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Photoassociation in trapped ultracold samples with realistic molecular potentials

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Introduction

We investigate the influence of a trap on the photoassociation process of two atoms. As an example the formation of $^6Li_2$ molecules is investigated. More specifically, photoassociation of spin-polarized ^{6}Li atoms (interacting via the $a^3\Sigma_u^+$ potential) into all vibrational bound states of the $1^3\Sigma_g^+$ state is considered. The results obtained with realistic molecular potentials are compared to those that are yielded, if the atomic interaction is modeled by a regularized δ function (with energy independent and dependent scattering length).

Questions

What is the influence of a trap on the photoassociation rate?

How good is the simplified modeling of atomic interactions (like the approximation with a pseudopotential) for the description of photoassociation in a trap.

Note: So far, the photoassociation of long-range states in a trap has been analyzed using the pseudopotential approximation for the initial state [1].

The validity of the pseudopotential approximation has only been discussed with respect to the energy [2].

Photoassociation:

Photoassociation is a collision of two atoms within a light field that leads to the formation of a molecule.

The problem of two atoms interacting through a two-body potential $V(r)$ confined in an isotropic harmonic trap can be reduced to solving the Schrödinger equation for the radial internal motion

$$\left[\frac{d^2}{dR^2} - \frac{J(J+1)}{R^2} + V_{\text{int}} + \frac{1}{2}\mu\omega^2 R^2\right]\Psi(R) = E\Psi(R) \quad . \tag{1}$$

In the trap-free case, the initial state for photoassociation is a continuum state describing two ground-state atoms. The corresponding wavefunction behaves asymptotically (for $R \to \infty$) as $\Psi_E = \sqrt{\frac{k}{\pi E}}\ \sin\left[k(R - a_{sc})\right]$. Within the trap all states are bound (non-dissociative). The lowest-lying discretized continuum state becomes the first "trap-induced" state (for $a^3\Sigma_u^+$ of $^6Li_2$ it is level $v' = 10$).

Influence of a trap on the continuum states:

- the wavefunctions decay exponentially at the trap wall,
- their nodal structure and
- their now bound-state normalization factors are preserved.

Influence of a trap on photoassociation rates:

The photoassociation rate to excited vibrational level v in case of trap frequency ω is proportional to

$$I^v(\omega) = \left|\int_0^\infty \Psi^v(R;\omega)\ D(R)\ \Psi^{10'}(R;\omega)\ dR\right|^2 \quad . \tag{2}$$

The summation over all vibrational final states gives a sum rule

$$\widetilde{I} = \left\langle \Psi^{10'}(R;\omega)\left|D^2(R)\right|\Psi^{10'}(R;\omega)\right\rangle \quad , \tag{3}$$

which in the case of Franck-Condon factors is equal to one. Therefore the total photoassociation yield is constant (in the Franck-Condon approximation), it is only possible to shift transition probabilities between vibrational states.

The influence of a trap on photoassociation rates can be described with the help of the ratio

$$f^v(\omega) = \frac{I^v(\omega)}{I^v(1)}, \tag{4}$$

where the value of the trap frequency in the denominator is fixed to $\omega = 2\pi \times 1$kHz and the one in the nominator is variable. There are three characteristic regimes for this ratio:

- Constant regime: Since the trap has almost no influence on the lowest-lying vibrational levels of the $1^3\Sigma_g^+$ state, the only change in (2) is due to the wavefunction of the ground state. It turns out that for a certain R - range the wavefunction varies linearly with the trap frequency, $\Psi^{10'}(R;\omega) = C \cdot \Psi^{10'}(R;1)$. If $\Psi^v(R;\omega)$ is located within the R - range where this linear behavior occurs, one finds $f^v(\omega) = C^2$ and thus a constant change (with ω) for the photoassociation rates to all vibrational final states v fulfilling this condition.
- Non-constant regime: We found the following rule of thumb to determine those vibrational levels v for which the photoassociation rate varies non-linearly with the trap frequency: if we define a $\Delta(R) = \Psi^{10'}(R;\omega_1) - C \cdot \Psi^{10'}(R;\omega_2)$, then a non-linear variation with ω is found for those v whose classical turning point is larger than R_0 with $\Delta(R > R_0) \gtrsim 10^{-3}$. The universality of this rule was also checked for Rb and K.
- Cut-off regime: If the last lobe of the final state wavefunction is positioned outside the classical turning point of the trap-induced initial state, then the photoassociation rate vanishes. For increasing trap frequencies this cut-off moves to smaller v.

