Using nonresonant light to probe halo molecules

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Arbeitsgruppe Koch
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Outline

1. Structure of weakly-bound molecules
2. Molecules in nonresonant laser fields
3. Probing weakly-bound species by short laser pulses
4. Results for $^{85}\text{Rb}_2$ halo molecules
5. What about experiments?
6. Conclusions and outlook
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1. Structure of weakly-bound molecules
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4. Results for $^{85}$Rb$_2$ halo molecules
5. What about experiments?
6. Conclusions and outlook
Molecular potentials

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$n = 6$: two atoms (molecular potential)
What happens near the threshold?

Near-threshold states have large quantum numbers

Near threshold is anticlassical!
What happens near the threshold?

Near-threshold states have large quantum numbers

We like to think that this justifies the semiclassical (WKB) approximation

Harald Friedrich and Johannes Trost, "Working with WKB waves far from the semiclassical limit", Physics Reports 397, 359 (2004)

Mikhail Lemeshko (FHI)

Probing halo molecules

AG Koch seminar
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![V(r) graph with a shaded area labeled "Semiclassical region" and a curve labeled "r".](image.png)
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For molecules $n = 6$: WKB doesn’t work
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Vibrational structure of weakly-bound molecules

There were many attempts to describe vibrations of weakly-bound molecules.
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The first one: a classic paper by LeRoy and Bernstein:

Dissociation Energy and Long-Range Potential of Diatomic Molecules from Vibrational Spacings of Higher Levels*

Robert J. LeRoy and Richard B. Bernstein

Theoretical Chemistry Institute and Chemistry Department, University of Wisconsin, Madison, Wisconsin 53706

(Received 12 December 1969)

An expression is derived which relates the distribution of vibrational levels near the dissociation limit $D$ of a given diatomic species to the nature of the long-range interatomic potential, in the region where the latter may be approximated by $D = C_n/R^n$. Fitting experimental energies directly to this relationship yields values of $D$, $n$, and $C_n$. This procedure requires a knowledge of the relative energies and relative vibrational numbering for at least four rotationless levels lying near the dissociation limit. However, it requires no information on the rotational constants or on the number and energies of the deeply bound levels. $D$ can be evaluated with a much smaller uncertainty than heretofore obtainable from Birge–Sponer extrapolations. The formula predicts the energies of all vibrational levels lying above the highest one measured, with uncertainties no larger than that of the binding energy of the highest level. The validity of the method is tested with model potentials, and its usefulness is demonstrated by application to the precise data of Douglas, Møller, and Stoicheff for the $B^2\Pi_{\delta u}^+$ state of Cl₂.
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They used WKB.
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\begin{align*}
\text{THE JOURNAL OF CHEMICAL PHYSICS} & \quad \text{VOLUME 52, NUMBER 8} & \quad \text{15 APRIL 1970}

\text{Dissociation Energy and Long-Range Potential of Diatomic Molecules from Vibrational Spacings of Higher Levels}\text{\text{*}}

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More or less good results for density of states \( dv/dE_b \), but not for absolute values of \( E_b \).
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*An expression is derived which relates the distribution of vibrational levels near the dissociation limit $D$ of a given diatomic species to the nature of the long-range interatomic potential, in the region where the latter may be approximated by $D - C/R^6$. Fitting experimental energies directly to this relationship yields values of $D$, $C$, and $\Xi$. This procedure requires a knowledge of the relative energies and relative vibrational numbering of the four rotational levels lying near the dissociation limit. However, it requires no information of the relative positions of the numbers and energies of the deeply bound levels. $D$ can be evaluated with a much smaller uncertainty than heretofore obtainable from Birge–Sponer extrapolations. The formula predicts the energies of all vibrational levels lying above the highest one measured, with uncertainties no larger than that of the binding energy of the highest level. The validity of the method is tested with model potentials, and its usefulness is demonstrated by application to the precise data of Douglas, Møller, and Stoicheff for the $B^3\Pi_{u^+}$ state of $\text{Cl}_2$.*

