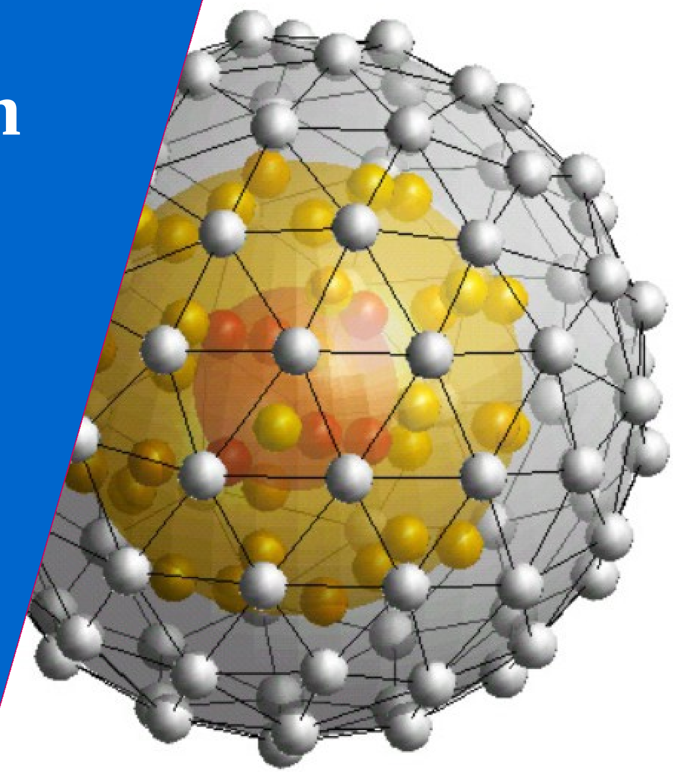
Simulating polaron biophysics with Rydberg atoms

ICQSIM2017, Paris, 15-11-2017

Servaas Kokkelmans



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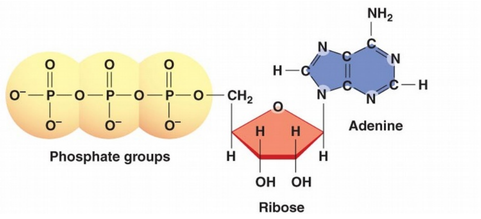
Where innovation starts

Outline

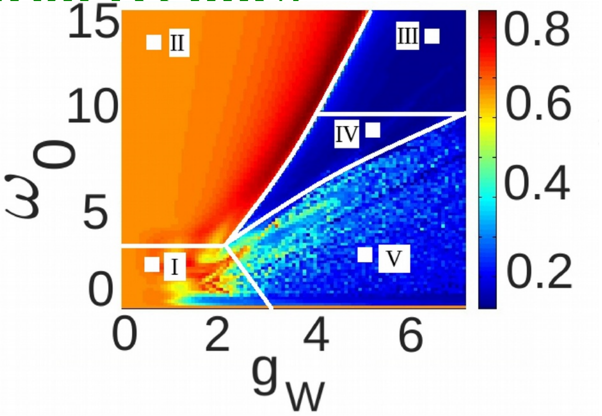


- **Transport problem in proteins**
- **Davydov solitons – semi-classical model**

- **Implement this model in a 1D optical lattice**
- **Obtain coupling parameters using Rydberg dressing**

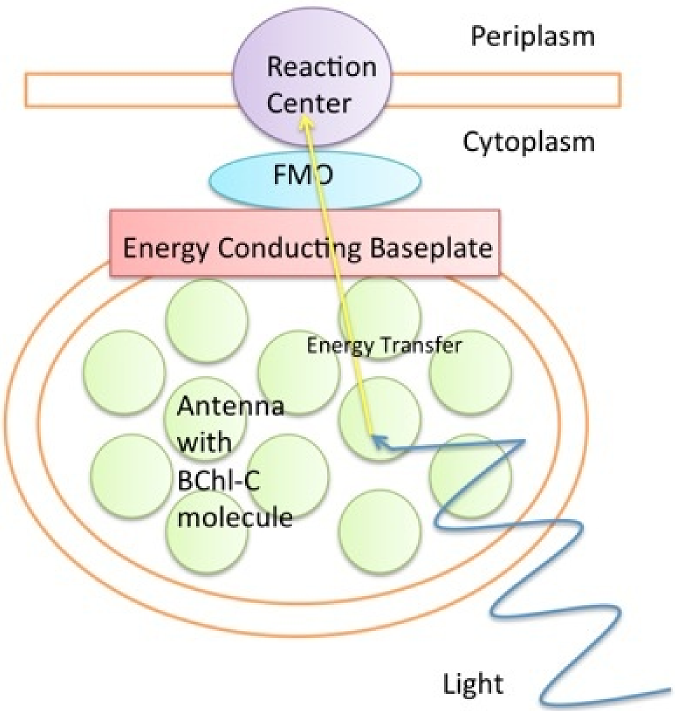
- **Phase diagram**
- **Spreading excitation, small and large polaron regimes**

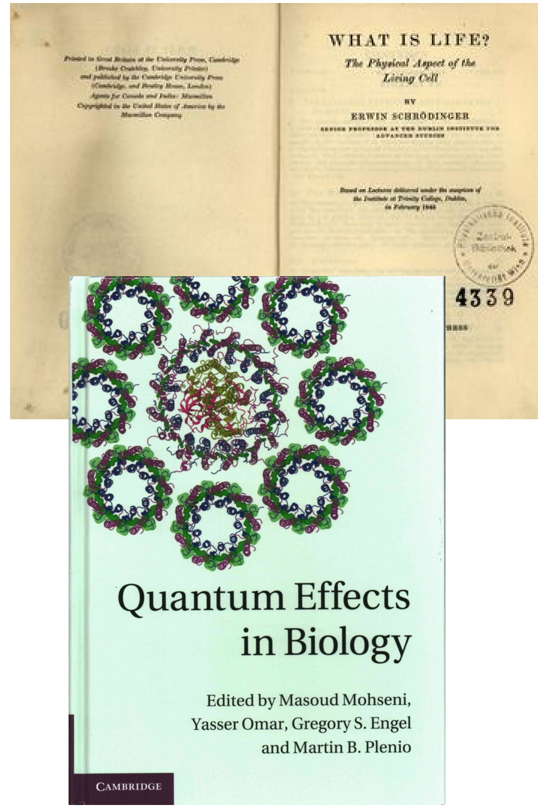
- **Possibilities for study with cold atoms**
- **Access the non-classical regime**



Quantum biology

- **Several applications**
- **Photosynthesis**





- **Efficiency of above 99% between the absorption of electrons and transfer to the reaction site**
- **Attributed to quantum coherence and entanglement**

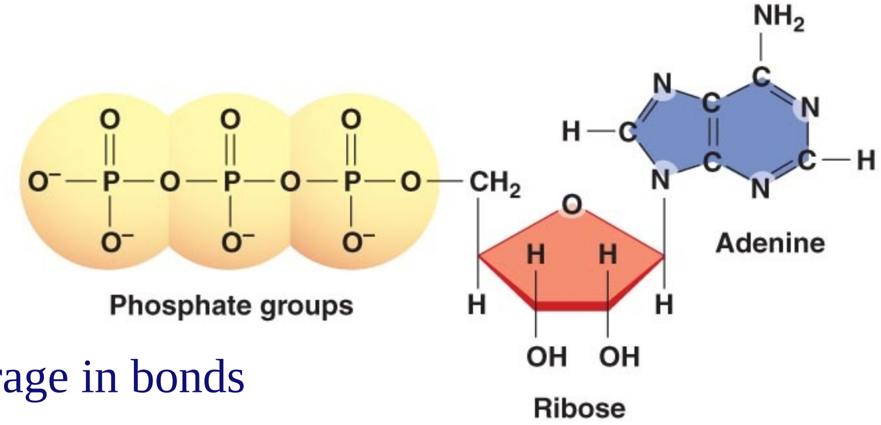
Proteins

Proteins are complex molecules of carbon, hydrogen, nitrogen, oxygen

Proteins perform key functions of cells:

- grab molecules and assemble them into cellular structures
- tear molecules apart for energy
- transport oxygen and other necessary items from one cell to another

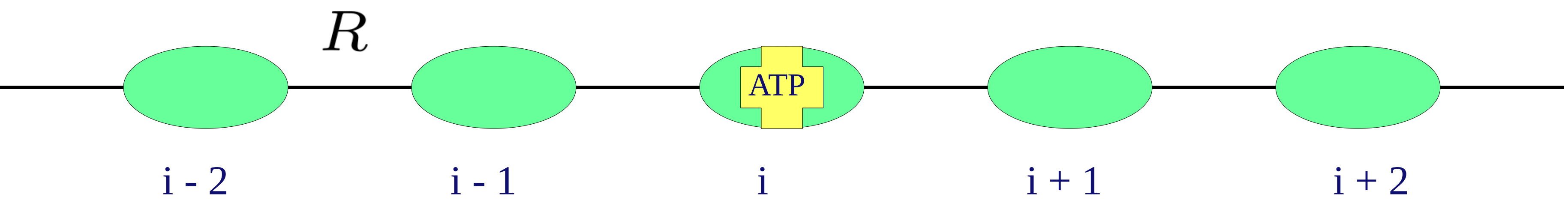
Proteins gain energy for activities by ATP hydrolisis.
ATP (adenosine triphosphate) is "molecular unit of currency" of intracellular energy transfer.



