

Quantum simulator for energy transport in proteins: polaron biophysics with Rydberg atoms

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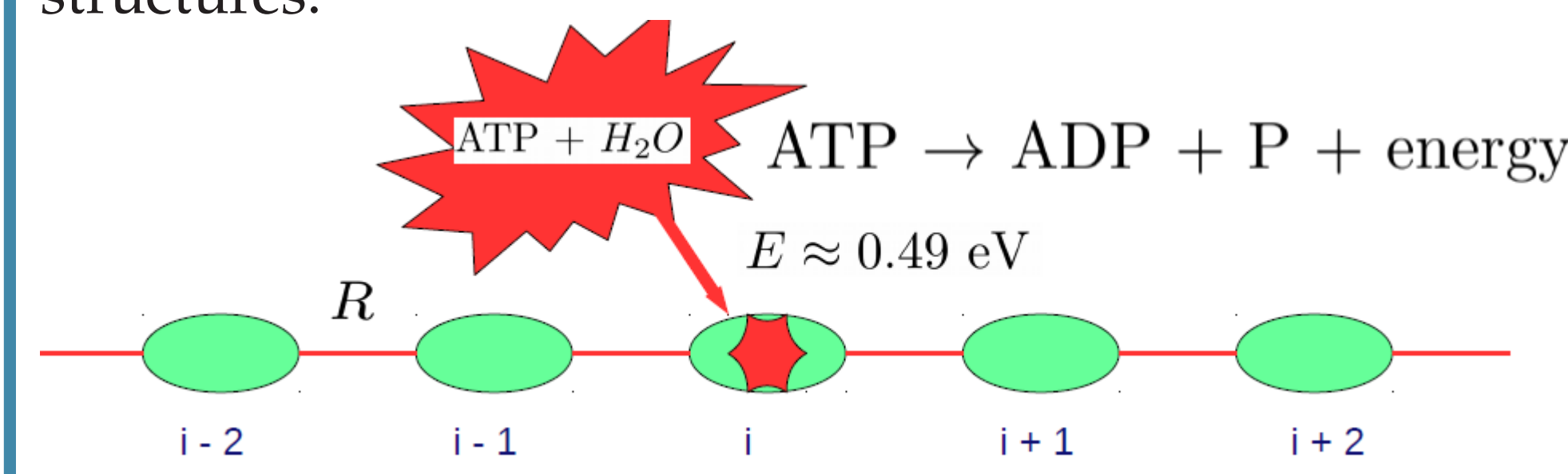
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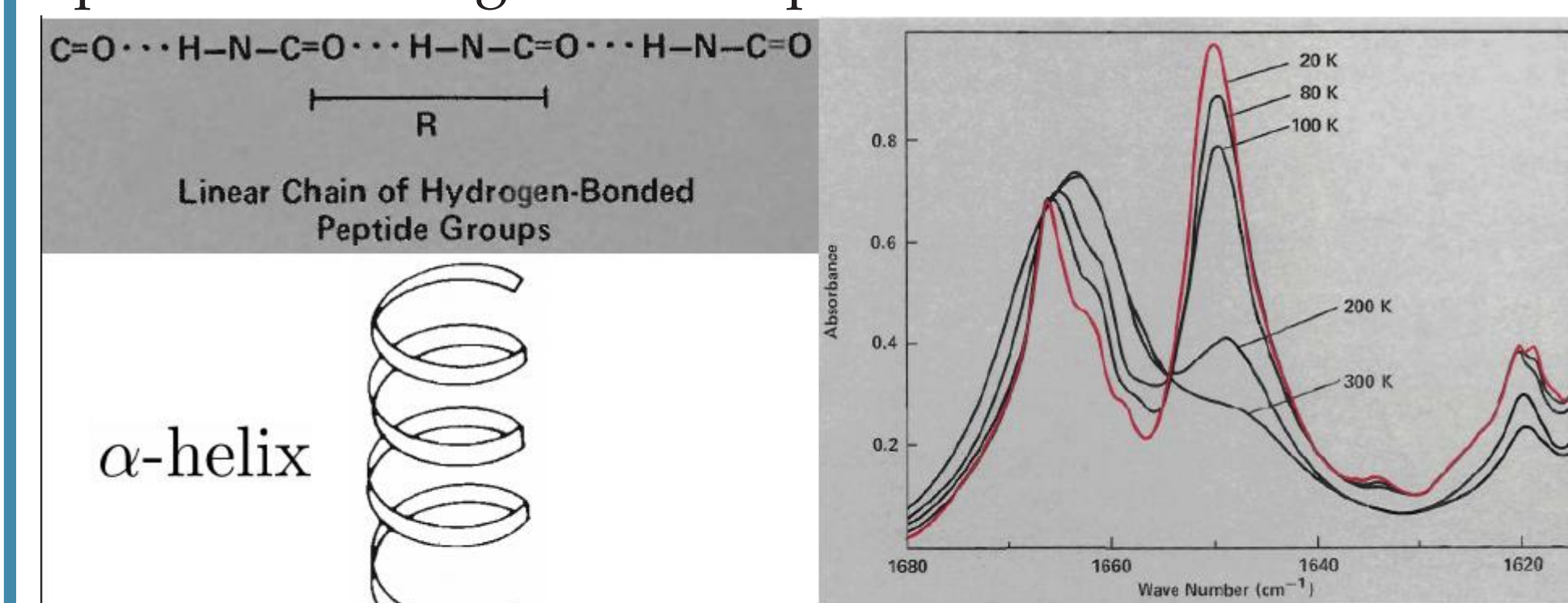
MOTIVATION

