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Wave packet dynamics under effect of a pulsed electric field

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ABSTRACT

We studied the dynamics of an electron in a crystalline one-dimensional model under effect of a time-dependent Gaussian field. The time evolution of an initially Gaussian wave packet it was obtained through the numerical solution of the time-dependent Schrödinger equation. Our analysis consists of computing the electronic centroid as well as the mean square displacement. We observe that the electrical pulse is able to promote a special kind of displacement along the chain. We demonstrated a direct relation between the group velocity of the wave packet and the applied electrical pulses. We compare those numerical calculations with a semi-classical approach.

1. Introduction

The dynamics of a quantum wave-packet on a one-dimensional model under effect of an electric field is a hot topic with several applications in general solid state physics [1–21]. Originally studied by Bloch and Zener about 70 years ago, the most famous phenomenology was obtained by investigating the effect of a constant electric field (DC) under the electronic dynamics in crystalline systems. The main result is the existence of a coherent oscillatory motion with frequency equal to intensity of the static electric field, also called Bloch Oscillations (BO). The experimental observation it was achieved in semiconductor super-lattices only in the nineties [2]. Due to technological advances, BOs have been experimentally studied in other systems, such as Bose–Einstein condensates [3], ultra-cold atoms [4] and optical super-lattices [5]. Within the theoretical point of view , an interesting analysis about the motion of a charged particle on a lattice in the presence of a generic electric field it was done in ref. [8]. The authors demonstrated the presence of a dynamic localization whenever the ratio of the magnitude and the frequency of the electric field is a root of the ordinary Bessel function of order [8]. The effect of scattering caused by imperfections of the lattice it was considered in ref. [9]. In ref. [11] it was shown a detailed analysis of the coherent electronic dynamics under effect of electric static and time-periodic (AC) fields. The authors demonstrated the possibility of to "push" a Gaussian wave-packet by using a oscillating field with frequency tuned at the Bloch frequency [11]. Recently, the properties of Bloch-oscillations in non-Hermitian lattices with a non-vanishing imaginary part of the band dispersion curve it was investigated in ref. [12]. The authors demonstrated by using a generalized acceleration theorem that a wave packet with narrow spectral distribution undergoes a periodic motion, but following a closed orbit in the complex plane. The competition between electron–electron interaction, electric field effect and dissipation terms it was studied in ref. [13]. By using the Keldysh Greens functions in cluster perturbation theory, the steady-state current it was computed. The authors demonstrated that the current properties are controlled by the Wannier-Stark resonances due to anti-ferromagnetic correlations [13].

The effect of the on-site Hubbard interaction U on the Bloch oscillations of two electrons under effect of an external electric field was investigated in refs. [16–18]. By solving the time-dependent Schrödinger equation for an initially localized two-electron state it was proven that the possibility of the wave packet develops Bloch oscillations where the dominant frequency is the twice of the Bloch frequency predicted by semi-classical approach [17]. It was proposed that this effect is strongly related with the set of two-electron bound states that appear for $U>0$. That hypothesis was investigated in detailed and proven in ref. [18]. Experimental investigations of Bloch oscillations in optical lattice and ring cavity were done in refs. [20,21]. By using interacting atoms in optical lattices, it was observed strongly correlated Bloch oscillations as well as correlations in two-particle quantum movement [21]. In special, the experiment conducted in ref. [21] proved the existence of Bloch oscillations with double frequency, previously obtained in ref. [17] through theoretical experiments.

In ref. [22] it was proposed that a superposition of a static field and a harmonic one can promote electronic dynamics in low-dimensional systems. It was also shown that the electronic velocity depends on the magnitudes of the AC and DC field

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components and the initial phase of the AC field. Transport over macroscopic distances has been recently reported in Bose-Einstein condensates with weak interaction in a tilted lattice under simultaneous influence of a DC and AC fields [23]. In this work we provide further studies about the specificity of the electronic dynamics under effect of time-dependent electric fields. We consider an electron moving in a regular one-dimensional(1D) lattice under effect of an external electric field $F(t)$. The external field consists of a Gaussian-pulse. We emphasize that pulsed external fields (including Gaussian–Pulses) have been used in several contexts of science [24–31]. For example, the effect of ultra short electric pulses on biological cells, tissues, and organs has attracted a great interest [29,30]. In our work, we will follow the time evolution of an initially Gaussian electronic wave packet under effect of an external Gaussian-electric pulse. We will compute typical tools that characterized the wave-packet dynamics along the chain, namely the electron's position and the mean-square displacement. Our calculations demonstrated an unusual electron dynamics quite related with the kind of pulse electric field we have considered. Our analysis suggests that the electrical pulse is able to promote a interesting electronic dynamics along the chain. Results revealed that the velocity of the particle can be controlled through the type electric pulses applied and it is possible to easily speed up or slow down the electron.