Energy storage in bonds

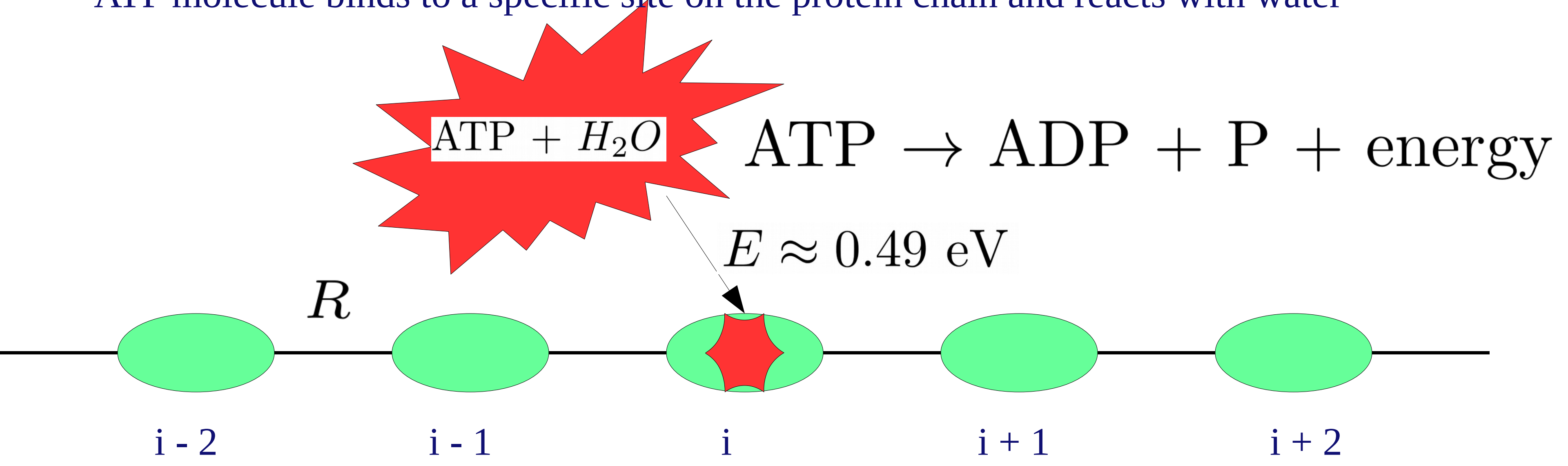
Energy transport in proteins

ATP molecule binds to a specific site on the protein chain



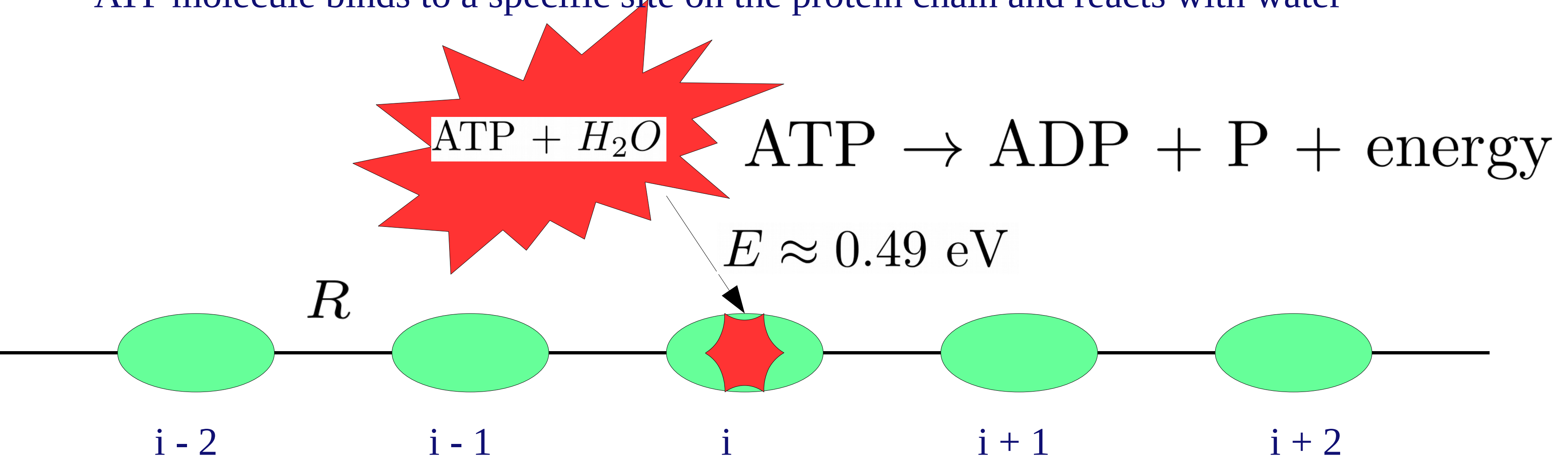
Energy transport in proteins

ATP molecule binds to a specific site on the protein chain and reacts with water



Energy transport in proteins

ATP molecule binds to a specific site on the protein chain and reacts with water



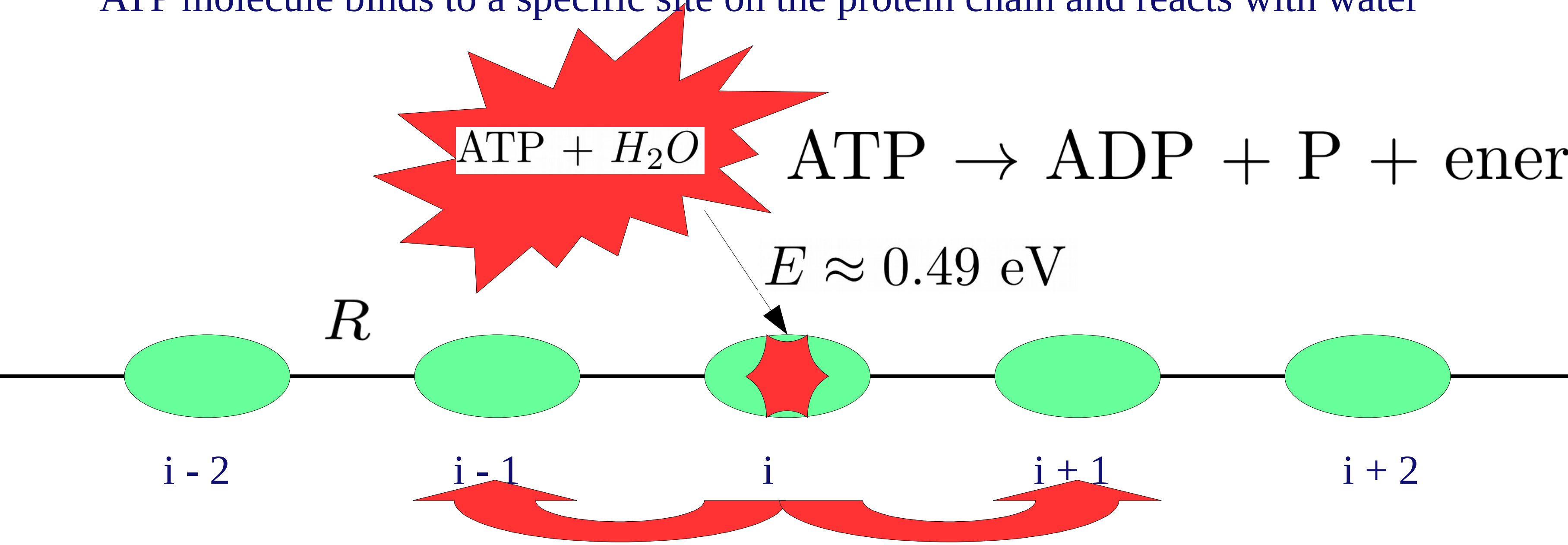
What happens to this Excitation ?