V_δ and V_{real} atom-atom interaction potentials

For the energy-independent regularized contact potential $V_{\text{int}} = \frac{4\pi a_{sc}}{2\mu}\delta^3(R)\frac{\partial}{\partial R}R$ the solution was found analytically by Busch $at\ al.$ [3],

$$\Psi_{n_t}(R) = \frac{1}{2}\pi^{-3/2}ARe^{-\bar{R}^2/2}\Gamma(-\nu)U(-\nu,\frac{3}{2},\bar{R}^2). \tag{5}$$

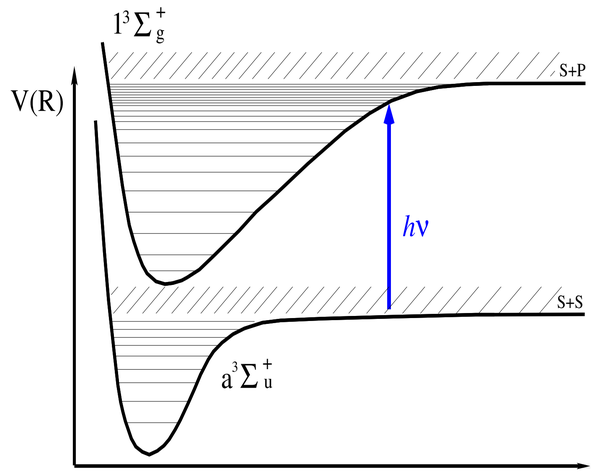
The energy-independent pseudopotential approximation is supposed to be valid when $\beta_6/a_{\text{ho}} \ll 1$, otherwise an energy-dependent pseudopotential should be used.

Difference in description with V_δ and V_{real} :

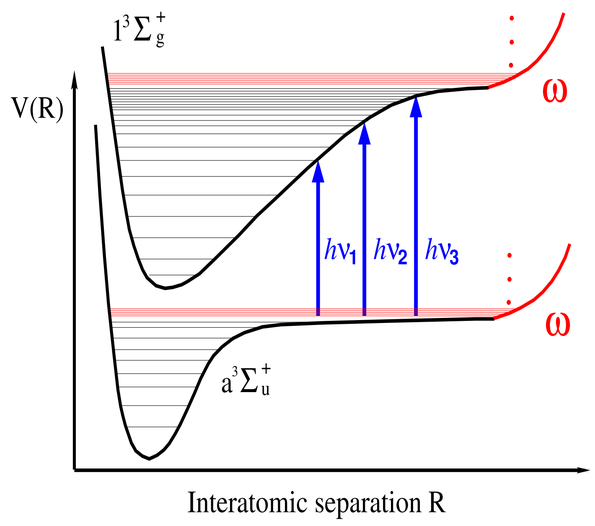
- Wavefunction $\Psi_{a_{\text{sc}}}$ ignores the nodal structure, but gives correct long-range behavior.
- Wavefunction $\Psi_{a_{\text{sc}}}$ has a phase shift compared to Ψ_{real}.
- Only photoassociation rates into long-range excited vibrational levels are relatively correct (in the case of $V_{a_{\text{E}}}$ they are correct).

There are some ways to change the photoassociation rate into a specific excited vibrational level: vary trap frequency, heat the sample, change a_{sc}.

