l = constant [5]. So, the operator acceleration $\hat{A}$ becomes, in that case,

$$\hat{A} = 2\sum_l \{|D_{l+1}|^2 - |D_l|^2\} \hat{C}_l^\dagger \hat{C}_l\,. \tag{6}$$

Equation (6), must be interpreted as equivalent to the Newton law, and defines the off-diagonal potential D in any particular problem. At this point, it is important to note that in the 'discretization' process we have preserved the Heisenberg equation of motion when the choice V_l = constant was made. Namely, the effect of an external field holds on the off-diagonal potential D_l rather than V_l.

For example, a DC electric field F is related to the choice

$$D_l = -\sqrt{Fl/2 + c}\, e^{i\phi_l} \qquad V_l = 0 \tag{7}$$

where c is a constant and ϕ_l an arbitrary phase. The choice (7) gives us $\hat{A} = F\hat{I}$ ($\hat{I}$ = identity) in accord with the continuous case and then, we could consider (4) and (7), equivalent to the continuous Schrödinger equation (5) with electric field $V(x) = Fx$.

Now, we discuss briefly the elimination of the arbitrary phase ϕ_l. This could be carried out by the unitary transformation

$$\psi_l \to \psi_l\, e^{i\alpha_l} \qquad \alpha_l = \sum_{s=s_0}^{l} \phi_s \tag{8}$$

which gives us the discrete Schrödinger equation

$$\sqrt{F(l+1)/2 + c}\,\psi_{l+1} + \sqrt{Fl/2 + c}\,\psi_{l-1} = E\psi_l\,. \tag{9}$$

Transformation (8) must be interpreted as a gauge transformation in a similar way to the continuous problem with electromagnetic fields.

Spectral properties of (9) will be studied in the following sections.

2. Particles in DC electric field ($c = 0$): spectral properties

Here, we will discuss spectral properties of the Schrödinger equation (9). For this we consider a sample of finite size N and we put $c = 0$. Namely, we consider the Schrödinger-type equation

$$\sqrt{F(l+1)}\psi_{l+1} + \sqrt{Fl}\psi_{l-1} = \sqrt{2}E\psi_l \qquad N \geqslant l \geqslant 0\,. \tag{10}$$

Moreover, we consider boundary conditions $\psi_0 = 1$ and $\psi_N = 0$.

The physical interpretation of (10) could be the following: the external field F produces a deformation on every 'atomic-like orbital' at position l in such a way that overlap between nearest-neighbour orbitals exists. Namely, if $F \doteq 0$ tunnelling does not exist.

The solution of (10) becomes direct if we consider the transformation

$$\psi_l = H_l/\sqrt{2^l l!} \tag{11}$$

which gives

$$H_{l+1} = 2\{E/\sqrt{2F}\}H_l - 2lH_{l-1}\,. \tag{12}$$

Relation (12) corresponds to the well known recurrence formula for Hermite polynomials. The boundary condition $\psi_N = 0$ gives $H_N(E/\sqrt{2F}) = 0$. Thus, the eigenvalues of the Schrödinger equation are just zeros of H_N. In the limit $N \gg 1$, we have the spectrum

$$E_s = \frac{\sqrt{2F}}{2\sqrt{2N+1}}\pi\{2s - 1 - N\} \qquad s = 0, 1, 2 \ldots N \tag{13}$$

and then $-\pi\sqrt{FN} < E_s < \pi\sqrt{FN}$. The fact that (11) forms an orthonormal basis results from the Christoffel–Darboux formula [6]

$$\sum_{l=0}^{N} \frac{H_l(x)H_l(y)}{2^l l!} = \frac{H_{N+1}(x)H_N(y) - H_N(x)H_{N+1}(y)}{2^{N+1}(x-y)n!}\,. \tag{14}$$

In the semi-infinite case ($N = \infty$), the spacing $E_s - E_{s-1} \sim \sqrt{F/N}$ goes to zero and a continuous spectrum could be expected. We remark that spectral properties of our model are different from others corresponding to model (1) where the spectrum becomes discrete. Also, we note that spectral properties of our model are in good accord with continous models of periodic potentials in DC electric fields [4].

3. Particles in DC electric field ($c \neq 0$): spectral properties

In this section we conjecture that the spectrun (13) could be also expected in our model when $c \neq 0$.

As we have conjectured, the choice (7) represents a particle in a DC electric field because the equation $\hat{A} = F\hat{I}$ is verified. The study of spectral properties of (9) ($c \neq 0$), for a system of finite size N, becomes direct from section 2: as $D_l \to \sqrt{Fl/2}$

in the limit $l \to \infty$, equation (10) of section 2 is asymptotically correct. Then, the spectrum E_s (13) must be expected when the boundary condition $\psi_N = 0$ holds ($N \gg 1$). In the same way, in the limit $N = \infty$, a continuous spectrum could be conjectured (section 2).

At this point it is important to note that spatial translation in (9) changes c by $F/2$. A similar situation occurs in the continuous model where the energy E changes by Fd. This suggests that the role of c, in our model, could be more important than an arbitrary constant.

4. Conclusions and discussions

The Heisenberg equation of motion ($A = [H, [H, x]]$) is preserved, in the 'discretization' process, only if the Schrödinger equation, and its associated Hamiltonian

$$- D_{l+1}\psi_{l+1} - D_l^*\psi_{l-1} = E\psi_l \tag{15}$$

are considered. In that case, the accceleration operator commutes with the position operator as in the continuous problem (5) and, in the space representation, is given by

$$A_l = 2\{|D_{l+1}|^2 - |D_l|^2\} . \tag{16}$$

Equation (16) must be considered as equivalent to the Newton law in classical mechanics. For instance, for a DC electric field, the choice (7) gives $A_l = F$, namely a constant acceleration. Spectral properties for that system were studied in section 2 ($c = 0$) and III ($c \neq 0$). Thus, a continuous spectrum could be expected at the semi-infinite limit (size $N = \infty$).

At this point, we can consider two different ways of 'discretizing' a given Schrödinger equation: *(a) using the 'similar' discrete Schrödinger equation*

$$V_l\psi_l - \psi_{l+1} - \psi_{l-1} = E\psi_l \tag{17}$$

which does not give the same Heisenberg equation as in the continuous case or (*b*) using (15) where D_l is determined by demanding a similar Heisenberg equation to that in the continuous case (5).

We remark that our goal was related to considering conceptual impositions on discrete systems rather than particular physical restrictions as is usual in tight-binding theory (solid state physics).

Finally a discussion related to discrete and continuous Schrödinger equations of one particle in a DC electric field becomes necessary. Our discrete model could not be defined on the whole space; off-diagonal potentials are defined by $|D_{l+1}|^2 - |D_l|^2 = F$ ($F > 0$) and then if $l \to -\infty$ a solution does not exist. That gives us a lack of translation invariance which needs to be investigated. Moreover, for the continuous model of a particle in a periodic potential with a DC electric field (for instance $V(x) = Fx + \cos x2\pi/d$), it is clear that the Schrödinger equation is invariant under the transformation $x \to x + d$, $E \to E + Fd$. Conversely, our equation is invariant under $l \to l + n$, $c \to c - Fn/2$. That suggests that the role of c could be more important than an arbitrary constant ($c \sim E$?). Finally, we remark that if we consider a finite system (size N), the lack of translation invariance does not necessarily become an obstacle.

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