Multipole Analysis of Radio-Frequency Reactions in Ultracold Atoms

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Outline

1 Introduction
   - Photo Reactions
   - Efimov Physics and Ultracold Atoms

2 Multipole Expansion

3 Dimer Photoassociation

4 Trimer Photoassociation

5 Experimental Realization

6 Conclusions

References:
- E. Liverts, B. Bazak, and N. Barnea, Phys. Rev. Lett. 108, 112501 (2012)
- B. Bazak, E. Liverts, and N. Barnea, Phys. Rev. A 86, 043611 (2012)
- B. Bazak, E. Liverts, and N. Barnea, Few Body Syst. 54, 667 (2013)
- B. Bazak and N. Barnea, arXiv:1305.4368 [cond-mat.quant-gas]
What Can We Learn From Photo Reactions?

1. Understanding of the systems at hand.
2. A test of the Hamiltonian at regimes not accessible by elastic reactions.
3. Reaction rates as input for experiments or applications (e.g. astrophysics).
4. Underlying degrees of freedom.
5. The transition from single particle to collective behavior.

Betzalel Bazak (HUJI)

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EFB22, 9 September, 2013
The interaction Hamiltonian between the photon field $A(x)$ and the atomic/nuclear system

$$H_I = -\frac{e}{c} \int dx A(x) \cdot J(x)$$

The current is a sum of convection and spin currents

$$J(x) = J_c(x) + \nabla \times \mu(x)$$

$$H_I = -\frac{e}{c} \int dx \{ A(x) \cdot J_c(x) + B(x) \cdot \mu(x) \}$$

- Classically, the convection current $J_c = \sum_i Q_i v_i$ is the flow of the charged particles.
- In nuclear physics, the convection current is dominant at low energies.
- Ultracold atoms are neutral $J_c(x) = 0$ and the current $\mu(x)$ is dominated by the spins.
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Efimov Physics and Universality

- **Borromean regime**: A 3-body bound state exists even when the 2-body system is unbound.
- In nuclear physics, $^6$He is bound while $^5$He, n-n - not.

- **The unitary limit**: $E_2 = 0, a_s \to \infty$.
- In 1970 V. Efimov found out that if $E_2 = 0$ the 3-body system will have an infinite number of bound states.
- The 3-body spectrum is $E_n = E_0 e^{-2\pi n/s_0}$ with $s_0 = 1.00624$.
- In atomic traps, $a_s$ can be manipulated through the Feshbach resonance.
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  ![He isotopes](image)

  *from ANL site*

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RF-induce atom loss resonances for different values of bias magnetic fields.

RF association of $^7$Li dimers and trimers at 1.5 $\mu$K
O. Machtey, Z. Shotan, N. Gross and L. Khaykovich, Phys. Rev. Lett. 108, 210406 (2012)
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- The response of an A-particle system is closely related to the static moments of the charge density
  \[ \rho(x) = \sum_{i=1}^{A} Q_i \delta(x - r_i) \]

- The Fourier Transform
  \[ \rho(k) = \int dx \rho(x) e^{ikx} = \sum_{i=1}^{A} Q_i e^{ikr_i} \]

- In the long wavelength limit \( k \to 0 \)

- For a system of identical particles

- Conclusion A: In general the Dipole is the leading term.
- Conclusion B: For identical particles the leading terms are \( \hat{M} \) and \( \hat{Q} \).
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\[ \rho(k) \approx AQ_1 + iAQ_1 k \cdot R_{cm} - Q_1 \sum_{i=1}^{A} \left( \frac{k^2 r_i^2}{6} + 4\pi \frac{k^2 r_i^2}{15} \sum_m Y_{2-m}(\hat{k})Y_{2m}(\hat{r}_i) \right) \]

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For RF photons in the few MHz region the wavelength is meters so $kR \ll 1$.

The atoms reside in a strong magnetic field, with well defined $m_F,$

$$|\Psi_0\rangle = \Phi_0(r_i)|m_1^F m_2^F \ldots m_A^F\rangle$$

In the final state the photon can either change one of the spins or leave them untouched.