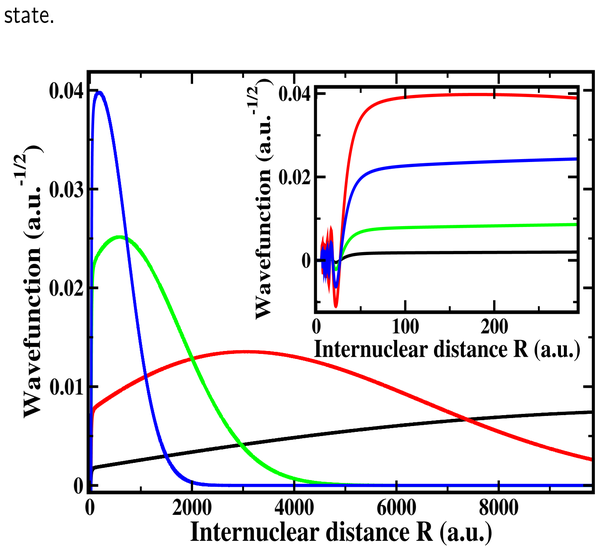
Schemes and figures



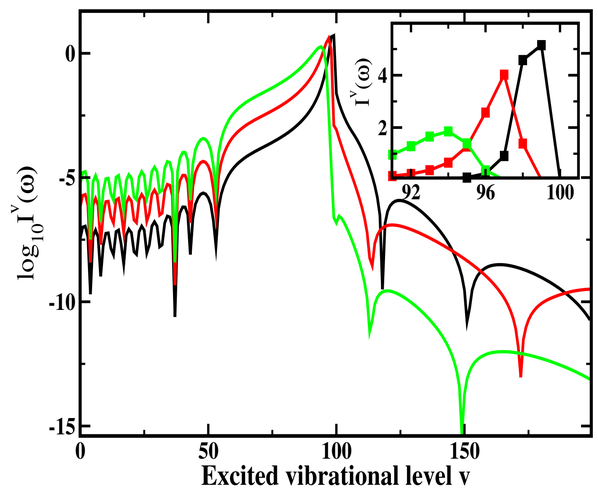
In the trap-free case the photoassociation is induced from the ground-state asymptote into vibrational level of $1^3\Sigma_g^+$.



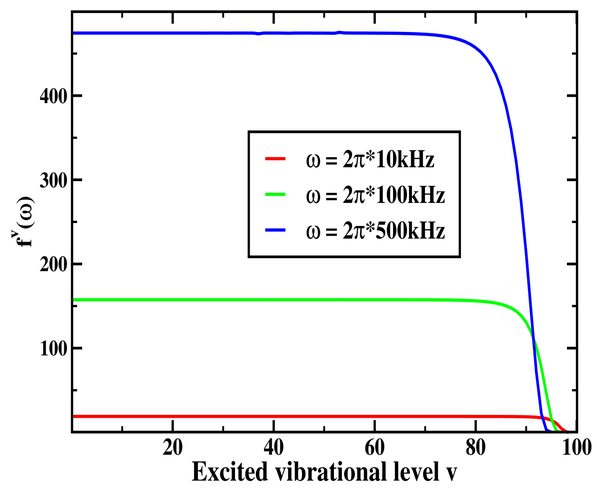
Photoassociation in a trap. There are no continuum states anymore — only bound states are present. The lowest-lying state is the first "trap induced" bound state.



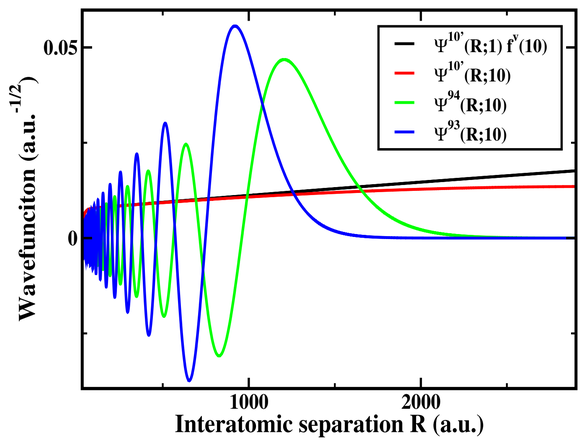
Wavefunction in a trap of frequency $\omega = 2\pi \times 1$kHz, $\omega = 2\pi \times 10$kHz, $\omega = 2\pi \times 100$kHz, $\omega = 2\pi \times 500$kHz . At intermediate interatomic separation the behavior of the wavefunction is linear (see inset).



Photoassociation rate for different trap frequencies.



The ratio $f^v(\omega)$ of equation (4) for different trap frequencies.



If the excited-state vibrational wavefunction extends in the region of the linear behavior of the first "trap-induced" initial state, then $f^v(\omega)$ is constant.