2. Time-dependent Schrödinger equation and formalism

Our model consists of an electron moving in a regular one-dimensional chain with N sites driven by an external field $F(t)$. The internal distance between the nearest neighbors is a. The tight-binding Hamiltonian that describe our model can be written as

$$H = J\sum_{n=1}^{N}(|n\rangle\langle n+1| + |n+1\rangle\langle n|)\sum_{n=1}^{N}(\epsilon_n - eF(t)na)|n\rangle\langle n|, \quad (1)$$

where $|n\rangle$ is a Wannier state localized at site i with energy ϵ_n, J is the inter-site coupling restricted to nearest-neighbors, e is the particle charge. The temporal evolution of the wave-function components in the Wannier representation ($|\psi(t)\rangle = \sum_n \psi_n|n\rangle$) is governed by the time-dependent Schrödinger equation

$$i\dot{\psi}_n = \psi_{n+1} + \psi_{n-1} - eF(t)n\psi_n. \quad (2)$$

Here, we will use units such that $\hbar = e = a = J = 1$. The on-site energies ϵ_n were taken as the reference energy ($\epsilon_n = 0$) and time is expressed in units of $\hbar/J$. The external field consists of a Gaussian-pulse [31], which can be expressed as

$$F(t) = B(\rho)\exp\left[-\frac{(t-\tau)^2}{4\rho^2}\right], \quad (3)$$

where ρ controls the duration of each pulse and τ is the time of reference. We can observe that for a finite and small ρ and a single value of τ, $F(t)$ represent a single pulse around $t \approx \tau$. We are interested in consider a collections of pulses, i.e., we will consider some distinct values of τ. The above set of equations were solved numerically by using fourth order Runge–Kutta method with step-size about 10^{-4} in order to to keep the wave-function norm conservation $(1 - \sum_n |\psi_n(t)|^2 \le 10^{-13})$ along the entire time interval considered. The initial wave-packet will be consider a Gaussian wave packet with width σ defined as

$$\psi_n(t=0) = \frac{1}{A(\sigma)}\exp\left[-\frac{(n-n_0)^2}{4\sigma^2}\right], \quad (4)$$

where the initial position of the particle (n_0) is the center of chain (i.e $n_0 = N/2$). After solving the set of equations we will compute the centroid $\overline{x}(t)$ and the mean-square displacement $\xi(t)$ i.e., typical quantities that can bring information about the eigenstates and wave-packet time-evolution. These tools are defined as:

$$\overline{x}(t) = \sum_n n|\psi_n(t)|^2, \quad (5)$$

and

$$\xi(t) = \sqrt{\sum_n [n - \overline{x}(t)]^2 |\psi_n(t)|^2} \quad (6)$$

The centroid $\overline{x}(t)$ represent the electronic position and $\xi(t)$ is a measurement of the spread of the wave-function. We will also analyzing the wave-function profile $|\psi_n(t)|^2$ versus t and n in order to understand better the effect of Gaussian-pulse electric field under the electronic dynamics.