Spin-flip reaction

$$|m_1^F m_2^F \ldots m_A^F\rangle \longrightarrow |m_1^F m_2^F \pm 1 \ldots m_A^F\rangle$$

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N. Gross and L. Khaykovich,
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\[
R(\omega) = C k \sum_{f,\lambda} |\langle \Phi_f | \Phi_0 \rangle|^2 \delta(E_f - E_0 - \omega)
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- For Frozen-Spin reactions we get a sum of the monopole operator \( \hat{M} = R^2 = \sum r_i^2 \) and the Quadrupole operator \( \hat{Q} = \sum r_i^2 Y_2(\hat{r}_i) \)

\[
O = \alpha \hat{M} + \beta \hat{Q}
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- The response is given by

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R(\omega) = k^5 \sum_{f,\lambda} |\langle \Phi_f | O | \Phi_0 \rangle|^2 \delta(E_f - E_0 - \omega)
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\[ R(\omega) = C\omega^5 \left[ \frac{1}{6^2} |\langle \psi_0 | \hat{M} | \varphi_0(q) \rangle|^2 + \frac{1}{5 \cdot 15^2} |\langle \psi_0 | \hat{Q} | \varphi_2(q) \rangle|^2 \right] \]

The bound state wave function is

\[ \psi_0 = Y_0 \sqrt{2\kappa} e^{-\kappa r} / r ; \quad \kappa \approx 1/a_s \]

The continuum state wave function is

\[ \varphi_{lm}(q) = Y_{lm}(\hat{r}) 2q [\cos \delta_{lj}(qr) - \sin \delta_{lj}(qr)] \]

The \( l = 0 \) matrix element

\[ |\langle \psi_0 | \hat{M} | \varphi_0(q) \rangle|^2 = \frac{1}{4\pi} \left( \frac{4q \sqrt{2\kappa}}{(q^2 + \kappa^2)^3} \right)^2 \left[ \cos \delta_0 (3\kappa^2 - q^2) - \sin \delta_0 \frac{\kappa}{q} (3q^2 - \kappa^2) \right]^2 \]

The \( \ell = 2 \) matrix element, assuming \( \delta_2 = 0 \)

\[ |\langle \psi_0 | \hat{Q} | \varphi_2(q) \rangle|^2 = \frac{5}{4\pi} \left[ \frac{16q^3 \sqrt{2\kappa}}{(q^2 + \kappa^2)^3} \right]^2 \]
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\[ |\langle \psi_0 | \hat{Q} | \varphi_2(q) \rangle|^2 = \frac{5}{4\pi} \left( \frac{16q^3 \sqrt{2\kappa}}{(q^2 + \kappa^2)^3} \right)^2 \]
For the dimer case, the response function can be written as

\[ R(\omega) = C\omega^5 \left[ \frac{1}{6^2} |\langle \psi_0 | \hat{M} | \varphi_0(q) \rangle|^2 + \frac{1}{5 \cdot 15^2} |\langle \psi_0 | \hat{Q} | \varphi_2(q) \rangle|^2 \right] \]

The bound state wave function is

\[ \psi_0 = Y_0 \sqrt{2\kappa} e^{-\kappa r} / r ; \quad \kappa \approx 1/a_s \]

The continuum state wave function is

\[ \varphi_{lm}(q) = Y_{lm}(\hat{r}) 2q[\cos \delta_{lj}(qr) - \sin \delta_{ln}(qr)] \]

The \( l = 0 \) matrix element

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Photoassociation of the Atomic Dimer

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The s-wave and d-wave components in the response function

- upper panel $a/r_{\text{eff}} = 2$
- lower panel $a/r_{\text{eff}} = 200$
- red - $r^2$ monopole
- blue - quadrupole
- black - their sum
Photoassociation of $^7\text{Li}$ dimers

$a_s = 1000a_0$

$T = 25\mu\text{K}$ (upper panel)
$T = 5\mu\text{K}$ (lower panel)