Energy transport in proteins (naive approach)

ATP molecule binds to a specific site on the protein chain and reacts with water

$$\mathrm{ATP} \rightarrow \mathrm{ADP} + \mathrm{P} + \mathrm{energy}$$

$$E \approx 0.49 \text{ eV}$$

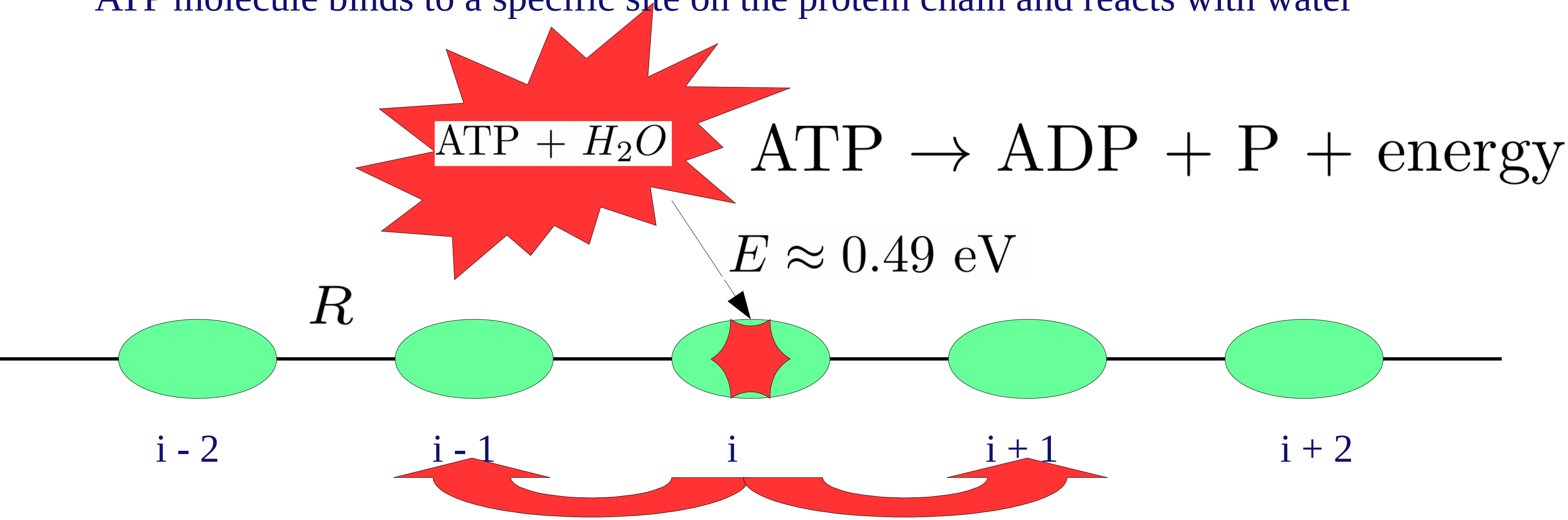


Excitation hopping

$$H = \sum_{<i,j>} J_{ij} \left(|i\rangle\langle j| + |j\rangle\langle i| \right)$$

Energy transport in proteins (naive approach)

ATP molecule binds to a specific site on the protein chain and reacts with water



Excitation hopping

$$H = \sum_{<i,j>} J_{ij} \left(|i\rangle\langle j| + |j\rangle\langle i| \right)$$

Excitation is smeared out through the chain: no directional transport

Energy transport in proteins

Davydov (70'): **coupling between excitation and proteins vibration**

Proteins building blocks have
permanent dipole moment ~ 4 Debye

$$J_{ij} = \frac{J}{|R_i - R_j|^3}$$

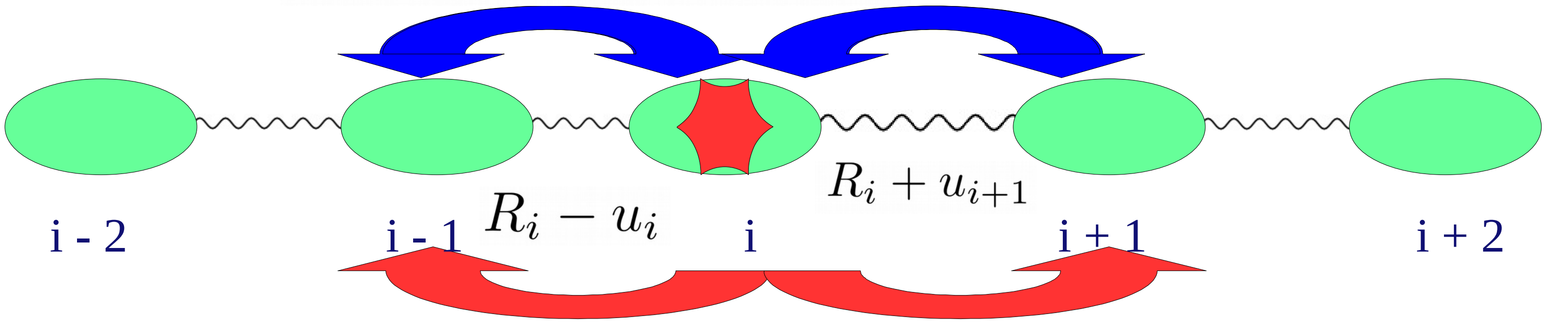
Energy transport in proteins

Davydov (70’): **coupling between excitation and proteins vibration**

Proteins building blocks have permanent dipole moment ~ 4 Debye

$$J_{ij} = \frac{J}{|R_i - R_j|^3}$$

$$U = \frac{K}{2}(R + u_{i+1} - u_i)^2$$



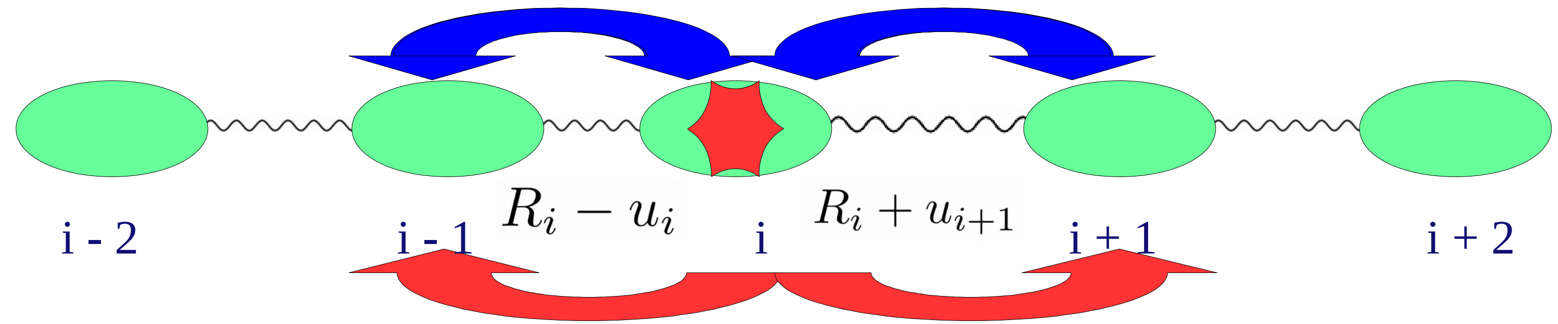
Excitation hopping (dipole-dipole)

Davydov, ***"The theory of contraction of proteins under their excitation"***. Journal of Theoretical Biology. 38 (3): 559–56, (1973).Davydov, ***"Quantum theory of muscular contraction"***. Biophysics. 19: 684–691, (1974).Davydov, ***"Solitons and energy transfer along protein molecules"***. Journal of Theoretical Biology. 66 (2): 379–387, (1977)Brizhik L, Eremko A, Piette B, Zakrzewski W ***"Solitons in α-helical proteins"***. Physical Review E.70: 031914, 1–16, (2004)Scott, ***"Davydov's soliton"***. Physics Reports. 217: 1–67, (1992). Cruzeiro-Hansson, Takeno, ***"Davydov model: the quantum, mixed quantum-classical, and full classical systems"***. Physical Review E. 56 (1): 894–906, (1997). Cruzeiro-Hansson L, ***"Influence of the nonlinearity and dipole strength on the amide I band of protein α-helices"***. The Journal of Chemical Physics. 123 (23): 234909, 1–7, (2005).

Energy transport in proteins: Hamiltonian

$$H = \sum_i H_i^{\mathrm{ex}} + H_i^{\mathrm{ph}} + H_i^{\mathrm{int}}$$

$$H_i^{\mathrm{ph}} = \frac{K}{2}(u_{i+1} - u_i)^2$$

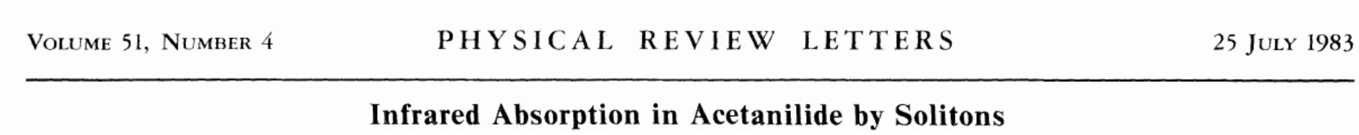


$$H_i^{\mathrm{ex}} = W a_i^\dagger a_i - J_0(a_{i+1}^\dagger a_i + h.c.) \qquad J_0 = \frac{J}{R^3}$$

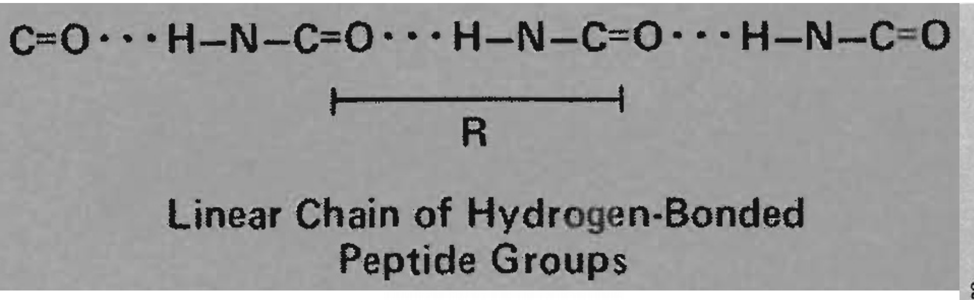
$$H_i^{\mathrm{int}} = \chi(u_{i+1} - u_i) a_i^\dagger a_i \qquad \chi = \frac{dW}{dR}$$

Davydov model!

