Sixth Workshop on the Critical Stability of Quantum Few-Body Systems

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Few-body structures of polar molecules in two dimensions

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Outline

1. Introduction
2. Two dipoles in two layers
3. Few body structures
4. Outlook

What is interesting about dipolar interaction in 2D?

New condensed-matter phases and new complex quantum dynamics [1], because it is

- long range;
- anisotropic.

Now the interaction can be controlled in the lab with

- atoms Cr with magnetic dipole moment [2];
- molecules with induced electric dipole KRb [3].

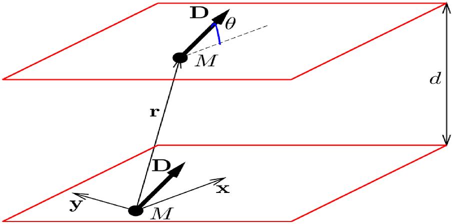
2D geometry

- supressed rate of the chemical reactions

[1]. T.Lahaye, C. Menotti, L.Santos, M.Lewenstein, and T.Pfau, *Rep. Prog. Phys.* **72**, 126401 (2009)
[2]. A. Griesmaier, J. Werner, S. Hensler, J. Stuhler, and T. Pfau, *PRL* **94**, 160401 (2005)
[3]. K.K.Ni et al. *Science* **322**, 231 (2008)

The System

- Two particles (mass M, dipole moment $\mathbf{D}$)
- $\mathbf{D}$ is aligned at angle θ
- 2D (parallel zero-width layers, separated by d)



It should be noted that the case $\theta = \pi/2$ can be found in the following papers
A. Pikovski, M. Klawunn, G. V. Shlyapnikov, and L. Santos, *PRL* **105**, 215302 (2010)

J. R. Armstrong, N. T. Zinner, D. V. Fedorov, A. S. Jensen, *EPL* **91**, 16001 (2010).

The Interaction

The interaction in Cartesian coordinates:

$$V(x,y) = D^2 \frac{x^2 + y^2 + d^2 - 3(x\cos\theta + d\sin\theta)^2}{(x^2 + y^2 + d^2)^{5/2}} \ ,$$

Properties of the interaction

- anisotropic,
- zero net volume: $\int V(x,y)\mathrm{d}x\mathrm{d}y = 0$,
- always provides a bound state*,
- for $D \to 0$ there exists just one bound state*.

* Simon B (1976) *Ann. Phys.* **97**, 279

The Interaction

The interaction in polar coordinates

$$V(r,\varphi) = D^2 \frac{3\sin^2\theta - 1}{2} \frac{r^2 - 2d^2}{(r^2+d^2)^{5/2}} - 3D^2 \frac{rd\sin(2\theta)\cos(\varphi)}{(r^2+d^2)^{5/2}} - \frac{3D^2}{2} \frac{r^2\cos^2\theta\cos(2\varphi)}{(r^2+d^2)^{5/2}} .$$

Interaction has three terms in $\cos(m\varphi)$ basis, except for three special polarization angles:

- $\theta = \pi/2$: just first term contributes, interaction is isotropic;
- $\theta_c = \arcsin\sqrt{1/3}$: first term vanishes;
- $\theta = 0$: second term vanishes.

Numerical procedure

Minimization of the functional

$$E[\Psi] = \frac{< \Psi|H|\Psi >}{< \Psi|\Psi >},$$

with the trial function

$$\Psi(\mathbf{r}) = \sum_{i=1}^{N} c_i e^{-(\mathbf{r}-\mathbf{s_i})^T A_i (\mathbf{r}-\mathbf{s_i})},$$

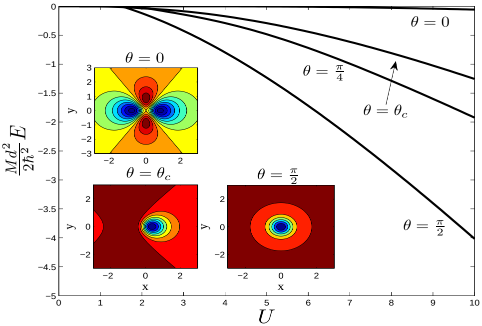
where c_i are the linear and $\mathbf{A_i}, \mathbf{s_i}$ are non-linear variational parameters.

