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Self-trapping of interacting electrons in crystalline nonlinear chains

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Abstract. Considering the nonlinearity arising from the interaction between electrons and lattice vibrations, an effective electronic model with a self-interaction cubic term is employed to study the interplay between electron-electron and electron-phonon interactions. Based on numerical solutions of the time-dependent nonlinear Schroedinger equation for an initially localized two-electron singlet state, we show that the magnitude of the electron-phonon coupling χ necessary to promote the self-trapping of the electronic wave packet decreases as a function of the electron-electron interaction U. We show that such dependence is directly linked to the narrowing of the band of bounded two-electron states as U increases. We obtain the transition line in the $\chi \times U$ parameter space separating the phases of self-trapped and delocalized electronic wave packets. The present results indicates that nonlinear contributions plays a relevant role in the electronic wave packet dynamics, particularly in the regime of strongly correlated electrons.

1 Introduction

The behavior of interacting electrons moving in low-dimensional systems has direct connections with the emergence of nontrivial magnetic, superconducting and optical properties [1–10]. Recently, a two-electrons tight-binding Hamiltonian in a linear chain has been investigated in detail providing a deeper understanding of some aspects of the competition between electron-electron interaction, compositional disorder and dynamical localization caused by electric fields [11–24]. In particular, by using analytical calculations [18–20], it was demonstrated that the two-electron Hamiltonian displays a band of bounded states in the energy range $U \leq E \leq \sqrt{U^2 + 16W^2}$, where U is on-site Coulomb interaction and W the hopping amplitude between first neighbors. Moreover, by using an extended dynamical mean-field theory [24], the effect of a large electric field on interacting electrons was studied, numerically demonstrating that the coherence of Bloch oscillations decays due to electron-electron correlations.

Besides the Coulombian interaction, the electron-phonon interaction also plays a relevant role on transport and thermodynamic properties. Concerning the electronic transport, the interaction between electrons and lattice vibrations leads to an effective nonlinearity [25–52]. In particular, a significant generalization of the polaron concept has been recently developed. It was demonstrated the existence of a *polaron-soliton* "quasiparticle". The coupling of self-trapped states (polaron states) with the lattice solitons has been generally termed as a *solectron* [25–33]. The solectron concept appears as a significant generalization of the original polaron concept that can mediate non-Ohmic supersonic electric conduction [33].

Usually, an effective cubic term in the time-dependent Schroedinger equation captures some essential features related to several physical scenarios, such as the electron-phonon dynamics, Bose-Einstein condensates (BEC), optical lattices, rogue waves and coupled optical waveguides [34–52]. Within the context of electron-phonon dynamics, the most important phenomenon associated with the effective nonlinearity incorporated into the Schroedinger equation is the so-called self-trapping of the electronic wave packet. It is also associated with the emergence of a wide class of topologically stable solutions such as solitons, vortex rings and breathers (oscillatory soliton-like solutions). Experimental investigations using photo-emission spectra have been widely used to investigate the effects of the electron-phonon interaction in pentacene films [53], graphene structures [54,55] and Pb thin films [56]. It has been pointed out that the phonon decay in an electron-hole pair can be used to estimate the strength of the electron-phonon coupling [57,58]. This decay leads to an extra width of the phonon that, after an average over all $\boldsymbol{q}$ vectors, provides the electron-phonon coupling strength. This width can be measured in experiments involving neutron [57,58] or Raman scattering [59–61].

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The influence of lattice vibrations on systems of interacting electrons has been a subject of recent investigations [62–66]. In particular, the interplay of electron-phonon interaction and electron-electron coupling was studied using dynamical mean-field theory to explore the effects of electronic correlations on the evolution of phonon kinks [62]. Depending on the degree of nonlinearity and Hubbard interaction, the slope of the electronic dispersion curve close to the Fermi level was shown to depict a significant decrease [62]. The time evolution of two correlated electrons of opposite spins moving in an anharmonic Morse-Toda lattice chain was investigated in reference [63]. It was observed that the degree of nonlinearity is a key ingredient to control the velocity of paired electrons [63]. Further, the problem of two interacting electrons coupled to dispersive phonons in a nonlinear lattice was numerically investigated [65]. It was observed an interesting collection of discrete breathers modes induced by the coupling between lattice vibrations and quasiparticles states. Moreover, it was demonstrated that the presence of anharmonicity in a two-electron Hamiltonian facilitates electron pairing in a localized state [66]. Such localized state appears as singlet state of two electrons bounded with the traveling local lattice soliton distortion. This state survives when Coulomb repulsion is included [66].