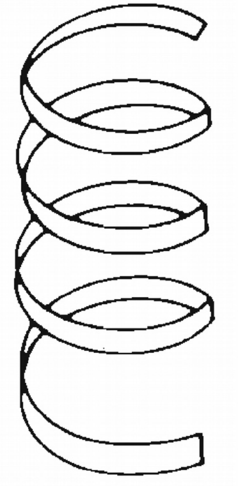
Experimental evidence: alpha-helix protein

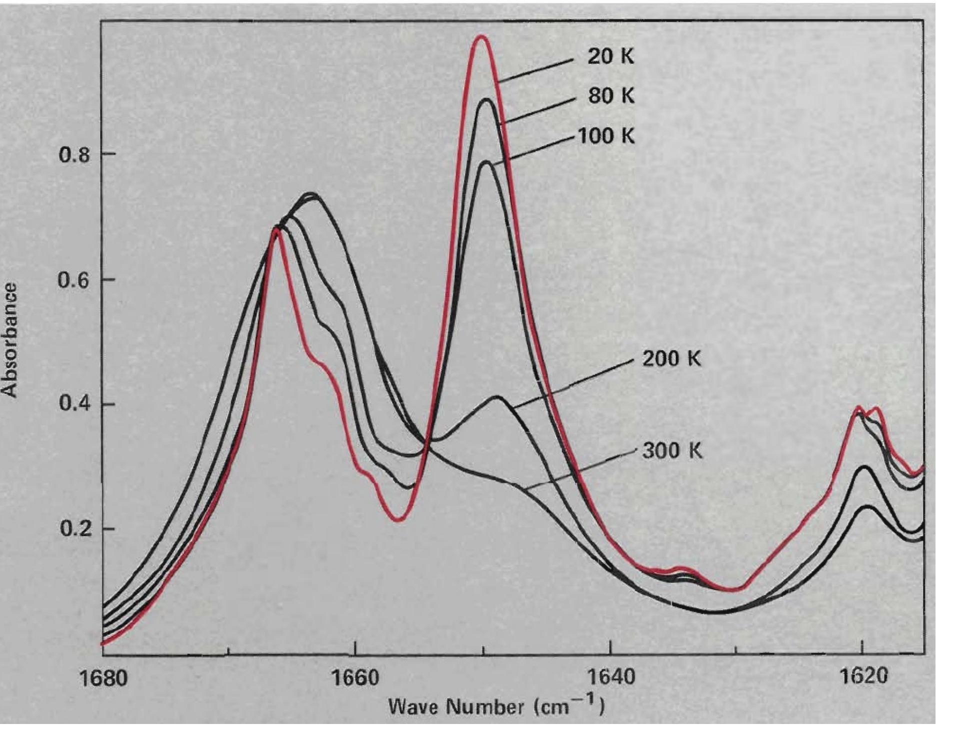

VOLUME 51, NUMBER 4 PHYSICAL REVIEW LETTERS 25 JULY 1983

Infrared Absorption in Acetanilide by Solitons



α-helix





Emerging absorption peak corresponds to exciton-phonon soliton energy

Indirect evidence of soliton mechanism

Solitons in the alpha-helix protein

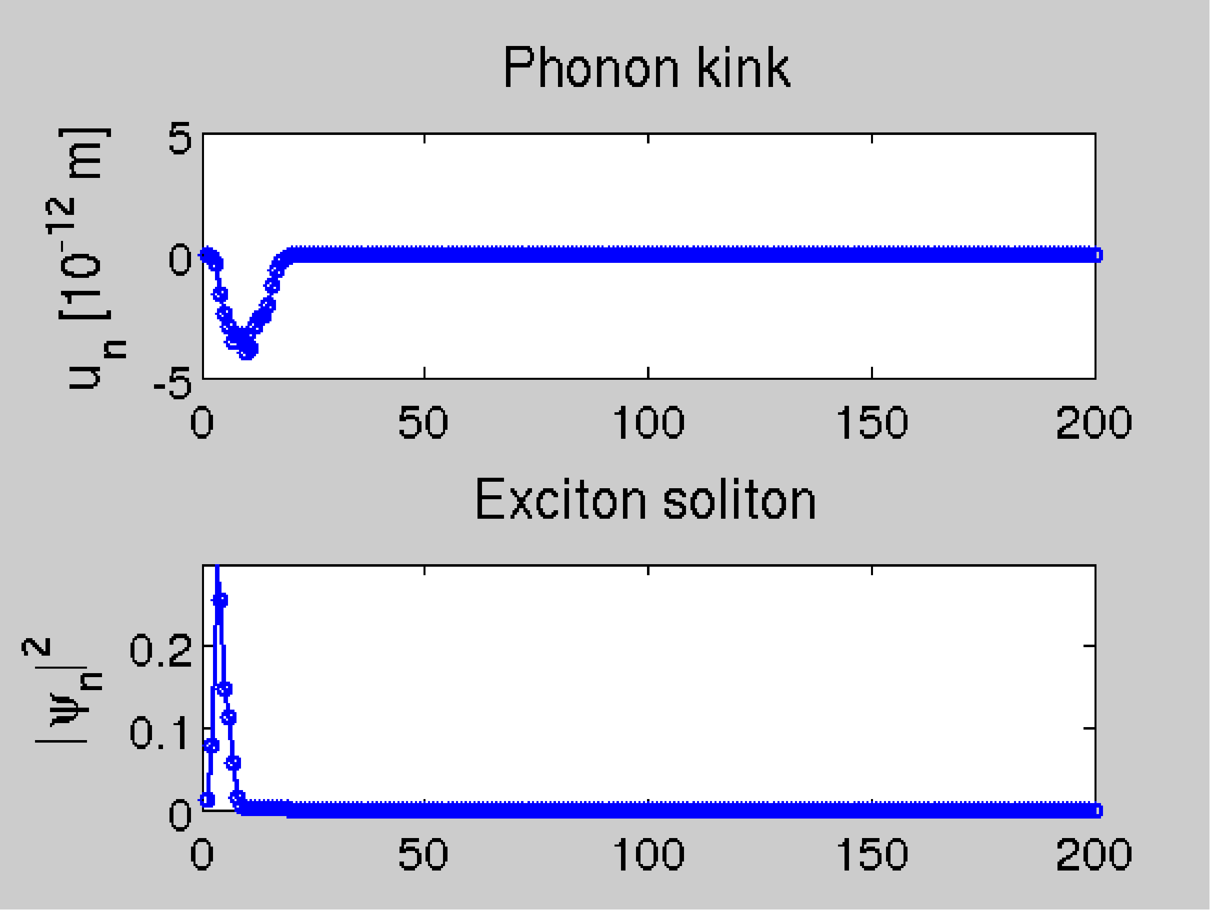
$$m = 114 \ \mathrm{m_p}$$

$$J_0 = 0.967 \ \mathrm{meV}$$

$$K = 13 \ \frac{\mathrm{N}}{\mathrm{m}}$$

$$\chi = 3 \times 10^{-11} \ \mathrm{N}$$

$$\tau = \frac{\hbar}{J_0} = 0.7 \times 10^{-12} \mathrm{s}$$



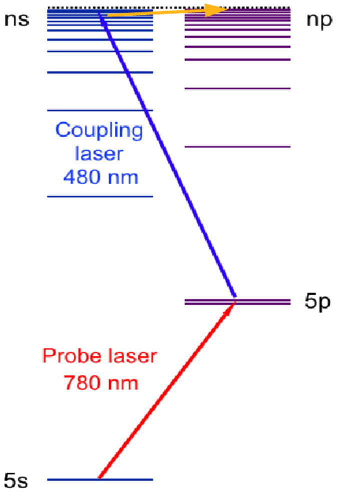
Can we be of help to bio-physics?

"[…] understanding of how proteins function is a lot like [...] understanding of how a car works. We know you put in gas and the gas is burned to make things turn but the details are all pretty vague."

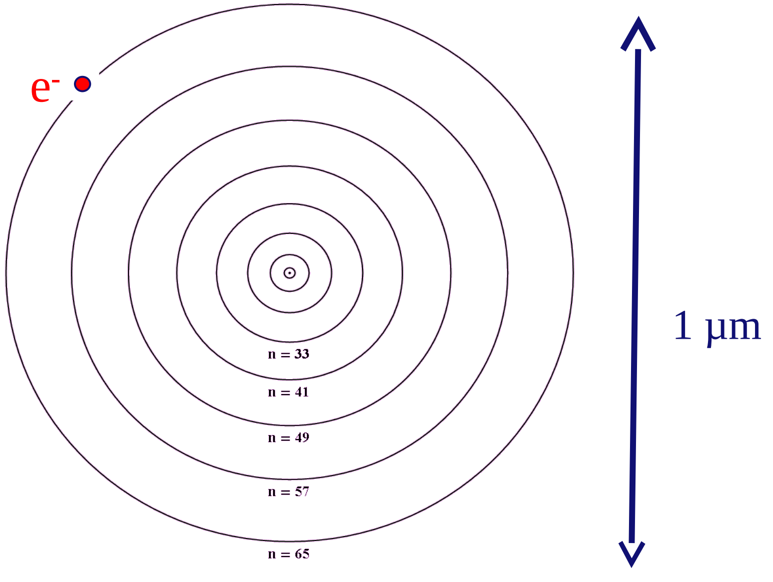
(Alwyn C. Scott in Discover Magazine, Vol. 15 No. 12, Dec. 1994)