Numerical procedure

- stochastically pick N Gaussians $\mathbf{A_i}, \mathbf{s_i}$
- determine c_i from the condition $\delta E = \sum \frac{\partial E}{\partial c_i} \delta c_i = 0$
- stochastically create new element $\mathbf{A_{new}}, \mathbf{s_{new}}$
- $E[(\mathbf{A_{new}}, \mathbf{s_{new}}), (\mathbf{A_2}, \mathbf{s_2}), ..., (\mathbf{A_N}, \mathbf{s_N})] <$ $E[(\mathbf{A_1}, \mathbf{s_1}), (\mathbf{A_2}, \mathbf{s_2}), ..., (\mathbf{A_N}, \mathbf{s_N})]$?, pick the best basis
- do as long as needed

Numerical solution

We get the energy E of the system for different polarization angles as function of the dimensionless strength of the interaction $U = MD^2/(\hbar^2 d)$.



Analytical approach

When $U \to 0$:

- $< r^2 > \to \infty$, so we have to enlarge sample basis;
- tail properties becomes very important, and the tail is not Gaussian.

Consequently, the convergence of the numerical method slows down. To get the energy we solve the Schrödinger equation

- decompose wave function

$$\Psi(r,\varphi) = \frac{1}{\sqrt{r}} \sum_{m=0}^{\infty} a_m \Phi_m(r) \cos(m\varphi), \; \lim_{r\to 0} \frac{\Phi_m(r)}{r^{m+1/2}} = 1,$$

- expand the coefficients, a_m, and the functions, Φ_m

$$\begin{aligned} a_m &= U a_m^{(1)} + U^2 a_m^{(2)} + \ldots, \\ \Phi_m &= \Phi_m^{(0)} + U\Phi_m^{(1)} + U^2 \Phi_m^{(2)} + \ldots, \end{aligned}$$

Analytical approach

- the potential in the basis $\cos(m\varphi)$ has just three terms so we assume that $a_m = 0$ for $m > 2$.
- we assume that the ground state wave function vanish at infinity

finally we get the energy*, which in the lowest order can be written as

$$E = -\frac{4\hbar^2}{Md^2}\exp(-2\gamma)\exp(-\frac{2}{U^2 A}) ,$$

$$A = \frac{1}{16}(3\sin^2\theta - 1)^2 + \frac{1}{8}\sin^2(2\theta) + \frac{1}{32}\cos^4\theta .$$

* Volosniev A G, Zinner N T, Fedorov D V, Jensen A S and Wunsch B (2011) *J. Phys. B:At. Mol.Opt.Phys.* **44**, 125301

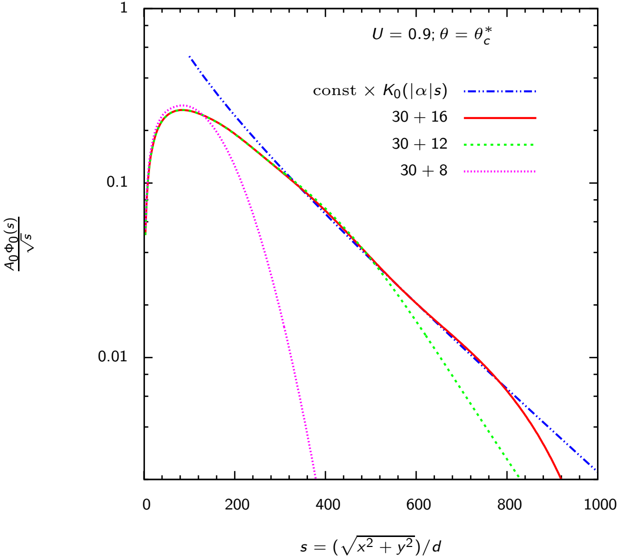
The wave function in the weakly-bound regime

The wave function in the weak binding regime *

- strongly delocalized ($< r^2 > \sim \exp(\mathrm{const}/U^2)$);
- has symmetric tail $\sim K_0(\alpha r/d)$, $\alpha = \frac{|Md^2E|}{\hbar^2}^{1/2}$.