3. Results

We will show initially our results for the temporal wave packet profile $|\psi_n(t)|^2$ versus t and n (see Fig. 1) . Calculations were done for N=400. The initial wave packet it was a Gaussian with $\sigma = 1.0$. In our first numerical experiment we have considered four electric pulses with $\rho = 1$, and $\tau = 10, 25, 45, 55$ time units. We adjusted the value of $B(\rho = 1)$ in order to impose that the impulse I of each pulse is given by: $I = \int_{-\infty}^{\infty} \mathbf{F}(t)\,dt = \pi/2$. In fig. 1 we observe the behavior of the electronic function in time and space. We note that in the early stages of temporal evolution ($t < 10$) the wave packet widens on the lattice. For short times, the electric field is absent and therefore the wave-function moves without any interaction. However, after the first pulse be applied, the wave packet seems to be "pushed " for one of the chain edges. We observe that this driven motion is stopped after the application of the second pulse (t=25). After the second pulse, the wave packet seems to develops movement with small (almost null) group velocity. We also observe a kind of ondulatory behavior. After the third pulse at t=45 a counter-intuitive behavior is observed. The particle restarts its movement however, in the opposite orientation. For t=55 time units, the wave packet is subjected to a new electric field pulse and an interruption of the particle movement can be observed again. This behavior can be understood following semi-classical

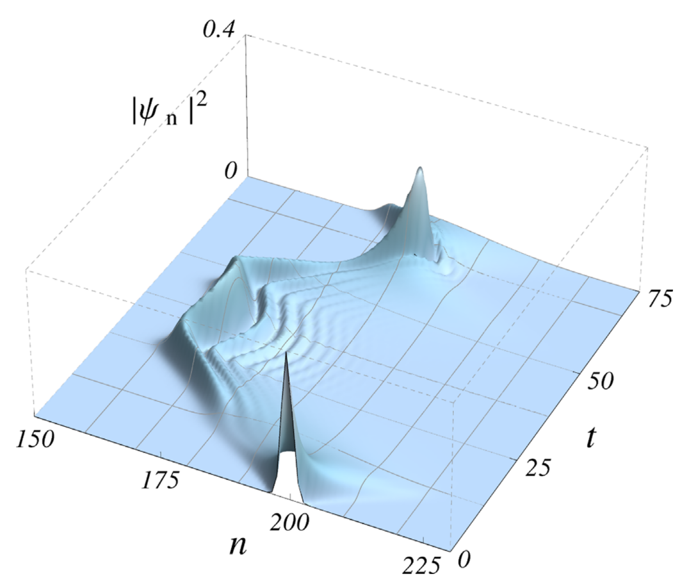

Fig. 1. (Color online) Time evolution of the wave packet with N=400 sites. The initial condition was a gaussian wave packet width $\sigma = 1.0$. We have used four pulses each one with impulses $I = \pi/2$. The pulses were applied at times $\tau = 10, 25, 45, 55$ time units.

arguments. For a particle of charge e, we can use the acceleration theorem and written the wave vector k as :

$$k = k_o + \frac{e}{\hbar}\int_{t_i}^{t_f} \mathbf{F}(t)\, dt. \tag{7}$$

The group velocity of wave-packet centered around some k' state is given by the gradient of the dispersion relation

$$v(k') = \frac{1}{\hbar}\frac{\partial E(k)}{\partial k}\bigg|_{k'}. \tag{8}$$

Therefore, by using the energy dispersion obtained in our case ($E(\mathbf{k}) = 2J\,\cos(ka)$), we can written $v(k)$ as

$$v(k) = -\frac{2Ja}{\hbar}\,\sin\left(k_o a + \frac{ea}{\hbar}I\right), \tag{9}$$