In this paper, we report further progress on the study of correlated electron systems coupled with lattice vibrations. We will provide a detailed analysis of the interplay between the on-site electron-electron Coulomb coupling and the effective nonlinearity arising from an underlying electron-phonon interaction within the context of self-trapping in low-dimensional systems. To this end, we will focus on the wave-packet dynamics of two electrons moving in a 1D crystalline nonlinear chain. We will use numerical methods to solve the time dependent Schroedinger equation to follow the time-evolution of the two-electrons wave packet. For initially close electrons in a singlet state, it is observed that the magnitude of the electron-phonon coupling χ necessary to promote the self-trapping decreases as the electron-electron interaction U is increased. Based on the long-time behavior of the two-electrons wave packet, we obtain the transition line corresponding to the self-trapped to delocalized transition.

2 Model and formalism

The vibrations in a lattice can be classified as acoustic phonon modes associated with the relative displacement of unitary cells and the optical phonons accounting for the displacement of atoms inside a single cell. Concerning the electronic tight binding Hamiltonian, the on-site potentials as well as hopping integrals depend upon these vibrations [40–42]. Following the Su-Schrieffer-Heeger model [67,68], the Hubbard Hamiltonian for two-interacting electrons coupled to the vibrations of a linear closed chain (periodic boundary condition) can be written as:

$$\begin{aligned} H = & \sum_n \left\{ \frac{{p_n}^2}{2M} + \frac{1}{2} M\omega_s^2 (u_{n+1} - u_n)^2 \right\} \\ & + \sum_n \left\{ \frac{{P_n}^2}{2M} + \frac{1}{2} M\omega_0^2 {\nu_n}^2 \right\} \\ & + \sum_n \alpha(V_0 + u_{n+1} - u_n)(c_{n+1}^\dagger c_n + c_n c_{n+1}^\dagger) \\ & + \sum_m \alpha(V_0 + u_{m+1} - u_m)(c_{m+1}^\dagger c_m + c_m^\dagger c_{m+1}) \\ & + \sum_n (E_n + \gamma_n \nu_n) c_n^\dagger c_n + \sum_m (E_m + \gamma_m \nu_m) c_m^\dagger c_m \\ & + \sum_n U c_{n,\uparrow}^\dagger c_{n,\uparrow} c_{n,\downarrow}^\dagger c_{n,\downarrow}. \end{aligned} \tag{1}$$

Here u_n and ν_n are the overall displacement and the internal vibration coordinates of the nth unit cell, respectively. p_n and P_n are, in order, their conjugated momentum. M is the mass of the unit cell, while ω_0 and ω_s are the oscillation frequency of the optical and acoustical phonons, respectively. $c_{n(m)}^\dagger$ and $c_{n(m)}$ are the creation and annihilation operators for the electron at site $n(m)$. Here α and $\gamma_{m(n)}$ are the coupling constants while V_0 is the bare hopping amplitude. $E_{m(n)}$ are the on-site energies and U is the on-site Hubbard electron-electron interaction. We will consider $\gamma_n = \gamma_m = \gamma$. In order to follow the time evolution of two-electron wave packets, we solve the time dependent Schroedinger equation by expanding the wave-function in the Wannier representation $|\Phi(t)\rangle = \sum_{n,m} \phi_{n,m}(t)|n\ s_1, m\ s_2\rangle$. From this, we can derive the equations of motion:

$$\begin{aligned} \frac{d^2 u_n(t)}{dt^2} = & -\omega_s^2 \left[2u_n(t) - u_{n+1}(t) - u_{n-1}(t)\right] \\ & + \frac{2\alpha}{M} \Re[\phi_{n+1,m}^*(t)\phi_{n,m}(t) - \phi_{n-1,m}^*(t)\phi_{n,m}(t) \\ & + \phi_{n,m+1}^*(t)\phi_{n,m}(t) - \phi_{n,m-1}^*(t)\phi_{n,m}(t)] \end{aligned} \tag{2}$$