Rydberg atoms

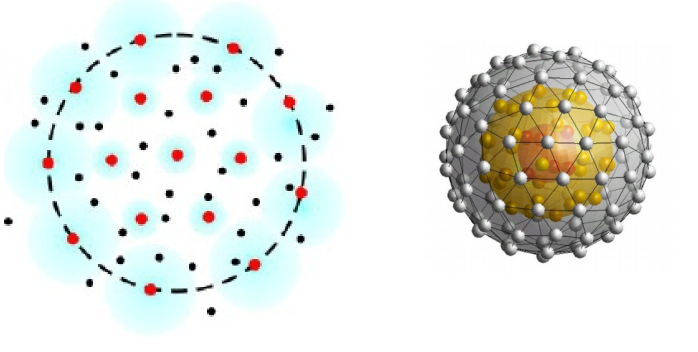
- **High principal quantum number**
- **Extreme properties**
- **long lifetime** n^3
- **Size: order of micrometer**
- **Very strong van der Waals interaction**



$C_6 \sim n^{11}$

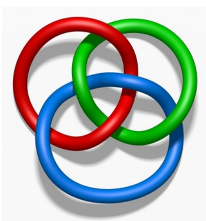


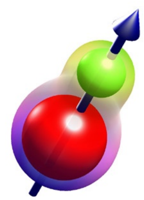
Use interaction to make crystals

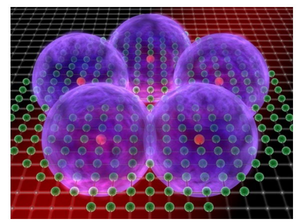


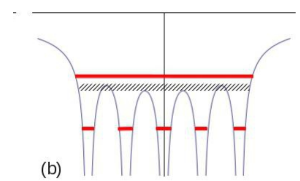
Strong interactions at different ranges

Particles with different ranges of interaction









short range → **long range**

quantum gases

dipolar molecules

Rydberg atoms

quantum plasmas

quarks

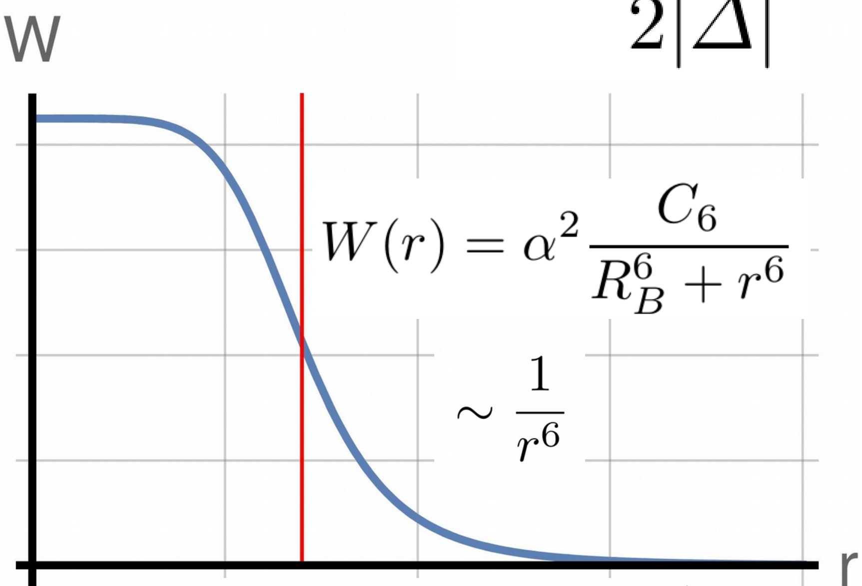
electrons and ions

Rydberg Dressing

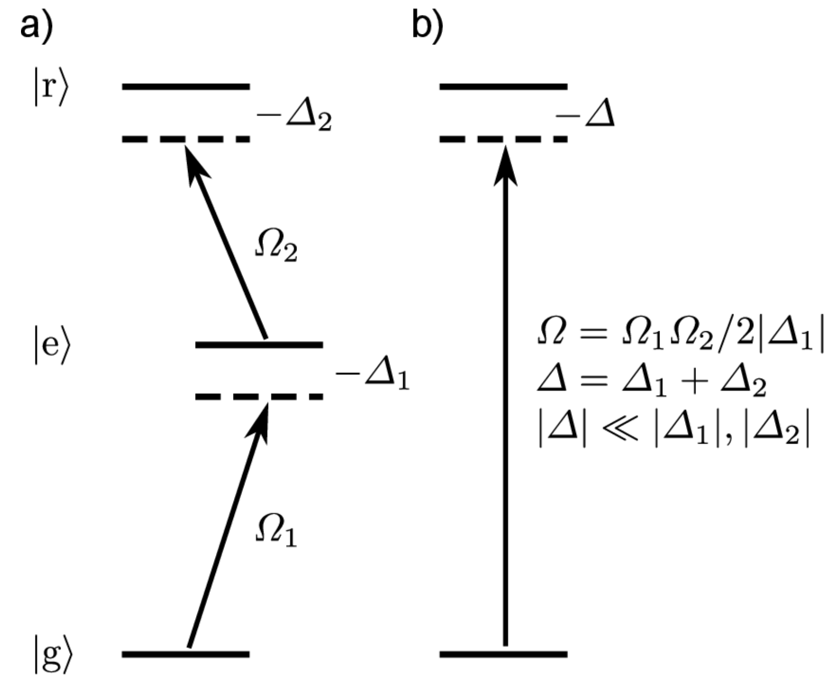
Admixture properties of Rydberg state to atom ground state

$$|\psi\rangle \approx |g\rangle + \alpha |nS\rangle$$

$$\alpha = \frac{\Omega}{2|\Delta|}$$



$$R_B \approx (C_6/2\hbar|\Delta|)^{1/6}$$

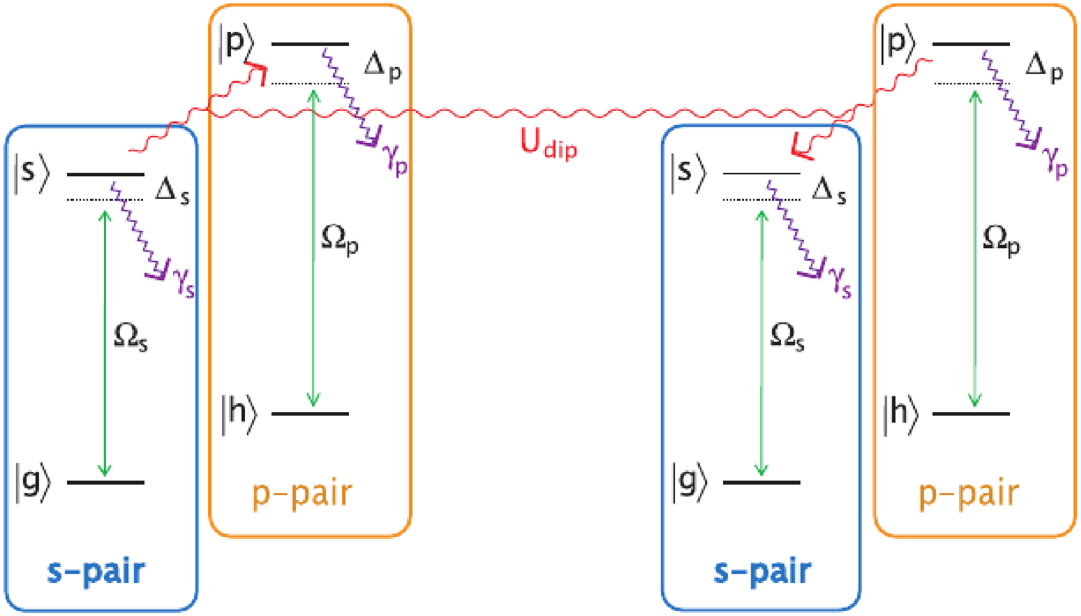


Dressed state acquires life-time:

$$\tau_{eff}^{-1} = \left(\frac{\Omega}{2\Delta}\right)^2 \tau_{|nS\rangle}^{-1} + \left(\frac{\Omega_1}{2\Delta_1}\right)^2 \Gamma_{5P_{3/2}}$$

Henkel, et. al PRL **104,** 195302 (2010)

Realization scheme : Hopping process



$$\alpha_{s,p} = \frac{\Omega_{s,p}}{2\Delta_{s,p}}$$

$$|\mathbf{k}\rangle \equiv |k_1 \ldots k_N\rangle \equiv |k_1\rangle \otimes \ldots \otimes |k_N\rangle$$

$$k_j \in \{g, h, s, p\}$$

$$\hat{\sigma}^{(n)}_{kk'} = |k_n\rangle\langle k'_n|$$

$$|gh\rangle \rightarrow |sp\rangle \rightsquigarrow |ps\rangle \rightarrow |hg\rangle$$

$$\hat{H} = \hat{H}_0 + \hat{V}$$

$$\hat{H}_0 = -\Delta_s \sum \hat{\sigma}^{(n)}_{ss} - \Delta_p \sum \hat{\sigma}^{(n)}_{pp} + \sum U_{nl} \hat{\sigma}^{(n)}_{sp} \hat{\sigma}^{(l)}_{ps}$$

$$\hat{V} = \sum_n \left(\frac{\Omega_s}{2} \hat{\sigma}^{(n)}_{gs} + \frac{\Omega^*_s}{2} \hat{\sigma}^{(n)}_{sg} \right) + \sum_n \left(\frac{\Omega_p}{2} \hat{\sigma}^{(n)}_{hp} + \frac{\Omega^*_p}{2} \hat{\sigma}^{(n)}_{ph} \right)$$