Due to the remarkable progress in our understanding of molecular structures, a tremendous development in life sciences has succeeded in providing explanations of different cell-biology phenomena. On a current stage of description a biological complexity of mesoscopic objects along with quantum behavior of the simplest elements lead together to many unsolved questions awaiting comprehensive answers. In this way, a brand new interdisciplinary field of ‘quantum biology’ become natural area for combining quantum physical methods and tools to investigate, model and simulate biological systems on a mesoscopic level

The most fundamental biological processes, such a protein folding, DNA repair and muscle contractions are related to transduction of the energy relased in the chemical reaction into work. Many biological processes takes energy from hydrolisis of adenosine triphosphate (ATP). An ATP molecule binds to a specific site on the protein, react with water and releases 0.49 eV of energy. Each site on the protein has permanent dipole moment which is responsible for energy excitation due to dipole-dipole interactions. There arises important question about quantum description of energy transport in biological structures.



In 1970's Davydov proposed a mechanism for the localization and transport of vibrational energy in α -helix region of a proteins. Such a region is a chain of amino acids held in helical shape by longitudinal hydrogen bonds where the vibrational degrees of freedom are coupled to exciton energy operator forming a exciton-phonon localized state - a soliton.



Emerging absorption peak corresponds to exciton-phonon soliton energy

Proposed model has been used for theoretical description of experimentally observed unconventional absorption band of model for protein. However, direct experimental evidence of soliton mechanism is still missing. Can we construct quantum simulator for such a system ?

QUANTUM DESCRIPTION

System Hamiltonian is given by

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{exc}} + \hat{\mathcal{H}}_{\text{vib}} \quad (1)$$

$$\hat{\mathcal{H}}_{\text{vib}} = \sum_i \hbar \omega_0 \hat{b}_i^\dagger \hat{b}_i, \quad (2)$$

$$\hat{\mathcal{H}}_{\text{exc}} = \sum_i W_i \hat{a}_i^\dagger \hat{a}_i + \sum_i J_{i+1,i} (\hat{a}_{i+1}^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{a}_{i+1}), \quad (3)$$

where on-site and hopping energies depends on relative distance changes $W_i = W_0 + g_W(u_{i+1} + u_{i-1})$, $J_{i+1,i} = -J_0 + g_J(u_{i+1} - u_i)$