where $I = \int_{t_i}^{t_f} \mathbf{F}(t)\, dt$ is the impulse. Therefore by using this semi-classical formalism we can understand the effect of pulsed electric field on the electronic transport. We can observe that after the first pulse be applied, the wave packet changes its initial wave vector from ($k_0 = 0$) to $k = \pi/2$ thus implying in a change of its group velocity. Following the same arguments, we can conclude that, after the second pulse be applied, the wave-vector change to $k = \pi$, in good agreements with the absence of group velocity found in Fig. 1. The change of orientation found after the third pulse be applied is related with o wave-vector values $k = 3\pi/2$. After the fourth pulse, the wave-vector changes to $k = 2\pi$ and the group velocity vanishes again in good agreements with Fig. 1. A more quantitative study is shown at Fig. 2. We show in Fig. 2(a) the plot of the electric field versus time. We can see clearly that the four pulses were considered for $t = 10, 25, 45, 55$ (the same case as in Fig. 1). In Fig. 2(b) and (c) we plot respectively the centroid and the mean-square displacement versus time (t). In good agreements with the description showed in Fig. 1, the centroid displays an interesting dynamics, strongly dependent on the electric pulses. The mean-square displacement dynamics reveals an increasing for short times (i.e. , in the absence of electric field). After the pulses are applied, this tendency is weakened or even reversed. Due to the change in the movement direction, the electronic wave-packet suffers interference and can decreases the width ξ as can be seen in Fig. 2c. In order to elucidate better the correspondence between the quantum mechanical description and the semi-classical approach, we shown in Fig. 3(a,b) the electronic centroid $\overline{x}(t)$ and $\xi(t)$ for two distinct experiments. We consider two distinct types of time dependent electric field: the first one is a sequence of four pulses each one with impulse $I = \pi/4$. Our calculations are shown in Fig. 3(a,b) (solid line) and the electric field temporal profile can be found in Fig. 3(c).The second experiment we have performed consisted of a sequence of two pulses each one with $I = \pi/2$ (see results in Fig. 3(a,b) dashed line). The electric field profile can be found in Fig. 3(d). Calculations were done for an initial wave packet with $\sigma = 1.0$ and N=400. We emphasize that the total impulse transferred for the wave-packet in both experiments was 2π therefore, from the qualitatively point of view , the results should be similar. By analyzing the Fig. 3(a,b) we observed a qualitative agreements between the dashed and solid curve. However, from the quantitative point of view, we observe that the case with $I = \pi/2$ promotes a biggest change at the wave-packet's velocity, in good agreements with the semi-classical approach. Moreover, we also observed that the mean square displacement ξ exhibits a roughly controlled behavior. In contrast with the case without electric field in which that the electron wave-packet spreads ballistically , the wave-packet here seems to keep trapped in a finite fraction of the lattice. It is an interesting key point because suggests that the pulsed electric field can be used to “push” the wave-packet and keeping its width finite. We can use this superposition of pulsed electric fields as tweezers to electronic manipulation.

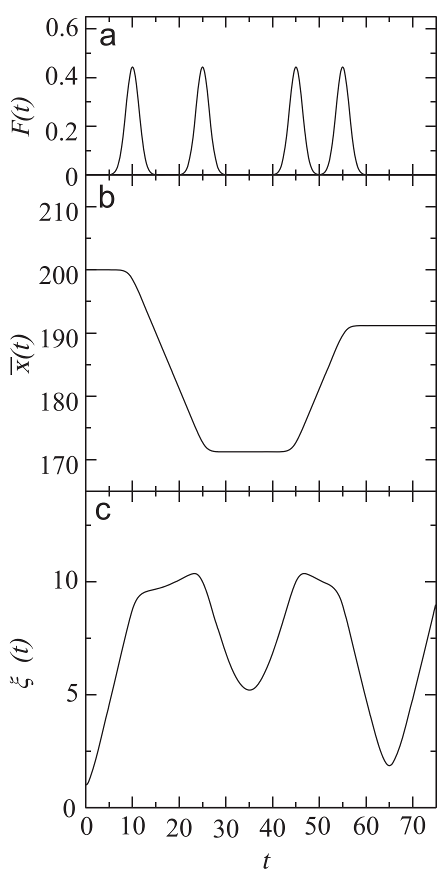

Fig. 2. Calculations of centroid and the mean square displacement for the same case of the Fig. 1. In (a) we plot the electric field versus time. We can see clearly the four pulses considered for $t = 10, 25, 45, 55$.

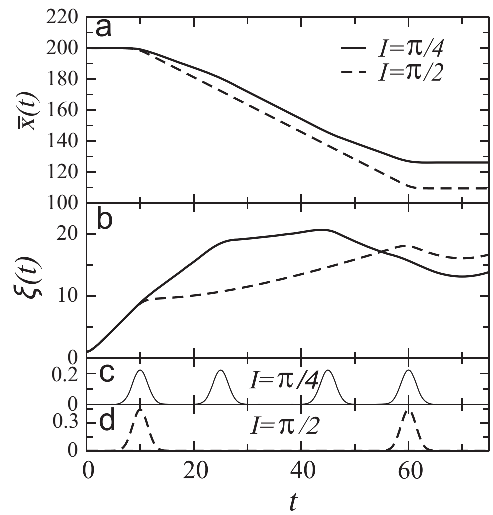

Fig. 3. (a,b) Numerical calculations of the centroid and mean square displacement. The experiments were done by considering two distinct types of time dependent electric field: The first one is a sequence of four pulses each one with impulse $I = \pi/4$ (see results showed in solid line and the electric field profile in (c)); the second case is a sequence of two pulses each one with $I = \pi/2$ (see results in dashed line and the electric field profile (d)). Calculations were done for an initial Gaussian wave packet with $\sigma = 1.0$ and N=400.