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The relative contribution to the peak

Normalized photoassociation rate $\left[\text{n.d.}\right]$
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The relative contribution to the peak

![Graph showing relative contribution to the peak](image-url)
Road-map for Efimov Physics

To get analytic results for the 3-body problem,

- **Assume short-range interaction and large scattering length**

- Remove center of mass and adopt the hyper-spherical coordinates

\[(r_1, r_2, r_3) \rightarrow (R_{CM}, x_i, y_i) \rightarrow (R_{CM}, \rho, \alpha_i, \hat{x}_i, \hat{y}_i)\]

- Use the adiabatic expansion (Born-Oppenheimer like), where \(\rho\) is the slow coordinate

\[\Psi(\rho, \Omega) = \sum_n \rho^{-5/2} f_n(\rho) \Phi_n(\rho, \Omega)\]

- Decompose into Faddeev amplitudes to impose symmetry and boundary condition

\[\Phi_n(\rho, \Omega) = \sum_i \phi_{n,i}(\rho, \Omega_i)\]

- For given \(\rho\), solve the hyper-angular equation,

\[\left(\hat{K}^2 + \frac{2m}{\hbar^2} \rho^2 \sum_i V(\sqrt{2}\rho \sin \alpha_i) + 4\right) \Phi_n(\rho, \Omega) = \nu_n^2 \Phi_n(\rho, \Omega).\]
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We assume our interaction is of zero range and s-wave only, and solve for low energy. Therefore, the potential is expressed as boundary condition,

\[
\frac{1}{2\alpha_i\Phi} \frac{\partial}{\partial\alpha_i} 2\alpha_i\Phi \bigg|_{\alpha_i=0} = -\sqrt{2\rho} \frac{1}{a_s}
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(negative \( \nu = \) imaginary values)
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\]

The result is a 1-D equation for \( f(\rho) \) and \( E \), with an effective \( \frac{1}{\rho^2} \) potential,

\[
\left( -\frac{\partial^2}{\partial \rho^2} + \frac{2m}{\hbar^2} \left( \frac{\hbar^2}{2m} \frac{v_n^2(\rho)}{\rho^2} - \frac{1}{4} - Q_{nn} - E \right) \right) f_n(\rho) = \sum_{n \neq n'} (2P_{nn'} \frac{\partial}{\partial \rho} + Q_{nn'}) f_{n'}(\rho)
\]

(negative \( \nu = \) imaginary values)
The Unitary Limit

- In the unitary limit, $|a| \to \infty$, $\nu$ does not depend on $\rho$, and the channels decouples.
- The hyper-radial equation is similar to the Bessel equation,

$$-\frac{d^2 f(\rho)}{d\rho^2} + \frac{\nu^2_L - 1/4}{\rho^2} f(\rho) = \epsilon f(\rho)$$

with $\nu_0 \approx 1.00624i$, and $\nu_2 \approx 2.82334$.

- Bound state, $E_n = -\hbar^2 \kappa_n^2 / 2m < 0$:

$$f_B^{(n)}(\rho) \propto \kappa_n \sqrt{\rho} K_{\nu_0}(\kappa_n \rho)$$

where to avoid the Thomas collapse, a 3-body repulsive force is to be introduced, for example $U(\rho \leq \rho_0) = \infty$ for some finite $\rho_0$, resulting in the famous Efimov spectrum,

$$\frac{E_n}{E_0} = e^{-2\pi n/|\nu_0|} \approx 515^{-n}.$$

- Scattering state, $E = \hbar^2 q^2 / 2m > 0$:

$$f_L(\rho) \propto \sqrt{\frac{q \rho}{R}} [\sin \delta_L J_{\nu_L}(q \rho) + \cos \delta_L Y_{\nu_L}(q \rho)]$$

where the 3-body phase shift is determined by $f_L(\rho_0) = 0$. 
The Unitary Limit

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Betzalel Bazak (HUJI)  Multipole analysis of RF reactions in ultracold atoms  EFB22, 9 September, 2013
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Matrix Elements Calculation