* Volosniev A G, Fedorov D V, Jensen A S and Zinner N T (2011) *PRL* **106**, 250401

Stochastic evaluation of the tail of the wave function



Universality in the weakly-bound regime

As approximation we use just the tail to estimate some observables.

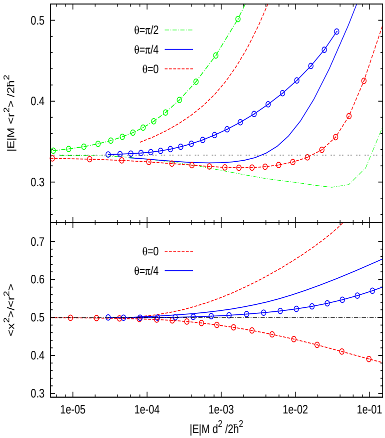
$$\Psi = \mathrm{const} \times K_0(\alpha r/d)$$

With this we get

- $< r^2 >= 2\hbar^2/(3M|E|)$
- $< x^2 > / < r^2 >= 1/2$

Numerical approach in the weakly-bound regime

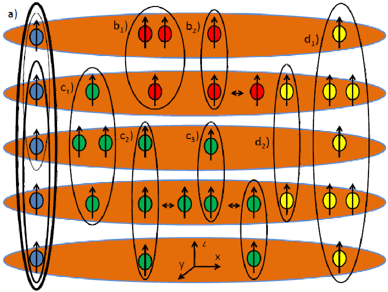
We compare results, obtained through the numerical minimization with results, given by this analytical approximation

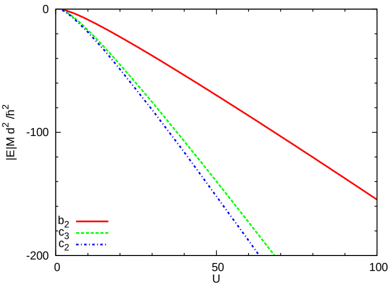


Two particles

- always bound
- energy increases as function of the polarization angle for $U \to 0$
- $E \sim -e^{-\frac{2}{U^2 A(\theta)}}$
- $\Psi(r) \sim K_0(\alpha r/d)$
- $E < r^2 >= \mathrm{const}$

Few body configurations with perpendicular polarization. Thresholds





Geometry of the interaction

- Perpendicular polarization;
- 2D

$$V(r,n) = \frac{r^2 - 2n^2d^2}{(r^2 + n^2d^2)^{5/2}}$$

where nd - distance in z direction

- $n = 0$: numerical problem

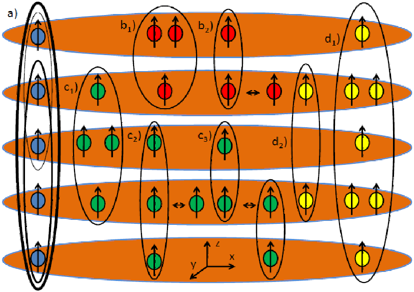
Regularization with $\Psi = \phi_{2D}\sqrt{\frac{1}{L\sqrt{\pi}}}e^{-\sum_i \frac{z_i^2}{2L^2}}$ *

$$V_r(r) = \frac{1}{2\sqrt{2}L^3}U\left(\frac{3}{2}, 1, \frac{r^2}{2L^2}\right),$$

* M.A. Baranov, H. Fehrmann, and M. Lewenstein, *PRL* **100**, 200402 (2008)

The System

- 2 particles $(\mathbf{r_1}, \mathbf{r_2})$ with dipole moment D_1 in one layer;
- 1 particle $(\mathbf{r_3})$ with dipole moment D_2 in another;
- all with the same mass M.