Wüster, et. al NJP **13,** 073044 **(2011)**

Realization scheme : Hopping process

Initial state

$$|\pi_i\rangle = |\cdots ggghggg\ldots\rangle$$

Dressing lasers

$$|0\rangle = c_S|nS\rangle + c_g|g\rangle$$

$$|1\rangle = c_P|nP\rangle + c_h|h\rangle$$

$$\hat{H} = \hat{H}_0 + \hat{V}$$

Van Vleck perturbation theory

$$H_{eff} = \sum_i W(R)\hat{a}_i^\dagger \hat{a}_i + J(R)(\hat{a}_{i+1}^\dagger \hat{a}_i + h.c.)$$

$$W(R) = \alpha_s^2\alpha_p^2 \frac{\Delta_S + \Delta_P}{1 - \bar{U}_{12}^2(R)}$$

$$J(R) = \alpha_s^2\alpha_p^2 \frac{U_{12}(R)}{1 - \bar{U}_{12}^2(R)}$$

$$\bar{U}_{\text{ij}} = U_{\text{ij}}/(\Delta_s + \Delta_p)$$

$$U_{kl} = U_{\text{dip}}(R_{kl}) = -\frac{\mu^2}{|\mathbf{R}_k - \mathbf{R}_l|^3}$$

Wüster, et. al NJP **13,** 073044 **(2011)**

Su-Schrieffer-Heeger (SSH) Hamiltonian

- **Sum of excitation and vibration energy**

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{exc}} + \hat{\mathcal{H}}_{\text{vib}}$$

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

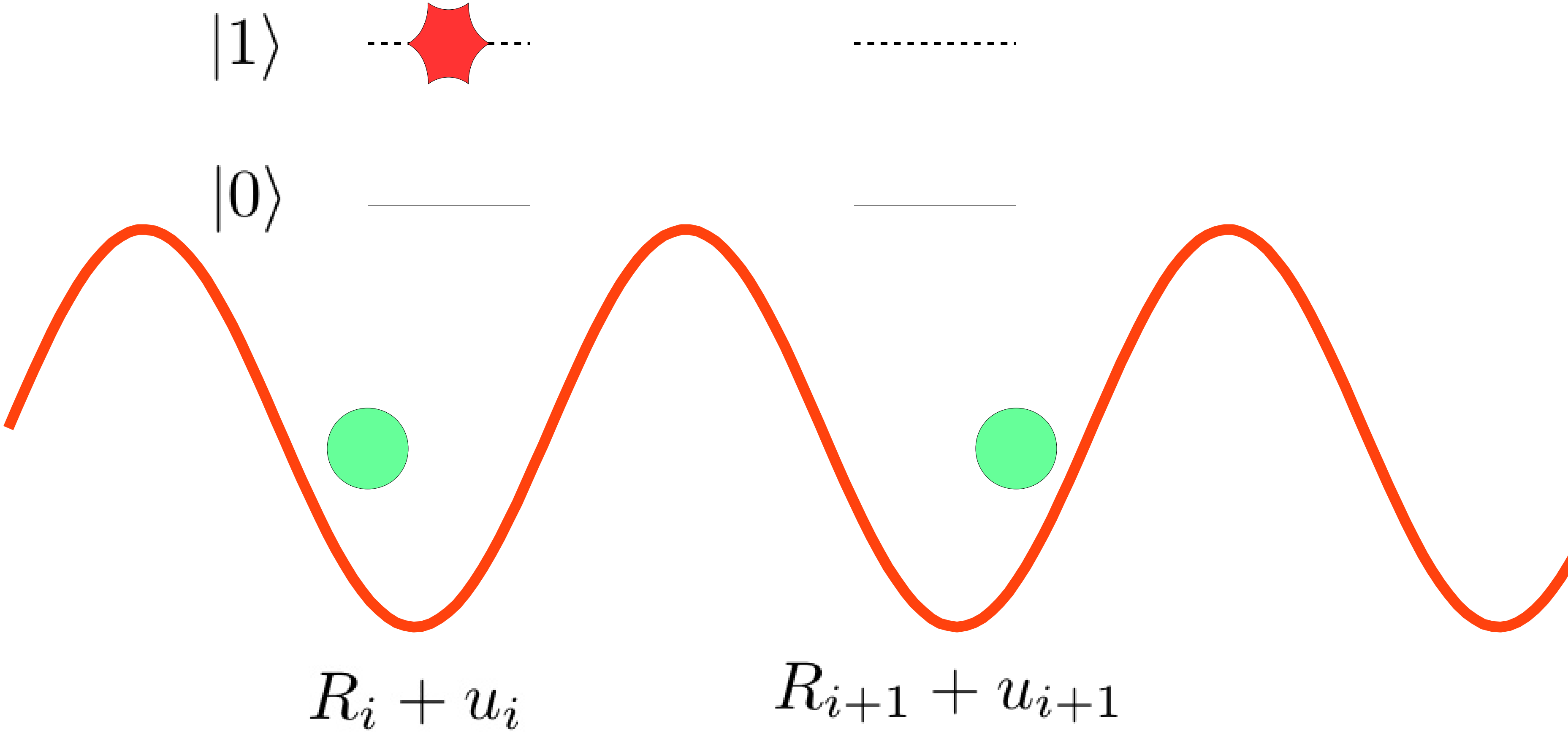
$$\hat{\mathcal{H}}_{\text{exc}} = \sum_i W_i \hat{a}_i^\dagger \hat{a}_i + \sum_i J_{i+1,i}(\hat{a}_{i+1}^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{a}_{i+1})$$

- **Interactions will be spatially dependent**

$$\hat{u}_i = l_0(\hat{b}_i^\dagger + \hat{b}_i)/\sqrt{2}$$

- **Davydov: classical motion atoms**

Realization scheme : Ry dressing +Optical Lattice



$$H_{ph} = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} K (u_{i+1} - u_i)^2$$

Position-dependent interactions

- **Spatial-dependent Rydberg dressing couplings**

$$W_i = \frac{\alpha^4 \hbar \Delta}{2} \left(\frac{1}{1-\kappa(R_0+u_{i+1}-u_i)^2} + \frac{1}{1-\kappa(R_0+u_i-u_{i-1})^2} \right),$$

$$J_{i+1,i} = \frac{\alpha^4 C_3^{sp}}{|R_0+u_{i+1}-u_i|^3} \frac{1}{1-\kappa(R_0+u_{i+1}-u_i)^2}$$

- **Lowest order expansion in position**

$$W_i = W_0 + \boxed{g_W}(u_{i+1}+u_{i-1}) \qquad J_{i+1,i} = -J_0 + \boxed{g_J}(u_{i+1}-u_i)$$

- **Control parameters**
- **On-site exciton-phonon coupling g_W (Holstein model)**
- **Exciton-phonon coupling via hopping g_J (SSH model)**

HSSH model!

Davydov equations

- **Davydov ansatz**

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

- **Semiclassical approach**

$$i\frac{\mathrm{d}\psi_i(t)}{\mathrm{d}t} = -(\psi_{i+1} + \psi_{i-1}) + g_W(u_{i+1} - u_{i-1})\psi_i$$
$$+ g_J[\psi_{i+1}(u_{i+1} - u_i) + \psi_{i-1}(u_i - u_{i-1})],$$