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Not applicable to really weakly-bound molecules
Improvements to the LeRoy-Bernstein quantization rule

Stimulated by the cold-molecules research, a lot of improvements were proposed:
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**Analytical correction to the WKB quantization condition for the highest levels in a molecular potential**

C. Boisseau¹, E. Audouard¹, J. Vigué¹,² and V.V. Flambaum²

¹ Laboratoire Collisions Agrégats Réactivité, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse Cedex, France
² School of Physics, University of New South Wales, Kensington, New South Wales 2033, Australia
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**Improved LeRoy–Bernstein near-dissociation expansion formula, and prospect for photoassociation spectroscopy**

Daniel Comparat⁴

*Laboratoire Aimé Cotton, CNRS II, Bât. 505, Campus d’Orsay, 91405 Orsay cedex, France*
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**Reexamination of the LeRoy-Bernstein formula for weakly bound molecules**

Haikel Jelassi, Bruno Viaris de Lesegno, and Laurence Pruvost

Laboratoire Aimé Cotton, CNRS II, Université Paris-Sud, Paris, France
Patrick Raab and Harald Friedrich derived the so-called “quantization function”

PHYSICAL REVIEW A 78, 022707 (2008)

Quantization function for deep potentials with attractive tails

Patrick Raab and Harald Friedrich
Physik Department, Technische Universität München, D-85747 Garching, Germany
Structure of weakly-bound molecules

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Their theory describes the vibrational structure of weakly bound molecules pretty well...
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Physikalische Zeitschrift der Sowjetunion, 28, 375 (1934)

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Their theory describes the vibrational structure of weakly bound molecules pretty well...

...but what does the “quantization function” mean?
The quantization function of Raab and Friedrich

We consider a state with vibrational quantum number $v$ and a binding energy $E_b$.
The quantization function of Raab and Friedrich

We consider a state with vibrational quantum number $v$ and a binding energy $E_b$.

We introduce a noninteger “threshold quantum number”, which corresponds to $E_b = 0$. 

![Diagram of molecular potential showing $E_b$, $v$, and $v_{th}$]
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Vice versa, \( v_{\text{th}} - v \) is some function of \( E_b \):
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The quantization function gives positions of weakly-bound vibrational levels
The quantization function of Raab and Friedrich

The analytic expression for the quantization function is:

\[ F(E_b) = F_{th}(\kappa) + F_{ip}(\kappa) \left[ F_{cr}(\kappa) + F_{WKB}(\kappa) \right] \]
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F_{WKB}(\kappa) = \frac{\kappa^{1-2/n}}{\sqrt{\pi} (n-2)} \frac{\Gamma\left(\frac{1}{2} + \frac{1}{n}\right)}{\Gamma\left(1 + \frac{1}{n}\right)} \quad \text{— pure WKB term}
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\[ F_{\text{th}}(\kappa) = \frac{2b\kappa - (p\kappa)^2}{2\pi [1 + (G\kappa)^4]} \] — near-threshold dependence

The expressions are very accurate and can be used for any binding energy \( E_b \).
Rotational structure of weakly-bound molecules

Now we know the vibrational structure. But what about rotation?
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Two years after introducing the quantization rule, LeRoy published an article:

Canadian Journal of Physics

Published by The National Research Council of Canada

VOLUME 50  MAY 15, 1972  NUMBER 10

Dependence of the Diatomic Rotational Constant $B_v$ on the Long-Range Internuclear Potential

Robert J. Le Ruy

Department of Physics, University of Toronto, Toronto 181, Ontario
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The WKB approximation was depressingly inaccurate, as LeRoy pointed out:

As a result, only upper and lower bounds could be given, rather than accurate predicted values for unobserved $B_v$'s for levels near $D$. 