$$\frac{d^2 \nu_n(t)}{dt^2} + \omega_0^2 \nu_n(t) = \gamma \sum_m |\phi_{n,m}(t)|^2 \tag{3}$$

$$\frac{d^2 \nu_m(t)}{dt^2} + \omega_0^2 \nu_m(t) = \gamma \sum_n |\phi_{n,m}(t)|^2 \tag{4}$$

$$\begin{aligned} i\hbar \frac{d\phi_{n,m}(t)}{dt} = & \left[E_n + \gamma \nu_n(t)\right] \phi_{n,m}(t) \\ & + \left[E_m + \gamma \nu_m(t)\right] \phi_{n,m}(t) \\ & + \sum_{p,n} t_{p,n} \phi_{p,n}(t) + \sum_{p,m} t_{p,m} \phi_{p,m}(t) \\ & + \delta_{n,m} U \phi_{n,m}(t), \end{aligned} \tag{5}$$

where $t_{p,n} = \alpha(V_0 + u_p - u_n)$ and $t_{p,m} = \alpha(V_0 + u_p - u_m)$. We assume that the dependence of hopping integrals on the u_n is so weak that it can be ignored and nearest

neighbors hopping integrals ($t_{p,n(m)} = W$ if $|p-n(m)| = 1$ and zero otherwise). After these considerations, we obtain

$$i\hbar\frac{d\phi_{n,m}}{dt} = [E_n + \gamma_n\nu_n(t) + E_m + \gamma_m\nu_m(t)]\,\phi_{n,m}(t) + W\,[\phi_{n-1,m}(t) + \phi_{n+1,m}(t) + \phi_{n,m-1}(t) + \phi_{n,m+1}(t)] + \delta_{n,m}U\phi_{n,m}(t). \quad (6)$$

We assume that the molecular vibrations on the lattice sites reach equilibrium on a time scale smaller than the scale of time for the evolution of the electronic wave packet. Therefore, we obtain $\omega_0^2\nu_n = \gamma\sum_m |\phi_{n,m}(t)|^2$ and $\omega_0^2\nu_m = \gamma\sum_n |\phi_{n,m}(t)|^2$. Substituting it in (6) and defining $\chi = \gamma/\omega_0^2$ we have

$$i\hbar\frac{d\phi_{n,m}}{dt} = [E_n + E_m]\,\phi_{n,m}(t) + \left[\chi\sum_m |\phi_{n,m}(t)|^2 + \chi\sum_n |\phi_{n,m}(t)|^2\right]\phi_{n,m}(t) + W\,[\phi_{n-1,m}(t) + \phi_{n+1,m}(t) + \phi_{n,m-1}(t) + \phi_{n,m+1}(t)] + \delta_{n,m}U\phi_{n,m}(t) \quad n,m = 1\ldots N \quad (7)$$

where N is the chain size. In the above equation we used units of $\hbar = 1$ and considered a unitary hopping amplitude between first-neighbor sites $W = 1$. χ represents the effective local electron-phonon coupling. In what follows, we will employ the eighth-order Runge-Kutta method to numerically integrate equation (7). We followed the time-evolution of an initially localized wave packet $\phi_{n,m} = \delta_{n,n_0}\delta_{m,m_0}$ where the initial position of the electron pair (n_0, m_0) will be considered to be centered at $(N/2-d_0, N/2+d_0)$. Aiming to characterize the dynamic behavior of the wave packet, we computed two typical quantities that can bring information about the possible self-trapping of the wave packet and its spacial extension, namely, the return probability and the participation function which are defined as

$$R_0(t) = |\phi_{n_0,m_0}(t)|^2, \quad (8)$$

and

$$\xi(t) = 1/\sum_{n,m} |\phi_{n,m}(t)|^4. \quad (9)$$

$R(t)$ gives the probability of finding the electron pair in the position corresponding to the center of the initial wave packet. In the long-time regime, its scaling behavior can also be used to distinguish between localized and delocalized wave packets [38,39]. We have used $t_{max} \approx 10^6$ in our calculations. Thus, $R(t \approx 10^6) \to 0$ means that the electronic wave function escapes from its initial location. Conversely, the return probability saturates at a finite value for a localized or a self-trapped wave packet. The participation function gives an estimate of the number of base states over which the wave packet is spread at time t. In particular, the asymptotic participation number becomes size-independent for localized wave packets. On the other hand, $\xi(t \approx 10^6) \propto N^2$ corresponds to the regime where the wave packet is uniformly distributed over the lattice and the two-electrons are uncorrelated.