In semi-classical approximation we assume that wave-function factorizes on excitation part $|\psi(t)\rangle = \sum_i \psi_i(t) \hat{a}_i^\dagger |\text{vac}\rangle$ and phonon part (which is in a coherent state) we can use Davydov anzatz:

$$|D\rangle \equiv \sum_i \psi_i(t) \hat{a}_i^\dagger e^{\sum_j \beta_j \hat{b}_j^\dagger - \beta_j^* \hat{b}_j} |0\rangle_{\text{ex}} |0\rangle_{\text{ph}}. \quad (4)$$

Time evolution of the Schrödinger for the full Hamiltonian reduces to time-evolution of Davydov's equations:

$$i \frac{d\psi_i(t)}{dt} = -(\psi_{i+1} + \psi_{i-1}) + g_W(u_{i+1} - u_{i-1})\psi_i \quad (5a)$$

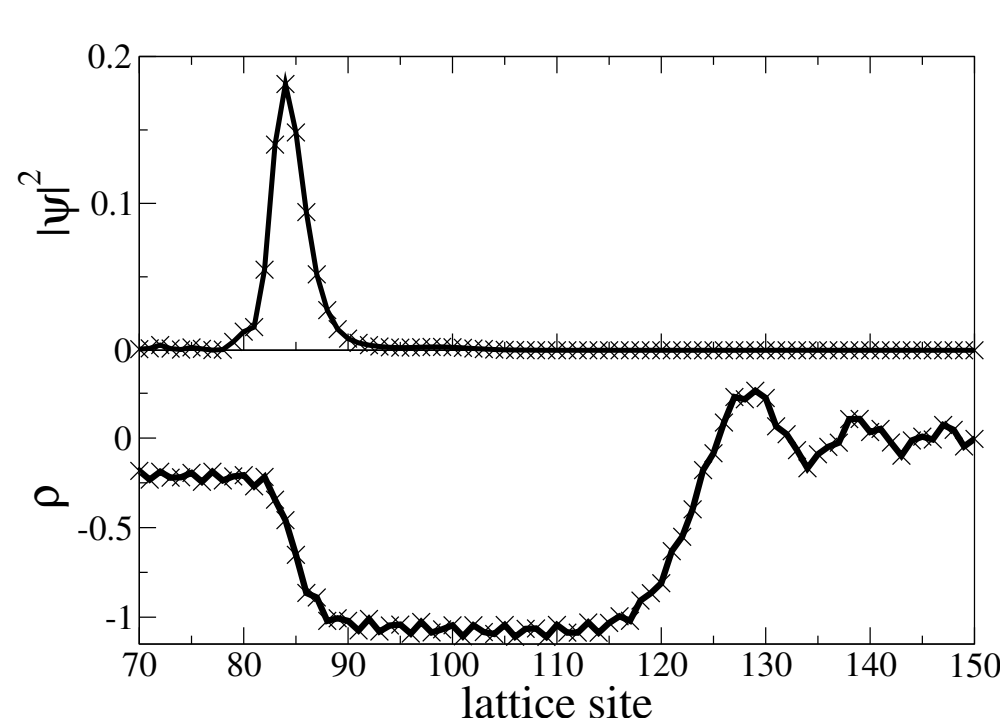
$$+ g_J[\psi_{i+1}(u_{i+1} - u_i) + \psi_{i-1}(u_i - u_{i-1})],$$

$$\frac{du_i(t)}{dt} = p_i(t), \quad (5b)$$

$$\frac{dp_i(t)}{dt} = -\omega_0^2 u_i(t) + g_W \omega_0 (|\psi_{i+1}|^2 - |\psi_{i-1}|^2) \quad (5c)$$

$$+ g_J \omega_0 [\psi_i^* (\psi_{i+1} - \psi_{i-1}) + \psi_i (\psi_{i+1}^* - \psi_{i-1}^*)],$$

where u_i is an expectation value of the displacement operator. Davydov equations give rise to self-stabilization mechanism for excitation.