Mikhail Lemeshko (FHI) Probing halo molecules AG Koch seminar
Rotational structure of weakly-bound molecules: our contribution

We follow Raab and Friedrich to study rotation of weakly-bound species.
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We consider a molecule in ground rotational state, $J = 0$, with a binding energy $E_b$.
Rotational structure of weakly-bound molecules: our contribution

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Rotation adds a centrifugal term to the potential, $V_{\text{cent}} = \frac{\hbar^2 J(J + 1)}{2mr^2}$

![Graph showing potential $V(r)$ with $E_b$ and $v(J=0)$]
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If the angular momentum $J$ is greater than some critical value $J^*$, the vibrational state is “pushed out” of the potential – the molecule dissociates.

![Diagram showing rotational potential energy $V(r)$ with binding energy $E_b$, vibrational states $v(J = 0)$ and $v(J > J^*)$, and critical angular momentum $J^*$]
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If the angular momentum \( J \) is greater than some critical value \( J^* \), the vibrational state is “pushed out” of the potential – the molecule dissociates.

Integer part of \( J^* \) gives the number of rotational states, supported by a given vibrational level.
Rotational structure of weakly-bound molecules: our contribution

- We derived a simple analytic expression for critical angular momentum:

\[ J^* = F(E_b)(n - 2), \]
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- When the molecule is rotationless?

We derived a simple criterion for that.

Molecule has only the ground rotational state if the binding energy satisfies:

\[ E_b < d_6 \frac{\hbar^3 m}{2}, \]

\( d_6 \approx 1.6 \) is a parameter

- Rotational constants of weakly-bound levels may be estimated as

\[ B = E_b J^*(J^* + 1) \]

These expressions are surprisingly accurate and were accepted as a PRA Rapid
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$m$ is the reduced mass, $d_6 \approx 1.6$ is a parameter

• Rotational constants of weakly-bound levels may be estimated as $B = \frac{E_b}{J^*(J^* + 1)}$

• These expressions are surprisingly accurate and were accepted as a PRA Rapid
What are “halo molecules”?

The weakest-bound molecules, which spend most of the vibrational period in the classically forbidden region, are called haloes.

![Graph showing the relationship between energy and distance for halo molecules.](image)
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The wavefunction extends up to $10 \ r_{\text{classical}}$

The molecule spends more than a half of the vibrational period beyond the classical turning point.

Most of haloes are rotationless – they support just the ground rotational state, $J = 0$
Outline

1. Structure of weakly-bound molecules
2. Molecules in nonresonant laser fields
3. Probing weakly-bound species by short laser pulses
4. Results for $^{85}\text{Rb}_2$ halo molecules
5. What about experiments?
6. Conclusions and outlook
Is angular momentum always quantized?

In the absence of a field, 

$$\langle J^2 \rangle = J(J+1)$$

is an integer for states with 

$$J = 0, 1, 2, ...$$

However, in the presence of a field, this is not true!

An external field, such as a laser field, hybridizes rotational levels, forming a "pendular state":

$$J = 0 \quad J = 2 \quad J = 4 \quad J = 0 \sim 0.87 \quad 0.48 \quad 0.06 \sim$$

Field imparts a noninteger value of 

$$\langle J^2 \rangle$$

in the example above 

$$\langle J^2 \rangle = 1.47$$.

The molecule is shaken by the field

Mikhail Lemeshko (FHI)

Probing halo molecules

AG Koch seminar 16 / 33
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\quad & \quad = & \quad \tilde{J}=0
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The molecule is shaken by the field
Can one make use of it?

Weakly-bound molecules usually support no rotation (no states with $J \geq 1$). For instance, the last vibrational state of $^{85}$Rb$_2$ dissociates for $\langle J^2 \rangle \geq 0.27$. The laser field adds a centrifugal term to the potential $V(r)$, so that the effective potential is:

$$U_{\text{eff}}(r) = V(r) + \langle J^2 \rangle \frac{\hbar^2}{2mr^2}$$

We may tune it by changing the intensity.
Can one make use of it?

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What happens when we apply the laser field? Let's see...
Can one make use of it?

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The laser is on...
Can one make use of it?

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a bit more intensity...
Can one make use of it?

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We may tune it by changing the intensity more!
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even more....
Can one make use of it?