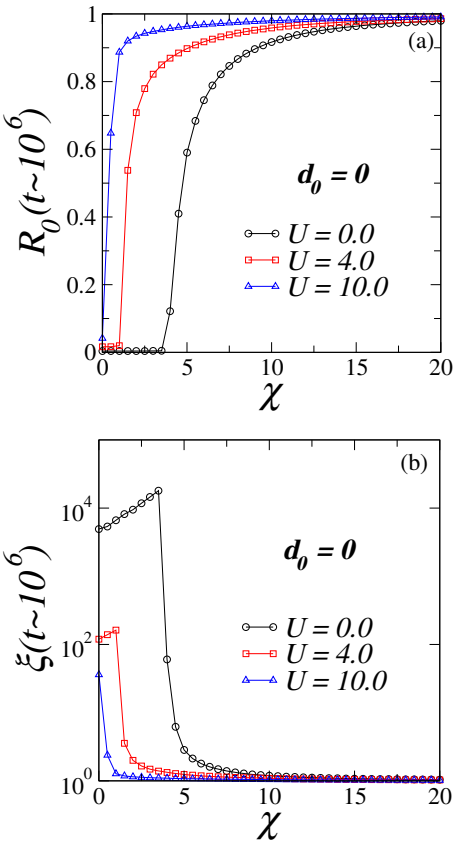

Fig. 1. (Color online) (a) Return probability at long times $R_0(t \approx 10^6)$ and (b) participation function $\xi(t \approx 10^6)$ versus the nonlinear strength χ for initially close electrons ($d_0 = 0.0$) with on-site Hubbard interaction $U = 0.0, 4.0, 10.0$. The results suggest that the presence of interaction promotes self-trapping for weaker nonlinearities.

3 Results

In Figures 1a–1b we plot the long-time return probability $R_0(t \approx 10^6)$ and the corresponding participation function $\xi(t \approx 10^6)$ versus the nonlinear strength χ for electrons initially localized on the same site ($d_0 = 0.0$). We report data for the non-interacting case together with two distinct values of the electron-electron coupling. The delocalized regime is signaled by a vanishingly small return probability and a finite participation function, while for self-trapped wave packets the return probability becomes finite and the participation function vanishes. We observe that the interaction promotes the wave packet self-trapping for weaker nonlinearities. Figures 2a–2b show similar data for the return probability $R_0(t \approx 10^6)$ and the participation function $\xi(t \approx 10^6)$ versus χ for electrons initially localized in well distant sites ($d_0 = 20.0$) with on-site Hubbard interaction $U = 0.0, 4.0$ and 10.0.

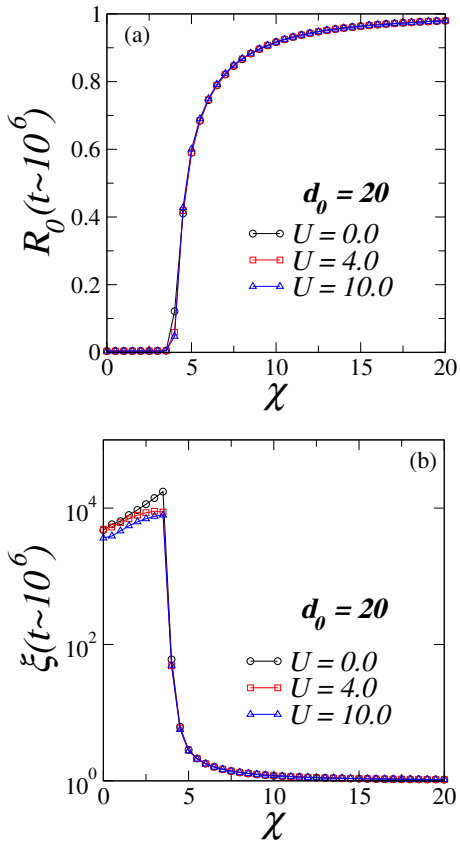

Fig. 2. (Color online) (a) Return probability at long times $R_0(t \approx 10^6)$ and (b) participation function $\xi(t \approx 10^6)$ versus the nonlinear strength χ for electrons initially far apart ($d_0 = 20.0$). For initially separated electrons, the Coulomb interaction does not significantly affect the wave packet dynamics.