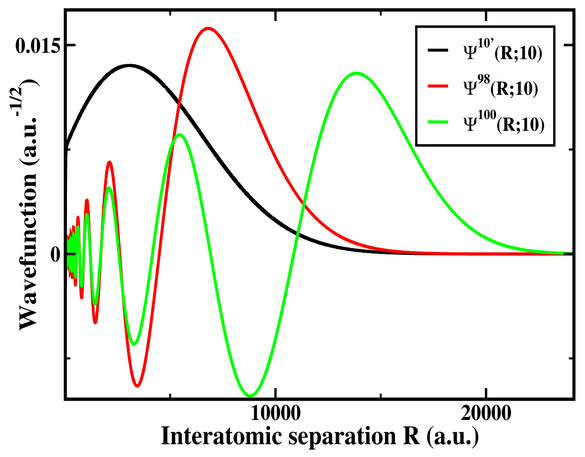
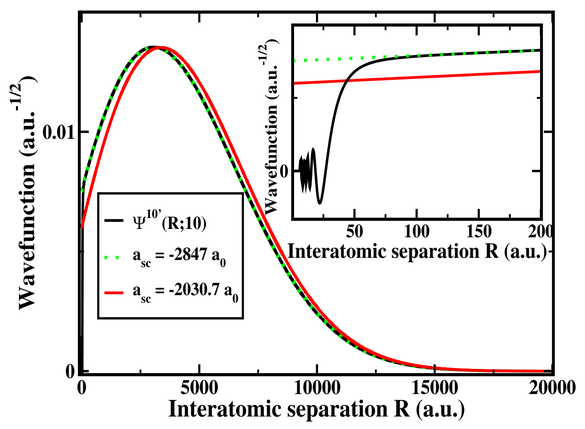
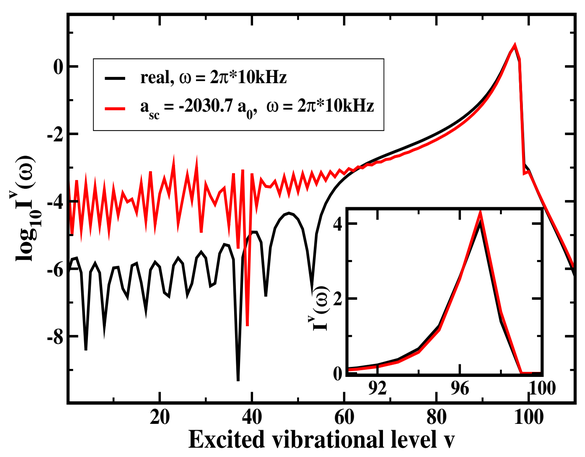


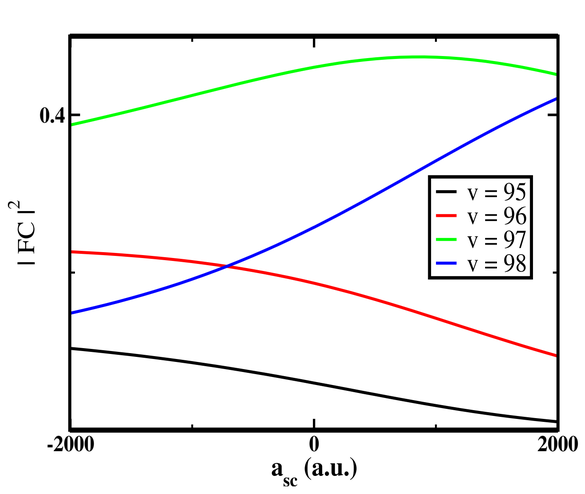
Illustration of the cut-off regime. For $\omega = 2\pi \times 10$kHz $v = 98$ is below the cut-off, $v = 100$ is beyond it.



The "correct" wavefunction is compared to the pseudopotential wavefunctions with different values of the scattering length (for trap frequency $\omega = 2\pi \times 10$kHz). Value $a_E = -2847a_0$ corresponds to the energy-dependent scattering length (obtained from the complete solution).



Comparison of the photoassociation rate (for trap frequency $\omega = 2\pi \times 10$kHz) using realistic or pseudopotential wavefunctions for the ground state.



A change of the scattering length shifts the outer turning points of the wave functions. This influences the photoassociation rate.

References

[1] B. Deb and L. You, Phys. Rev. A **68**, 033408 (2003).

[2] D. Blume and Chris H. Greene, Phys. Rev. A **65**, 043613 (2002).

[3] T. Busch, B.-G. Englert, K. Rzazewski, and M. Wilkens, Found. of Phys. **28**, 549 (1998).