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The molecule is shaken enough by the field to dissociate
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What happens if a laser pulse is short?
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“Short” means “shorter than the rotational period”
What happens if a laser pulse is short?

“Short” means “shorter than the rotational period”

For a cw-laser field, $\langle J^2 \rangle$ is constant
What happens if a laser pulse is short?

“Short” means “shorter than the rotational period”

If the pulse duration is longer than the rotational period, $\langle J^2 \rangle$ is transferred adiabatically.
What happens if a laser pulse is short?

“Short” means “shorter than the rotational period”

If the pulse duration is longer than the rotational period, \( \langle J^2 \rangle \) is transferred adiabatically.

The molecule has no angular momentum after the pulse has passed.
What happens if a laser pulse is short?

“Short” means “shorter than the rotational period”

If the pulse duration is shorter than the rotational period, the process is nonadiabatic.
What happens if a laser pulse is short?

“Short” means “shorter than the rotational period”

If the pulse duration is shorter than the rotational period, the process is nonadiabatic

A part of the angular momentum is transferred to the molecule forever
What happens if a laser pulse is short?

“Short” means “shorter than the rotational period”

In the case of very short pulses most of the angular momentum is imparted forever.
What happens if a laser pulse is short?

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In the case of very short pulses most of the angular momentum is imparted forever

This angular momentum remains unless the system is perturbed
What happens if a laser pulse is short?

“Short” means “shorter than the rotational period”

In the case of very short pulses most of the angular momentum is imparted forever.

This angular momentum remains unless the system is perturbed.

If the transferred angular momentum exceeds some critical value, the molecule will be shaken enough by the pulse to dissociate.
And... if the pulse is even shorter?
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If the pulse duration is shorter than the *vibrational* period, the transferred angular momentum depends on the internuclear distance.
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Consequently, the pulse intensity needed for dissociation depends on the distance which molecule had at the moment when the laser pulse struck.

![Graph showing relationship between pulse intensity and internuclear distance](image-url)
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We can probe the vibrational dynamics!
And... if the pulse is even shorter?

If the pulse duration is shorter than the *vibrational* period, the transferred angular momentum depends on the internuclear distance.

For any intensity $I$ there is some critical distance $r^*$. 

![Graph showing the relationship between intensity $I$ and internuclear distance $r^*$]
And... if the pulse is even shorter?

If the pulse duration is shorter than the *vibrational* period, the transferred angular momentum depends on the internuclear distance.

For any intensity $I$ there is some critical distance $r^*$. If the internuclear distance is smaller than $r^*$ at the moment when the pulse strikes, the molecule dissociates.
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No dissociation occurs for larger internuclear separations.

![Graph showing dissociation and no dissociation as a function of intensity and internuclear distance.]

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And... if the pulse is even shorter?

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For any intensity $I$ there is some critical distance $r^*$. If the internuclear distance is smaller than $r^*$ at the moment when the pulse strikes, the molecule dissociates.

No dissociation occurs for larger internuclear separations.

So, for any pulse intensity $I$ the probability of dissociation is the probability to have internuclear distances smaller than $r^*(I)$.

![Graph showing dissociation and no dissociation as a function of internuclear distance and laser intensity](image)
And... if the pulse is even shorter?

If the pulse duration is shorter than the *vibrational* period, the transferred angular momentum depends on the internuclear distance.

This is simply the integral of the squared wavefunction:

\[ F(r^*) = \int_0^{r^*} |\phi_v(r)|^2 \, dr. \]
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Here comes the idea:

In an experiment we can measure $F(I)$.
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We can calculate the dependence \( I(r^*) \)
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Hence, we can obtain the square of the vibrational wavefunction!
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Potential and wavefunction

We used a single Rb\(_2\) potential curve from ref. [Seto et al JCP, 113, 3067 (2000)], combining it with dispersion terms from ref. [van Kempen et al PRL 88, 093201 (2002)].
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The last vibrational state, $v = 123$, is bound by $E_b = -237$ kHz

We also developed an analytic model, based on the near-threshold expansion of the wavefunction
Dependence of dissociation probability from the intensity

The vibrational period of $^{85}\text{Rb}_2 (v = 123)$ molecule is about 0.67 $\mu$s, so it can be probed by ns pulses. We performed the calculation for 50 ps pulses.
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The maxima of $F(I)$ reflect the nodes of the vibrational wavefunction.
Results for $^{85}\text{Rb}_2$ halo molecules

**Dependence of dissociation probability from the intensity**

The vibrational period of $^{85}\text{Rb}_2$ ($v = 123$) molecule is about 0.67 µs, so it can be probed by ns pulses. We performed the calculation for 50 ps pulses.