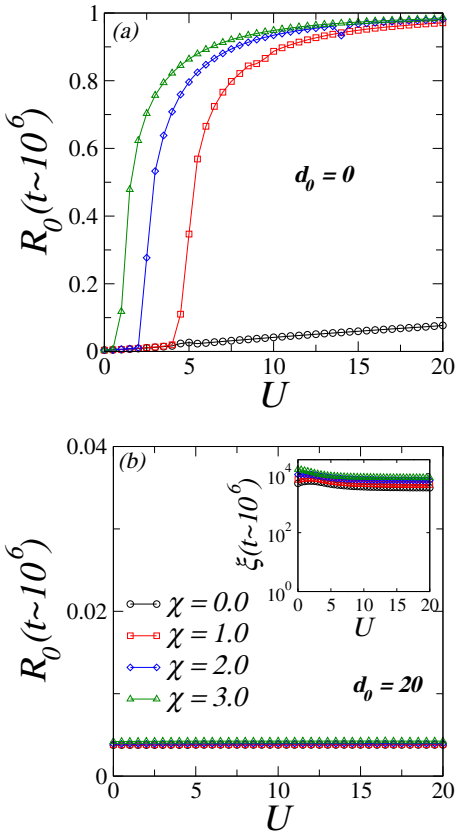

Fig. 3. (Color online) Return probability at long times $R_0(t \approx 10^6)$ versus the on-site Hubbard interaction U with $\chi = 0.0$ up to 3.0 for (a) initially close electrons ($d_0 = 0.0$) and (b) electrons initially far apart ($d_0 = 20.0$). For initially close electrons, it is observed that the magnitude of the electron-electron interaction necessary to promote the self-trapping becomes smaller in the presence of larger nonlinearities. The inset shows that the wave packet of initially far apart electrons becomes delocalized in the regime of small nonlinearities, irrespective to the valor of the Hubbard coupling.

The collapse of the data suggests that the on-site interaction does not play a significant role on the self-trapping in this case, indicating that local coupling is required to enhance the tendency of self-trapping due to the effective nonlinearity.

In order to further characterize the influence of the electron-electron coupling on the self-trapping phenomenon, we show in Figure 3 the asymptotic return probability $R_0(t \approx 10^6)$ versus the on-site Hubbard interaction U both in the linear regime $\chi = 0.0$ as well as in the nonlinear regime with χ up to 3.0 for electrons initially at the same site [2(a)] and electrons initially far apart [2(b)]. Notice that in the linear regime, the return probability is always small, signaling the absence of wave packet trapping. For electrons initially placed on distant sites, the return probability is of the order of $1/N^2$ irrespective to the coupling strength. This behavior is consistent with an uncorrelated spreading of both electrons throughout the chain. For electrons that are initially occupying the same site, we observe that above a critical coupling strength a self-trapping transition takes place even in the regime of weak nonlinearity. Therefore, our results show that the Hubbard coupling favors the self-trapping of the electronic wave packet. The smooth linear growth of the return probability in the linear case $\chi = 0$ is associated with the build up of electron-electron correlations as the coupling strength is increased. In this case, the vanishing of the asymptotic return probability changes from a $1/N^2$ scaling law typical of uncorrelated delocalized electrons to a slower $1/N$ decay for strongly correlated, although also delocalized, electrons.