- The $r^2$ operator reads $\sum_i r_i^2 = \rho^2 + 3R_{CM}^2$.
- For the $\hat{Q}$ operator, $r_i = R_{CM} - \sqrt{\frac{2}{3}} y_i$,
  
  \[ r_i^2 Y_M^M(\hat{r}_i) = \rho^2 \cos^2 \alpha_i Y_M^M(\hat{y}_i) \]

\[ |\langle f | \hat{H}_I | i \rangle|^2 \propto \frac{1}{6^2} |\langle \psi_B | \sum_i r_i^2 Y_0^0 \rangle|^2 + \frac{1}{15^2} |\langle \psi_B | \sum_i r_i^2 Y_2^2(\hat{r}) \rangle|^2 \]

(dashed line - full numerical calculation for finite $a$)
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Trimer Photoassociation: Results

\[ k_B T = E_3 \]

\[ k_B T = 0.2E_3 \]

Normalized transition rate

\[ \text{Normalized transition rate} \]

\[ 0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1.0 \]

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red - \( r^2 \) monopole, blue - quadrupole, and black - their sum
Log-periodic oscillations

- We found another fingerprint of the Efimov physics, a *log-periodic* oscillations:
  - For the s-wave, near threshold,
    \[ I \approx 1 + \frac{B_2}{2} \cos\left(2s_0 \ln \frac{q}{\kappa}\right), \quad B_2 \approx 8.5\% \]
  - For any multipole, at the high-frequency tail
  - The near threshold oscillations may be blurred by the finite energy width of the trimer.
  - The high-frequency tail oscillations are masked by rapid phase shift variation and \( q^4 \) factor.
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Outline

1 Introduction
   • Photo Reactions
   • Efimov Physics and Ultracold Atoms

2 Multipole Expansion

3 Dimer Photoassociation

4 Trimer Photoassociation

5 Experimental Realization

6 Conclusions
Experimental realization

- Magnetically Feshbach resonance based on the spin dependence of the molecular interaction.

Therefore, $m_f$ ceases to be a good quantum number, but $\sum m_f$ still is.

For example, the state $|11\rangle$ is mixed with $|02\rangle$ and $|20\rangle$.

However, this mixing involves high energy scale, and therefore its influence depends on the energy scales of the system.

Other effects not included: power broadening caused by high amplitude RF, finite time and finite energy width.
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![Energy vs. Interatomic distance graph](image)

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from Ketterle group site
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- Magnetically Feshbach resonance based on the spin dependence of the molecular interaction.

- Therefore, $m_f$ ceases to be good quantum number, but $\sum m_f$ still is.

- For example, the state $|11\rangle$ is mixed with $|02\rangle$ and $|20\rangle$

- However, this mixing involves high energy scale, and therefore its influence depends on the energy scales of the system.

- Other effects not included: power broadening caused by high amplitude RF, finite time and finite energy width.
Putting all together, fitting our model to the Khaykovich group data:

\[ a_s = 820a_0 \quad T = 3.9\, K \quad E_3 = 1.2E_2 \]

\[ a_s = 630a_0 \quad T = 3.5\, K \quad E_3 = 1.1E_2 \]
Summary and Conclusions

1. The new RF experiments in ultracold-atoms systems carry much in common with photo-reactions and charged current reactions in nuclei.

2. For spin-flip reaction, the Franck-Condon factor is the leading contribution to the cross-section, and $R(\omega) \propto \omega$.

3. For frozen-spin reactions the monopole $R^2$ and the quadrupole are the leading terms, and $R(\omega) \propto \omega^5$.

4. We have studied the dimer formation and found that the reaction mechanism changes from monopole to quadrupole with increasing gas temperature.