The “edge” of $F(I)$ gives the position of the wavefunction’s main maximum.
Two words about the analytic model

Near the threshold, everything is determined by the long-range potential, $-\frac{C_6}{r^6}$.
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However, there are solutions for $E_b = 0$, with the following asymptotic behavior:

\[
\psi_0(r) \sim r \to \infty 1
\]

\[
\psi_1(r) \sim r \to \infty r
\]

In the first order we can present the bound state wavefunction as:

\[
\psi_b(r) = \psi_0(r) - k\psi_1(r) \sim r \to \infty 1 - kr
\]

It solves the Schrödinger equation and has a correct asymptote, $\psi_b(r) \sim r \to \infty e^{-kr}$.

The model based on this wavefunction explains the main features of $F(I)$.

Mikhail Lemeshko (FHI)

Probing halo molecules

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Could the experimentalists have already seen the effect?
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Yes, they could have.
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Yes, they could have: example 1

The intensity of some optical dipole traps reaches $10^6 - 10^7 \text{ W/cm}^2$
What about experiments?

Could the experimentalists have already seen the effect?

Yes, they could have: example 1

The intensity of some optical dipole traps reaches $10^6 - 10^7$ W/cm$^2$

This may have already dissociated some of the weakest-bound molecules
Could the experimentalists have already seen the effect?

Yes, they could have: example 2

Lasers in optical dipole trap change the effective potential...
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Controlling the molecular size using nonresonant fields

Applying a cw-laser field we may decrease the binding energy...
Controlling the molecular size using nonresonant fields

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$^{85}\text{Rb}_2$ in the least-bound state already is a long-range molecule

![Graph showing $\langle r \rangle = 167 \text{ Å}$]
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However, it may be transferred to a “pure halo” regime using cw-laser field
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The intensity needed is $6.52 \times 10^8$ W/cm$^2$
Other possibilities

- Using nonresonant fields one can change the scattering length.
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- Thereby, one can tune the positions of Feshbach resonances

- One may preclude atoms from colliding, by creating a field-induced potential barrier between them

- Alternatively, one may create molecules by association of ultracold atoms via the shape resonance – an inverse procedure to the “dissociation by shaking”
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Conclusions

We showed that weakly bound Feshbach molecules can be probed by “shaking” in nonresonant laser fields.
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1. We showed that weakly bound Feshbach molecules can be probed by “shaking” in nonresonant laser fields.

2. Using short laser pulses it is possible to map out the square of the vibrational wavefunction.
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3. Using a cw-laser field one can control the molecular size, the atomic scattering length and the positions of Feshbach resonances.
Conclusions

1. We showed that weakly bound Feshbach molecules can be probed by “shaking” in nonresonant laser fields.

2. Using short laser pulses it is possible to map out the square of the vibrational wavefunction.

3. Using a cw-laser field one can control the molecular size, the atomic scattering length and the positions of Feshbach resonances.

4. As an aside, we derived simple expressions for a number of rotational states, supported by a weakly-bound molecule, and for the rotational constants.
Outlook

1. The experimentalists may have already observed some shaking due to the field of optical dipole traps.
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2. Manipulating Feshbach resonances with a cw-laser might be a straightforward proof of the shaking mechanism.

Further reading:
- arXiv: 0903.0811 (about probing halo molecules)
- arXiv: 0904.0567 (about rotational states of weakly-bound dimers)
Conclusions and outlook

Outlook

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Thank you for your attention!