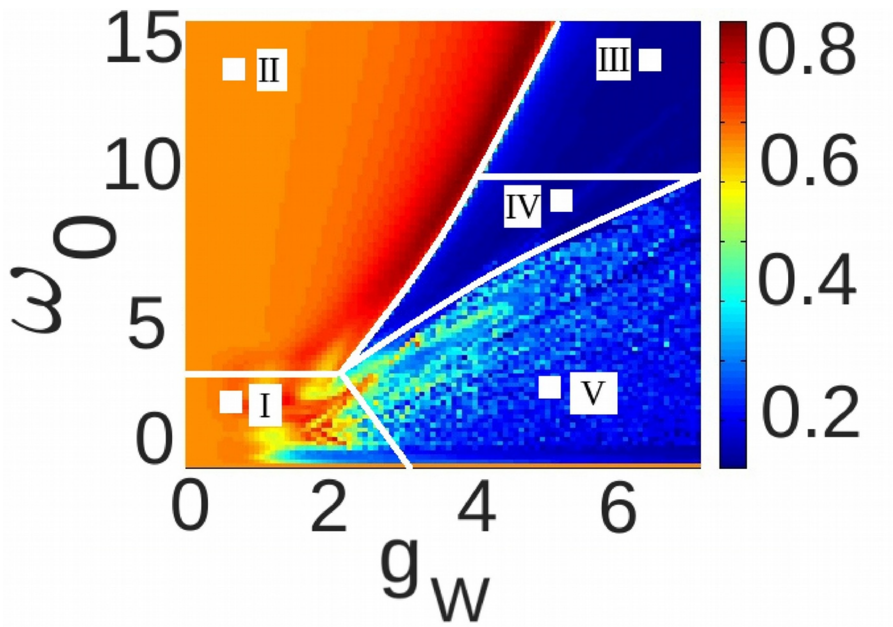
Schrodinger Equation For excitation

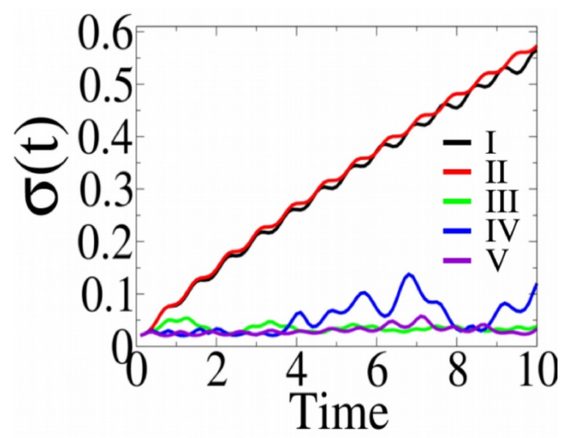
$$\frac{\mathrm{d}u_i(t)}{\mathrm{d}t} = p_i(t),$$
$$\frac{\mathrm{d}p_i(t)}{\mathrm{d}t} = -\omega_0^2 u_i(t) + g_W\omega_0(|\psi_{i+1}|^2 - |\psi_{i-1}|^2)$$
$$+ g_J\omega_0[\psi_i^*(\psi_{i+1} - \psi_{i-1}) + \psi_i(\psi_{i+1}^* - \psi_{i-1}^*)]$$

Wave equation for lattice displacement

Phase diagram

- **Investigate spreading excitation**
- **Define width excitation** $\sigma(t) = N / \sum_i \rho_i^2(t)$ $\rho_i(t) = \langle \Psi(t) | \hat{a}_i^\dagger \hat{a}_i | \Psi(t) \rangle$



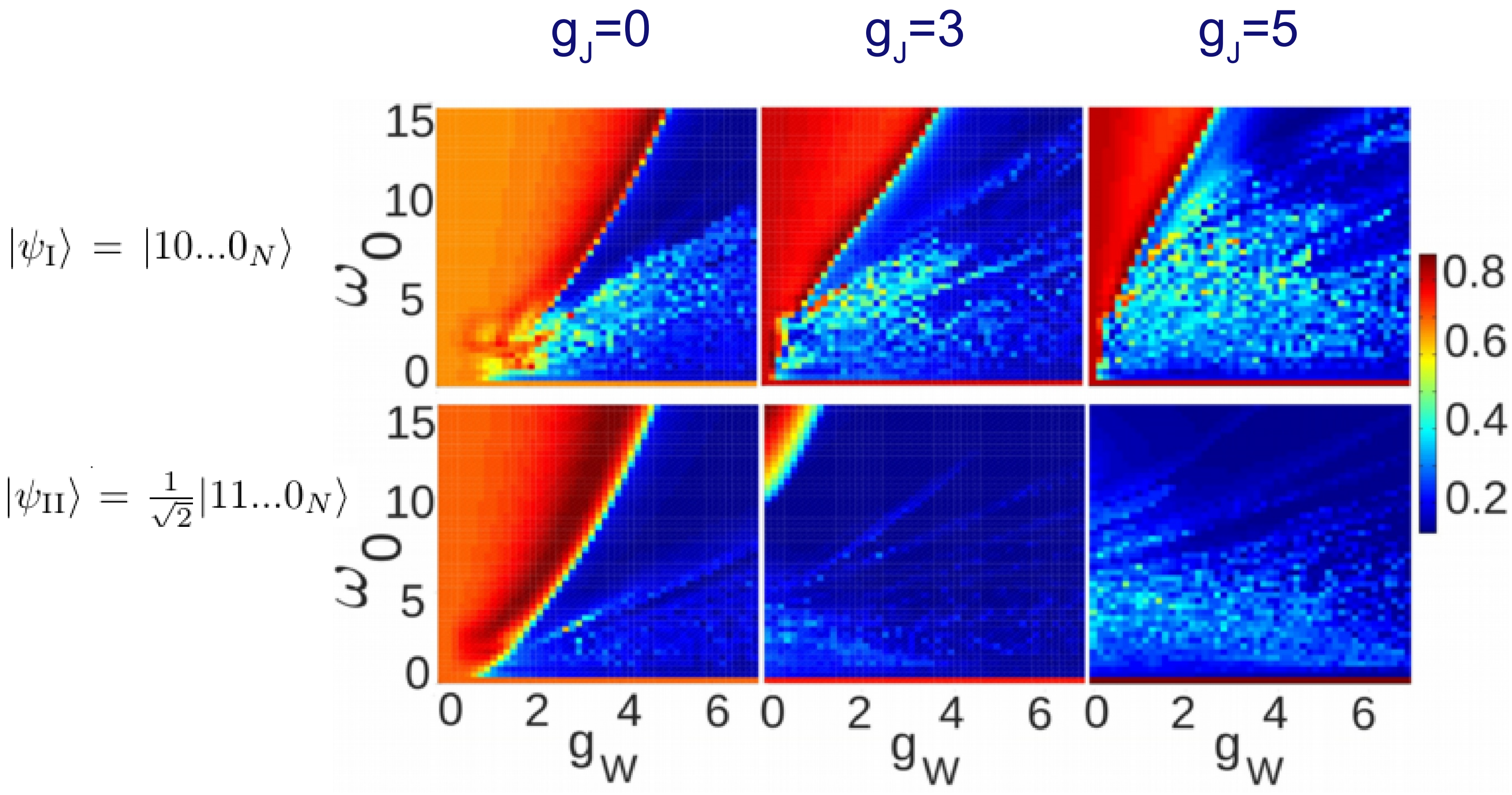


- **Energy units of J_0 (i.e. $J_0 = 1$)**

[M. Płodzień, T. Sowiński, S. Kokkelmans, arXiv:1707.04120]

Different parameters

- **Two different initial conditions**
- **Different coupling strengths**



Exact diagonalization method

$|\psi_{\mathrm{I}}\rangle = |10...0_N\rangle \quad |\psi_{\mathrm{II}}\rangle = \frac{1}{\sqrt{2}}|11...0_N\rangle$