In Fig. 4 we investigated the time evolution of an initial gaussian wave-packet with $\sigma = 1$ and 4 under effect of a single electric field pulse with several values of impulse I. In Fig. 4(a,c) we plot the centroid versus time for $I = \pi/2, 3\pi/2, 5\pi/4, \pi/4, \pi$. Calculations

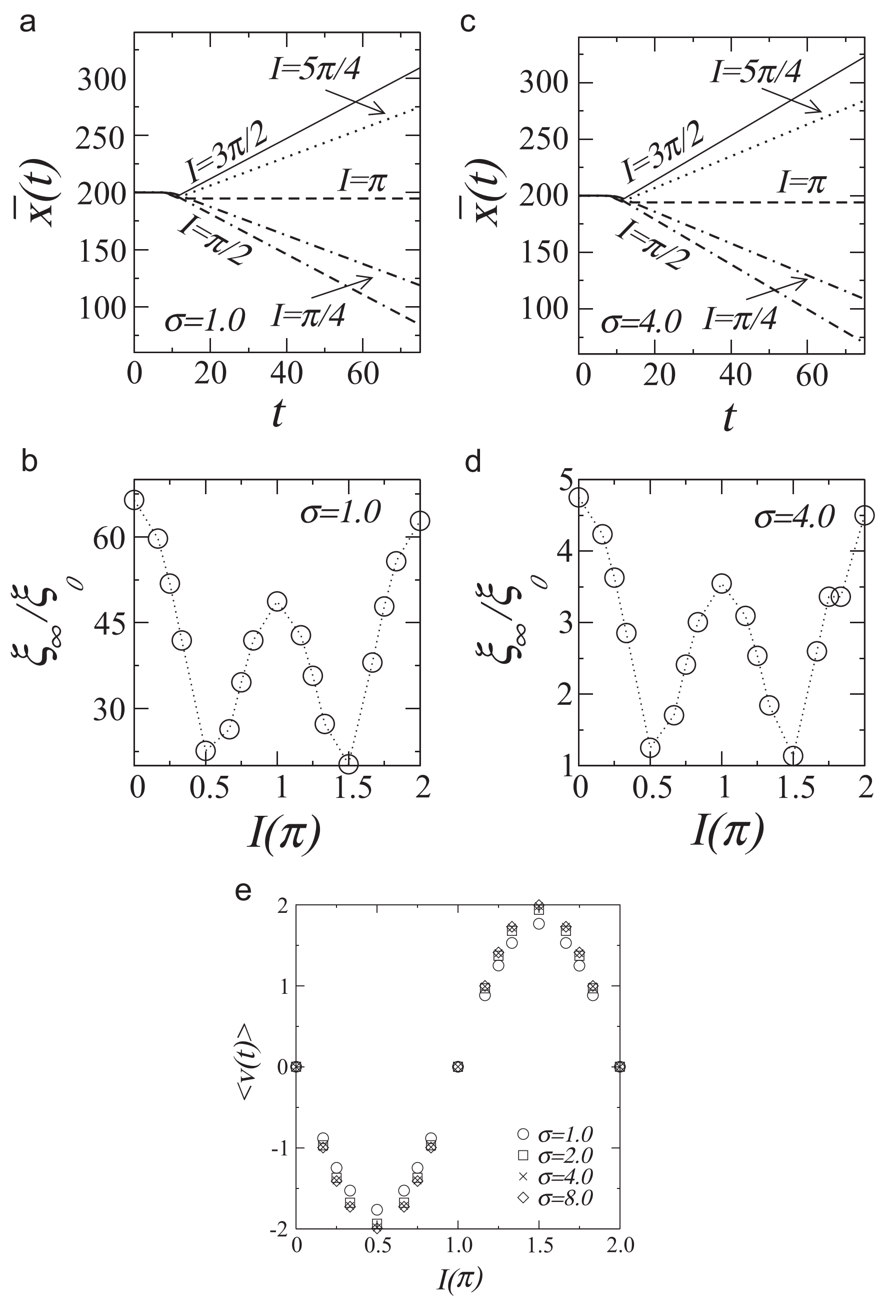

Fig. 4. (a,c) The centroid versus time for an initial gaussian with $\sigma = 1$ (a) and $\sigma - 4$ (c) under effect of a single pulse with $I = \pi/2, 3\pi/2, 5\pi/4, \pi/4, \pi$. (b,d) the ratio between the mean square displacement for long time and the initial mean square displacement (ξ_∞/ξ_0) ; calculations were done for $\sigma = 1$ (b) and $\sigma - 4$ (d). (e) The group velocity versus I for $\sigma = 1$ up to 8.

were done for $\sigma = 1$(a) and $\sigma = 4$(c). We observe that a single pulse with impulse I is able to promote the movement of the particle in several directions of the chain. The direction and the electronic velocity is strongly related with the intensity of impulse, in good agreements with our semi-classical formalism (see Eq. (9)). However, it is interesting to investigate also the wave-packet spread and its relation with the applied pulsed electric field. In Fig. 4(b,d) we plot the ratio ξ_∞/ξ_0 versus the impulse I. Here, ξ_∞ represent the mean square displacement for long time and ξ_0 the mean square displacement in the early stage of the time evolution ($t \approx 0$). We emphasize that the border effect here are numerically negligible. Our results reveals a richness of properties and an interesting dependence of the wave-packet spread with the impulse I. For both values of σ we observe that for the most values of I, the wave-packet spreads within the chain. For $I \approx \pi/2$ and $3\pi/2$ we can observe a decreasing of the ratio ξ_∞/ξ_0. For $\sigma = 4$ we can see that the wave-packet spreads less than the case with $\sigma = 1$ and for $I \approx \pi/2$ and $3\pi/2$ does not spread ($\xi_\infty \approx \xi_0$). We can give some heuristic arguments to understand those previous finds. For large σ (e.g. $\sigma = 4$), the initial wave-packet is narrow in frequencies. Therefore, for $\sigma \gg 1$, the initial wave-packet is a superposition of modes with small group velocity and therefore, the mobility is smaller thus promoting the decreasing of ratio ξ_∞/ξ_0. For $I \approx \pi/2$ and $3\pi/2$ we emphasize that the group velocity for these cases is maximum (see