EXCITATION STABILIZATION

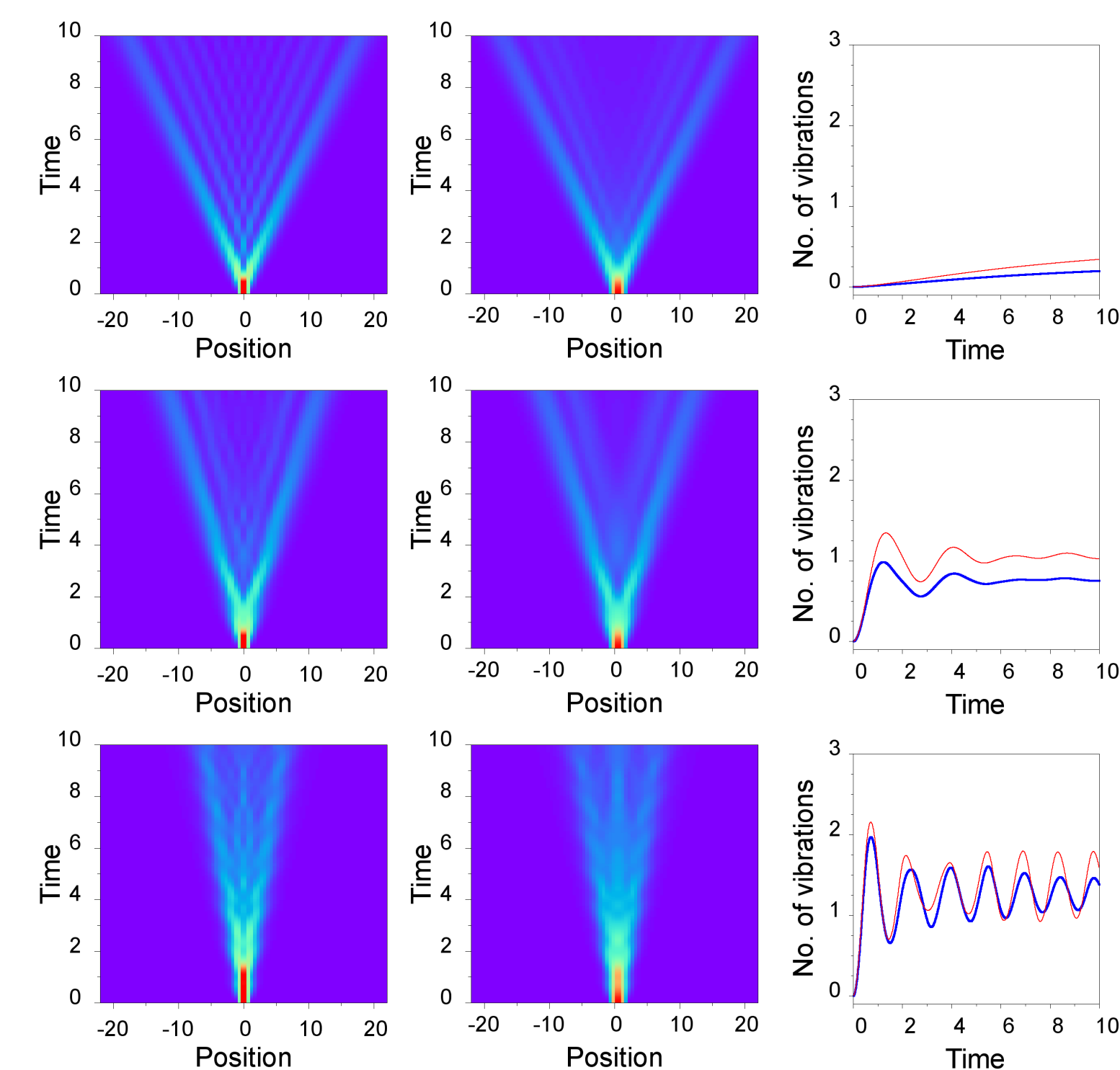
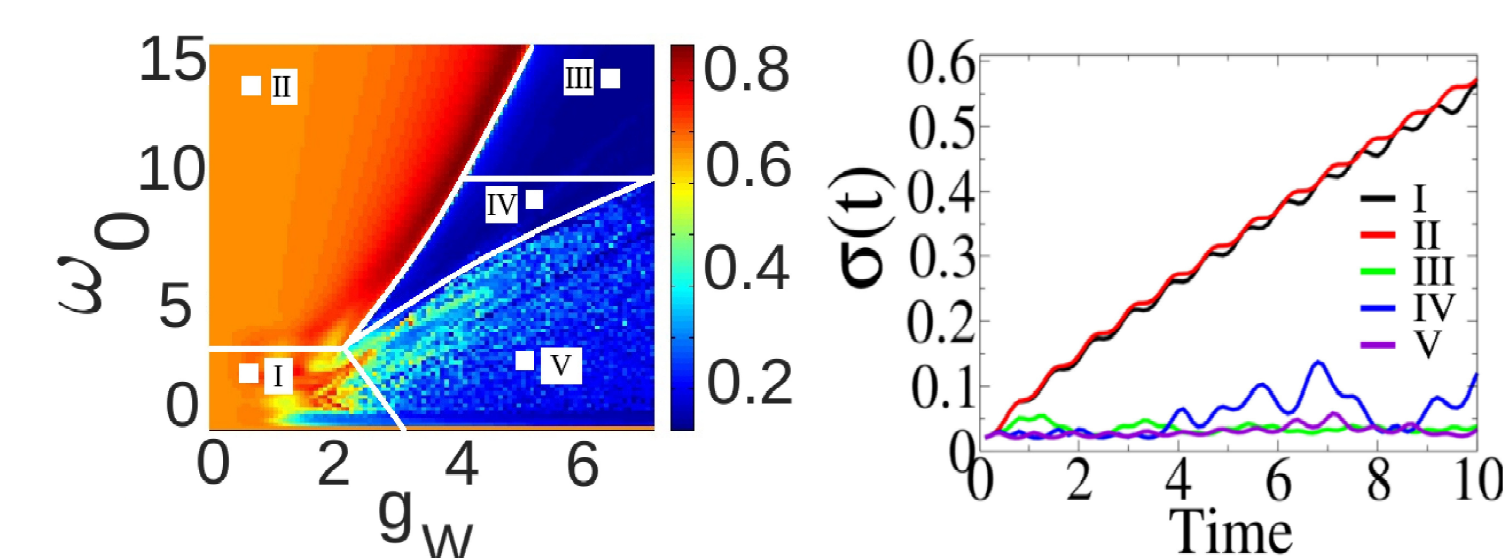
The general aim for the considered system described by the Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{vib}} + \hat{\mathcal{H}}_{\text{exc}}$ is to give predictive conclusions on its dynamical properties depending on the parameters g_W , g_J , and ω_0 . For example, one of the questions having no decisive answer is related to the problem of the spreading of the excitation initially being localized in a chosen site K $|\Psi_0\rangle = \hat{a}_K^\dagger |\text{vac}\rangle$, or it is slightly delocalized in neighboring sites $|\tilde{\Psi}_0\rangle = \frac{1}{\sqrt{2}}(\hat{a}_K^\dagger + \hat{a}_{K+1}^\dagger) |\text{vac}\rangle$, where $|\text{vac}\rangle$ is a vacuum state of the system fulfilling the condition $\hat{a}_i |\text{vac}\rangle = \hat{b}_i |\text{vac}\rangle = 0$ for any i . On mathematical level this property can be extracted from information encoded in the time-dependent density profile $\rho_i(t) = \langle \Psi(t) | \hat{a}_i^\dagger \hat{a}_i | \Psi(t) \rangle$, where the state of the system at given moment t can be formally written as