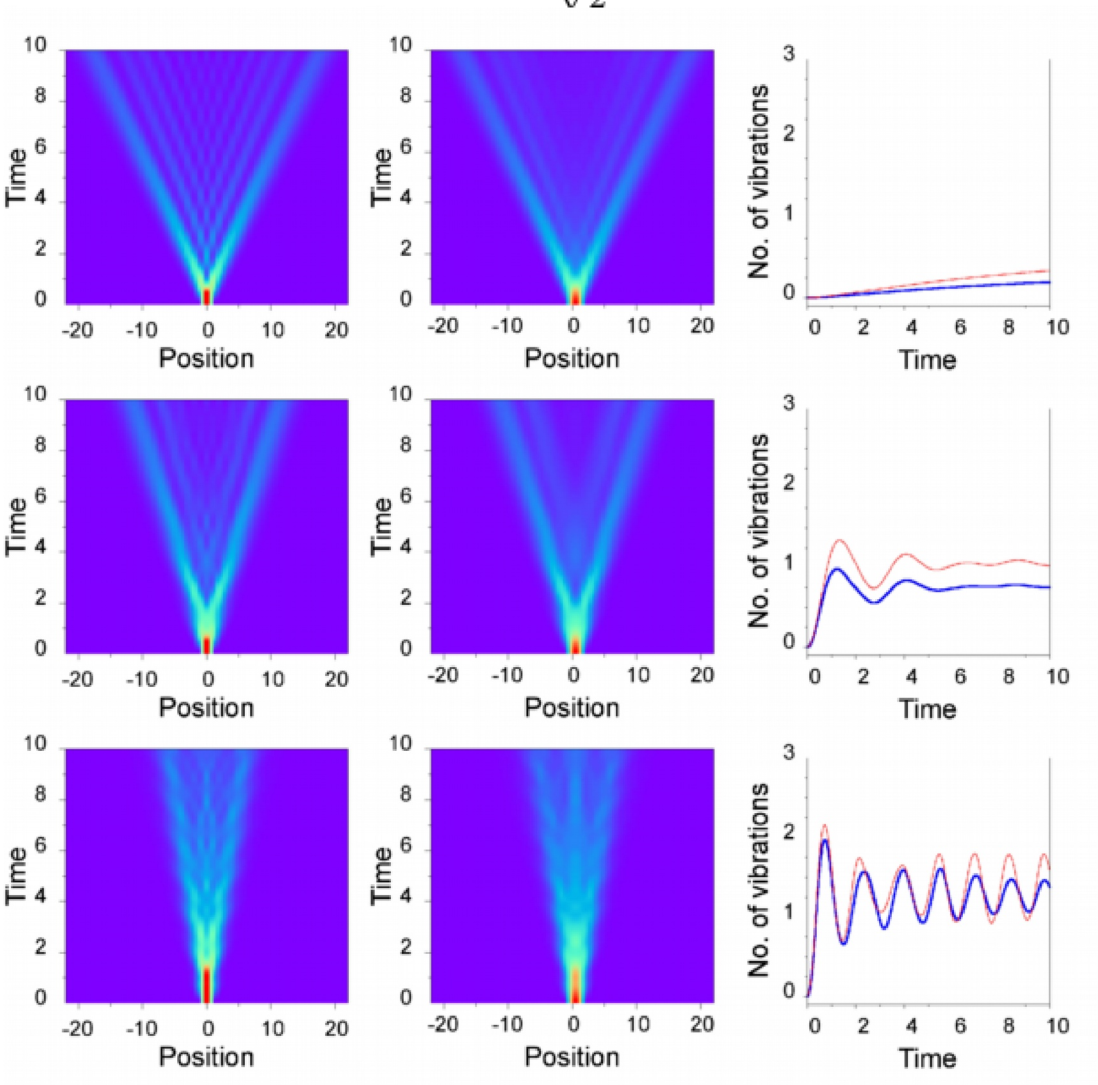
- **Basis states**

  $|i\rangle|m_1, \ldots, m_N\rangle$

$g_W = 0.1$

$g_W = 0.75$

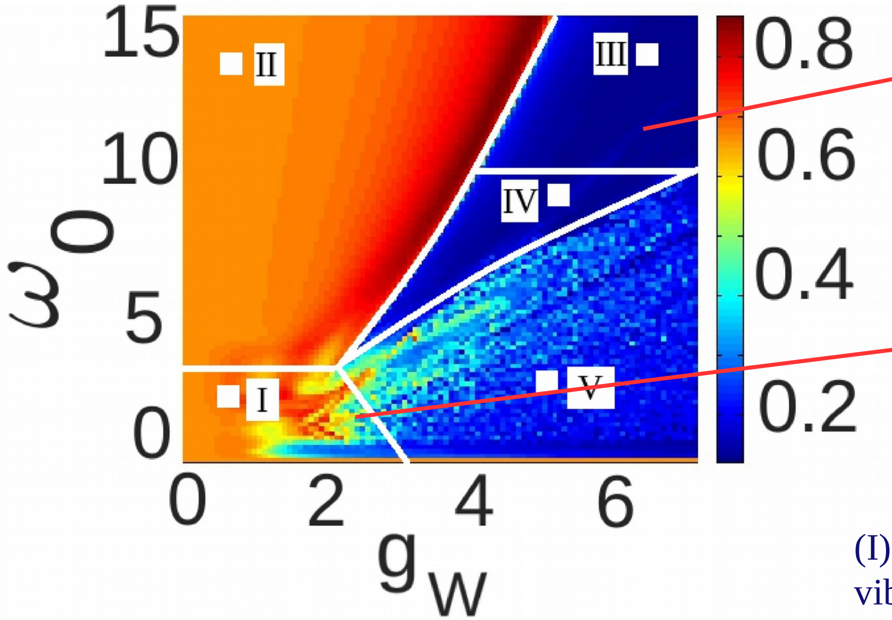
$g_W = 1.5$



[M. Płodzień, T. Sowiński, S. Kokkelmans, arXiv:1707.04120]

Phase diagram

- **Explore from quantum to semi-classical regime**



Large polaron

Small polaron

(I) and (II) excitation dressed by cloud of vibrations and spreads

(III) Excitation is localized

(IV) Davydov-like soliton behavior;

(V) $g_W \gtrsim \omega_0$ corresponding to Discrete Breathers behavior

[M. Płodzień, T. Sowiński, S. Kokkelmans, arXiv:1707.04120]

Experimental parameters

- **Rb-87 in optical lattice**

Excitation

n=50

$$C_3^{sp} = 3.224\,\mathrm{GHz}\,\mu\mathrm{m}^3$$

$$\Delta/2 = \Delta_s = \Delta_p = 2.5\,\mathrm{GHz}$$

$$\alpha = 0.015$$

Life-time@ $T = 300\ \mathrm{K}$

$\tau_S = 65\mu\mathrm{s}$ $\tau_P = 86\mu\mathrm{s}$

Optical lattice/phonons

$$R_0 = 1\,\mu\mathrm{m}$$

$$V_0 = 100 E_R$$

$$\omega_0 = \sqrt{2V_0/M}\pi/R$$

N=50

- **Good enough for ex** $\omega_0 = 4.7$ **e diagram**

$$g_W = 5.6$$

$$g_J = 5.6$$

Conclusions / outlook

- **Rydberg implementation of bio-physics transport problem**
- **Semiclassical Davydov regime (large polaron)**
- **Small # phonons: small polaron possible**
- **Non-perturbative regime in between small/large polaron**

- **Interesting phase diagram to explore experimentally**
- **Transport of Polarons**
- **Platform for study bi-polaron system**
- **Tune interactions from attractive to repulsive by tuning** g_W **&** g_J
- **Disorder effects in HSSH Hamiltonian with incommensurate optical lattices**

- **Possibility in other systems – ion crystals?**

[Simulating polaron biophysics with Rydberg atoms,
M. Płodzień, T. Sowiński, S. Kokkelmans, arXiv:1707.04120]

Thanks!

Rydberg physics
Edgar Vredenbregt
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Bart Hoekstra
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Yuri v/d Werf

Few-body physics
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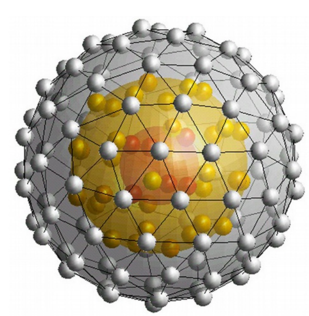


Holstein – Su – Schrieffer - Heeger Hamiltonian

$$H = H_{\mathrm{ex}} + H_{\mathrm{ph}} + H_{\mathrm{W}} + H_{\mathrm{J}}$$

$$H_{\mathrm{ex}} = J_0 \sum_j (\hat{a}_{i+1}^\dagger \hat{a}_i + h.c.)$$

$$H_{\mathrm{ph}} = \sum_k \epsilon_k \hat{b}_k^\dagger \hat{b}_k$$

$$H_{\mathrm{W}} = g_W \sum_{k,j} \hat{a}_j^\dagger \hat{a}_j (\kappa_{k,j}^* \hat{b}_k^\dagger + \kappa_{k,j} \hat{b}_k)$$

$$H_{\mathrm{J}} = g_J \sum_{k,j} (\hat{a}_{j+1}^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_j)(\kappa_{k,j}^* \hat{b}_k^\dagger + \kappa_{k,j} \hat{b}_k)$$

$$\epsilon_k = 2\sin\frac{kR}{2}$$

$$\kappa_{k,j} = \frac{2i\sin kR}{\sqrt{N\epsilon_k}} e^{ikjR}$$

$$J(R+u) = J_0 + \tfrac{dJ}{dR}u \equiv J_0 + \chi_J u$$

$$W(R+u) = W_0 + \tfrac{dW}{dR}u \equiv W_0 + \chi_W u$$

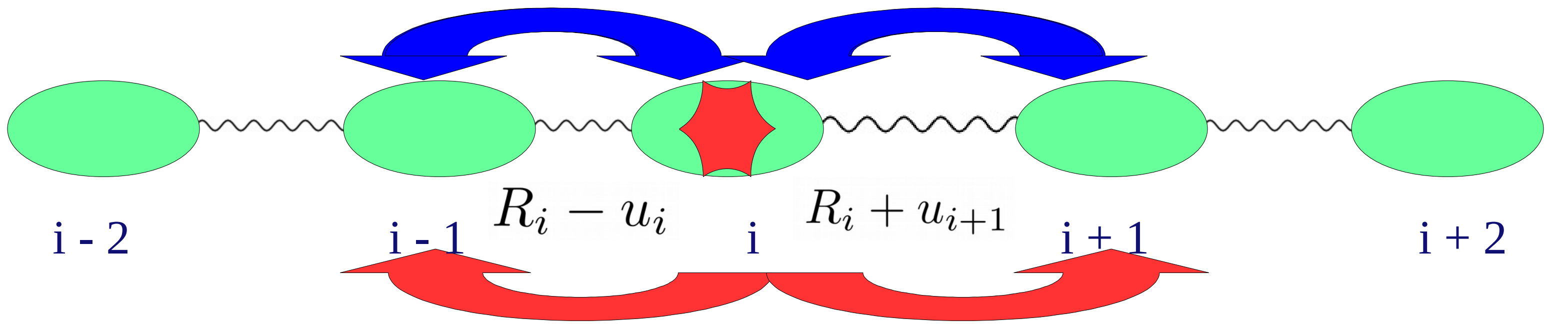
$$g_W = \chi_{\mathrm{W}} l_0, \; g_J = \chi_{\mathrm{J}} l_0$$

$$l_0 = \sqrt{\hbar/M\omega}$$

$$\omega = 2\sqrt{K/M}$$

Energy transport in proteins: Hamiltonian

$$H = \sum_i H_i^{\mathrm{ex}} + H_i^{\mathrm{ph}} + H_i^{\mathrm{int}} \qquad |\Psi\rangle = \sum_i \psi_i a_i^\dagger |0\rangle$$



$$i\hbar|\dot{\Psi}\rangle = H|\Psi\rangle$$
$$m\ddot{u} = -\partial_u\langle\Psi|H|\Psi\rangle$$
$$\Longrightarrow \quad i\hbar\partial_t\psi = -J_0\partial_x^2\psi - 4\frac{\chi^2}{K}|\psi|^2\psi$$

$$\psi = \frac{\chi}{\sqrt{2KJ_0}}\frac{1}{\mathrm{Cosh}\left(\frac{\chi^2}{KJ_0}x\right)}$$

Exciton-phonon soliton