System b_1

The Shrödinger equation

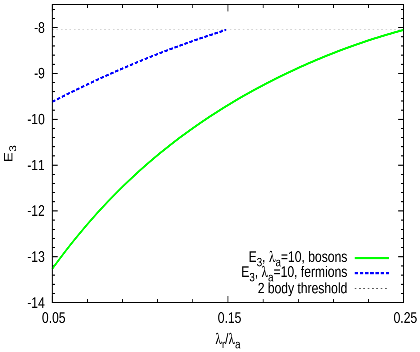
$$\Big(-\sum_{i=1}^{3} \frac{\hbar^2}{2M} \vec{\nabla}_i^2 + D_1 D_2 V(|\mathbf{r_1} - \mathbf{r_3}|, 1) + D_1 D_2 V(|\mathbf{r_2} - \mathbf{r_3}|, 1) + \\ + D_1 D_1 V_r(|\mathbf{r_1} - \mathbf{r_2}|) \Big) \phi_{2D} = \epsilon_3 \phi_{2D} \ ,$$

Two dimensionless parametres

- $\lambda_a = M \frac{D_1 D_2}{\hbar^2 d}$ - strength of the interaction with attractive core;
- $\lambda_r = M \frac{D_1 D_1}{\hbar^2 d}$ - strength of the repulsive interaction.

Energy dependence of the system of three dipoles

Using the same numerical procedure we get energy of the system $E_3 = \epsilon_i \frac{Md^2}{\hbar^2}$



In this example the system is unbound for $\lambda_r = \lambda_a$

Stability of the system for $\lambda_a = \lambda_r$

- the system is bound for sufficiently small ratio λ_r/λ_a
- the system is unbound for sufficiently big ratio λ_r/λ_a

For any given λ_a there exists a critical repulsive strength, $\lambda_r^{cr}(\lambda_a)$ such that $E_3(\lambda_r^{cr}(\lambda_a), \lambda_a) = E_2(\lambda_a)$

$$\lambda_r^{cr}(\lambda_a) = \frac{E_2(\lambda_a) - \langle \phi_{2D} | T + \lambda_a V_{13} + \lambda_a V_{23} | \phi_{2D} \rangle}{\langle \phi_{2D} | V_{12} | \phi_{2D} \rangle},$$

Stability of the system for $\lambda_a = \lambda_r$

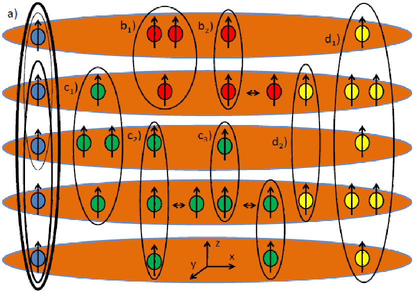
Proof of instability

- prove that $\frac{\partial \lambda_r^{cr}/\lambda_a}{\partial \lambda_a} \geq 0$ (direct calculation using that $\frac{\partial E}{\partial \lambda_a} < \phi_{2D}|\phi_{2D} > = < \phi_{2D}|\frac{\partial H}{\partial \lambda_a}|\phi_{2D} >$);
- show that for infinetely large value of λ_a the system is unstable (compare the minimum of the full potential for three body with the two body energy).

The system is unstable always for $\lambda_r > 0.375 \times \lambda_a$

The System

- 2 dipoles in one layer with dipole moment D_1;
- 1 dipole in layer above with dipole moment D_2;
- 1 dipole in layer below with dipole moment D_2.



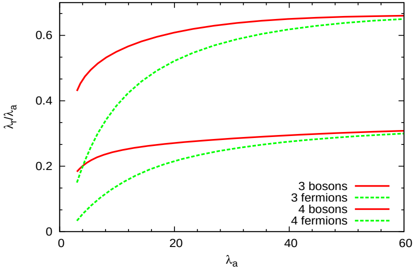
system c_1

Results

The same procedure shows that

- the system is unbound for $\lambda_a = \lambda_r$;
- system is more bound in a sense that $\lambda_r^{cr}(3) < \lambda_r^{cr}(4)$.

Numerical results for the critical strength *



* A. G. Volosniev, D. V. Fedorov, A. S. Jensen, N. T. Zinner arXiv:1109.4602v1 (2011)

Three and Four particles

- are always unbound for $\lambda_a = \lambda_r$;
- three particles are unbound for all $\lambda_r > 0.375\lambda_a$;
- four particles are unbound for all $\lambda_r > 0.75\lambda_a$.

Outlook

- more particles (7,10) can be bound;
- different polarization;
- external field;
- quasi 2D;
- ...