Eq. (9)) therefore, the intrinsic interference of the wave-packet during the push promotes the drastic decreasing of the mean square displacement. Fig. 4(e) shows the group velocity for each value of impulse I. The sine behavior of the group velocity is in good agreements with the semi-classical prediction described in the Eq. (9). We highlight these two factors as essential for using this technique for manipulating particles in lattices. So the velocity of the particle and its position within the lattice become predictable and controllable through adjustments to electric pulses applied.

4. Summary and conclusions

In this work we have considered a one-electron wave-packet confined in a regular one-dimensional chain under effect of an external time- dependent electric field $F(t)$. The external electric field $F(t)$ consisted of a collection of short Gaussian-pulses. We have followed the time evolution of an initially Gaussian wave packet and compute the electronic positions and the wave-packet spread. The Schrödinger equation it was solved by using a standard fourth order Runge–Kutta formalism. The numerical validation it was obtained by checking the wave-function normalization during the integration. Our calculations suggest that the electrical pulse can promote a new type of electronic dynamics along the chain. Our calculations also indicate that the velocity of the particle can be controlled by the specifities of the applied electric pulses . In our numerical experiments we have demonstrated the possibility of driving the electron along the chain, reverse the direction and also to brake the particle during a short interval. We also provide a detailed description of the time-dependent behavior of the width of the wave-function. Our calculations indicate the possibility of to keep the wave-function trapped in a finite fraction of lattice even at the cases in which that the centroid exhibits mobility. We emphasize that our calculations are interesting within the context of manipulate charged particles in low-dimensional systems. We have used a simple semi-classical formalism that explains in detail the phenomenology studied here. Our results provide a good agreement between the numerical calculations and semi-classical investigation. We hope that our work encourages further investigation about the manipulation of particles in low-dimensional systems using pulsed electric fields.

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