5. The trimer formation was studied, with similar dependence on temperature.

6. Log-periodic oscillations are predicted in the trimer photoassociation.
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The Hyper-Spherical Coordinates

- To eliminate center of mass, we use the Jacobi coordinates, $(r_1, r_2, r_3) \rightarrow (R_{CM}, x_i, y_i)$:

$$x_i = \frac{r_j - r_k}{\sqrt{2}}, \quad y_i = \sqrt{\frac{2}{3}} \left( -r_i + \frac{r_j + r_k}{2} \right)$$

- Now using the hyper-spherical coordinates, $(x_i, y_i) \rightarrow (\rho, \alpha_i, \hat{x}_i, \hat{y}_i)$:

$$\rho^2 = x_i^2 + y_i^2, \quad \tan \alpha_i = x_i / y_i,$$

- The Hamiltonian $\mathcal{H} = (T + \sum_{i<j} V(|r_i - r_j|)$ reads,

$$T = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial \rho^2} + \frac{5}{\rho} \frac{\partial}{\partial \rho} - \hat{K}^2 / \rho^2 \right)$$

where

$$\hat{K}^2 = -\frac{1}{\sin 2\alpha} \frac{\partial^2}{\partial \alpha^2} \sin 2\alpha + \frac{\hat{l}_x^2}{\sin^2 \alpha} + \frac{\hat{l}_y^2}{\cos^2 \alpha} - 4$$

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The Adiabatic Expansion

Next we apply the adiabatic expansion,

\[ \Psi(\rho, \Omega) = \sum_n \rho^{-5/2} f_n(\rho) \Phi_n(\rho, \Omega), \]

\( \Phi_n(\rho, \Omega) \) is the solution of the hyper angular equation corresponding to the eigenvalue \( \nu_n^2 \),

\[ \left( \hat{K}^2 + \frac{2m}{\hbar^2} \rho^2 \sum_i V(\sqrt{2}\rho \sin \alpha_i) + 4 \right) \Phi_n(\rho, \Omega) = \nu_n^2 \Phi_n(\rho, \Omega). \]

\( f_n(\rho) \) is the solution of the hyper-radial equation,

\[ \left( -\frac{\partial^2}{\partial \rho^2} + \frac{2m}{\hbar^2} (V_{\text{eff}}(\rho) - E) \right) f_n(\rho) = \sum_{n \neq n'} (2P_{nn'} \frac{\partial}{\partial \rho} + Q_{nn'}) f_{n'}(\rho) \]

where the effective potential is

\[ V_{\text{eff}}(\rho) = \frac{\hbar^2}{2m} \frac{\nu_n^2(\rho) - 1/4}{\rho^2} - Q_{nn} \]

and the non-adiabatic couplings are

\[ P_{nn'}(\rho) = \left\langle \Phi_n(\rho, \Omega) \left| \frac{\partial}{\partial \rho} \right| \Phi_{n'}(\rho, \Omega) \right\rangle_{\Omega} \]

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The Faddeev Decomposition

- Using Faddeev decomposition,

\[ \Phi_n(\rho, \Omega) = \sum_i \phi_{n,i}(\rho, \Omega_i) \]

- We assume our interaction is of zero range and s-wave only, Therefore the only partial wave to be considered for the bound state is \( l_x = 0, l_y = L \).

- Now the solution is,

\[ \phi_{n,i}(\rho, \Omega_i) = \frac{g_{\nu,L}(\alpha_i)}{\sin(2\alpha_i)} \gamma_{l_x,l_y}^{L,M}(\hat{x}_i, \hat{y}_i) \]

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\[ g_{\nu,L}(\alpha_i) = \cos^L \alpha \left( \frac{\partial}{\partial \alpha} \frac{1}{\cos \alpha} \right)^L \sin \left[ \nu \left( \alpha - \frac{\pi}{2} \right) \right], \]

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- In the low energy limit, the boundary condition reads

\[ \left[ \frac{1}{2\alpha_i \Phi} \frac{\partial}{\partial \alpha_i} 2\alpha_i \Phi \right]_{\alpha_i=0} = -\sqrt{2\rho} \frac{1}{a_s} \]

A. Cobis, D.V. Fedorov, and A.S. Jensen, Phys. Rev. Lett. 79, 2411 (1997).
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