To precisely locate the critical points of the delocalized to self-trapped transition, we employ a finite-size scaling analysis. In Figure 4 we plot the return probability at long time $R_0(t \approx 10^6)$ versus χ for $U = 2.5$, $d_0 = 0.0$ and $N = 100, 150, 200, 300, 500, 750$. Above $\chi_c = 1.85(5)$ the return probability becomes finite, indicating the self-trapped regime. Below χ_c, the asymptotic return probability is vanishingly small (of the order of $1/N$), which characterizes the regime of extended states. Finally, we plot the phase diagram in the $\chi \times U$ plane in Figure 5. In the absence of electron-electron coupling ($U = 0$) the critical nonlinear strength above which the electronic wave packet becomes self-trapped is of the order

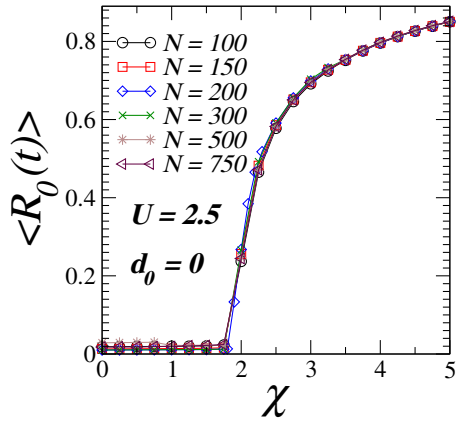

Fig. 4. (Color online) Return probability versus χ for $U = 2.5$, $d_0 = 0.0$ and $N = 100, 150, 200, 300, 500, 750$. For $\chi \geq 1.85(5)$ the return probability becomes finite, indicating the self-trapped regime.

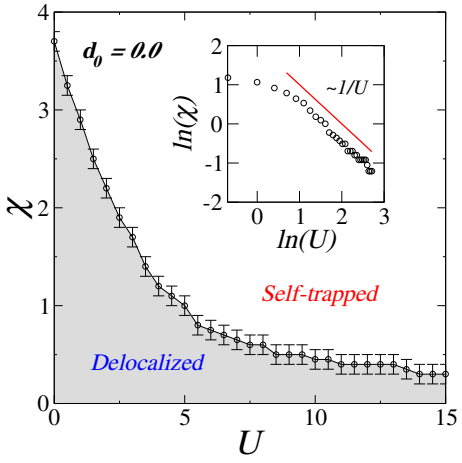

Fig. 5. (Color online) Phase diagram in the χ versus U parameter space showing the delocalized to self-trapped transition. In the absence of electron-electron interaction, the critical nonlinear strength is of the order of the single-electron bandwidth. The magnitude of the critical electron-phonon coupling χ decreases as the electron-electron coupling is increased. Inset shows the $\chi_c \propto 1/U$ asymptotic behavior.

of the single electron energy bandwidth, in agreement with previous results [38–42]. As the Hubbard coupling is turned on, the critical nonlinear strength decreases. Such decrease is linear with the Hubbard coupling in the regime of weakly interacting electrons. In the opposite regime of strongly correlated electrons, the critical nonlinear strength vanishes as $1/U$. It is worthy to recall that the energy band corresponding to bounded two-electrons states ranges from $U \leq E \leq \sqrt{U^2 + 16}$. Its width display the same limiting behaviors at weak and strong couplings. This feature indicates that the bounded two-electron states play a mayor role in the wave packet dynamics, being able to promote the wave packet trapping of strongly correlated electrons even in the presence of weak nonlinearities.

4 Summary

In summary, we investigated the influence of electron-electron correlations in the wave packet self-trapping phenomenon induced by an effective cubic nonlinearity arising from an underlying electron-phonon coupling. In particular, we considered the problem of two electrons in a singlet configuration moving on a nonlinear chain and interacting with each other through a local Hubbard coupling. We numerically solved the time dependent Schroedinger equation and followed the time-evolution of the two-electrons wave-packet. By exploring the asymptotic behavior of the return probability and the participation function, we showed that the Hubbard coupling has a negligible influence on the wave packet dynamics whenever the electrons are initially placed at large distances, even though double occupancy is produced by the wave packet spreading over the lattice in the regime of weak nonlinearities. The electron-electron coupling develops a significant influence on the wave packet dynamics when the electrons are initially localized on the same site. In this case, the critical nonlinear strength above which the wave packet becomes trapped continuously decrease as a function of the Hubbard coupling. In the regime of strongly correlated electrons, the critical nonlinear strength becomes of the order of the energy bandwidth associated with bounded two electron states. The present results adds to some recent works on the interplay between electron-electron and electron-phonon interactions [62–65]. In particular, we showed that the critical nonlinearity decays as $1/U$ thus indicating that the electron-phonon interaction acts as a relevant mechanism of electron localization in strongly correlated electron systems.

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