$$|\Psi(t)\rangle = \exp(-i\hat{\mathcal{H}}t) |\Psi_{\text{ini}}\rangle, \quad (6)$$

where $|\Psi_{\text{ini}}\rangle$ is one of considered initial states. Temporal spreading of the excitation is simply captured by the width of the excitation wave packet $\sigma(t) = N [\sum_i \rho_i^2(t)]^{-1}$. The quantity takes value $1/N$ for excitation localized at exactly one lattice site and 1 in a fully delocalized case. In principle, by analyzing time-dependence of $\sigma(t)$ one can easily settle if the excitation remains localized or it spreads across the system.

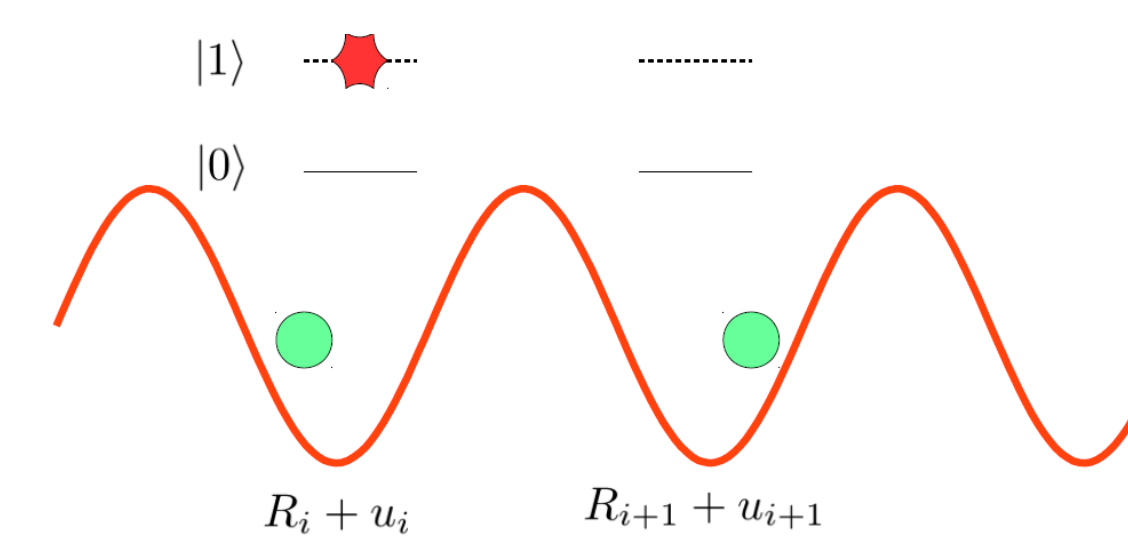
$$\rho_i(t) = \langle \Psi(t) | \hat{a}_i^\dagger \hat{a}_i | \Psi(t) \rangle \quad (7)$$

As a measure of excitation width we define $\sigma(t) = N [\sum_i \rho_i^2(t)]^{-1}$



Exact evolution of the excitation wave packet governed by the full Hamiltonian for the initial state $|\Psi_0\rangle$ (left column) and $|\tilde{\Psi}_0\rangle$ (middle column). Right column shows the total number of vibrations \hat{N}_{vib} created in the system during the evolution (thick blue and thin red line for left and middle column, respectively). Consecutive rows corresponds to different local couplings $g_W = \{0.1, 0.75, 1.5\}$. All calculations performed for $g_J = 0$ and $\omega_0 = 3$. Note that for stronger interactions evident stabilization of the excitation density profile, along with increasing number of created vibrations, is observed.

DRESSED RYDBERG ATOMS IN OPTICAL LATTICE



We consider off-resonant coupling of two different but degenerated internal Zeeman ground states $|g\rangle$ and $|g'\rangle$ to two precisely selected, highly excited Rydberg states $|nS\rangle$ or $|nP\rangle$ with principal quantum number equal n and angular momentum equal 0 or \hbar . In consequence an atom can be found in one of the two dressed states:

$$|0\rangle \approx |g\rangle + \alpha_s |nS\rangle, \quad |1\rangle \approx |g'\rangle + \alpha_p |nP\rangle, \quad (8)$$

where amplitudes $\alpha_l = \Theta_l / 2\Delta_l$ ($l \in \{s, p\}$) are determined by a total Rabi frequency of a driving field Θ_l and a total laser detuning Δ_l . In this basis of dressed states the dipole-dipole interaction between neighboring atoms C_3^{sp}/R^3 may induce transitions between internal states of neighboring atoms $|0_i\rangle |1_{i+1}\rangle \leftrightarrow |1_i\rangle |0_{i+1}\rangle$.

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