A diagrammatic approach to composite, rotating impurities.

G. Bighin and M. Lemeshko
Institute of Science and Technology Austria

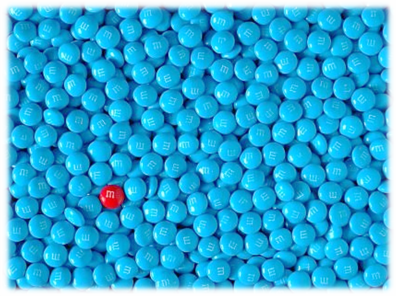
Trieste, July 4th, 2017

Impurity problems

Definition: one (or a few particles) interacting with a many-body environment.

How are the properties of the particle modified by the interaction?

Still $\mathcal{O}(10^{23})$ degrees of freedom...



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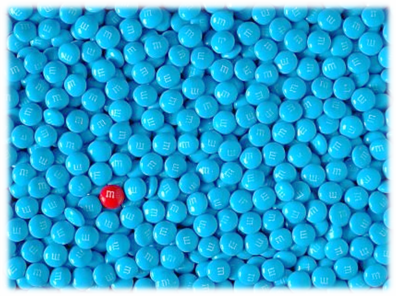
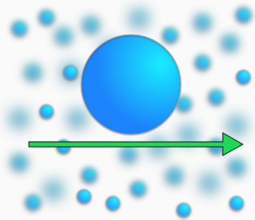
Quasiparticle description?



From impurities to quasiparticles

Structureless impurity: translational degrees of freedom/linear momentum exchange with the bath.

Most common cases: electron in a solid, atomic impurities in a BEC.



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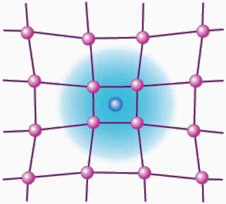

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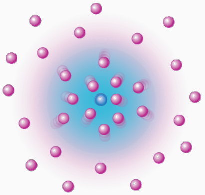

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Structureless impurity: translational degrees of momentum

This scenario can be formalized in terms of quasiparticles using the polaron.

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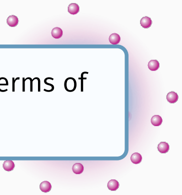

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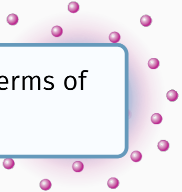

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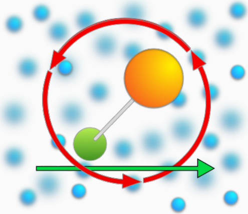

Composite impurity: translational *and internal* (i.e. rotational) degrees of freedom/linear and angular momentum exchange.

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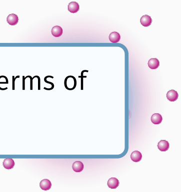

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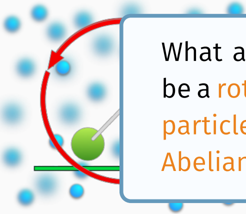

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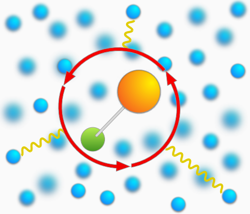
What about a rotating particle? Can there be a rotating analogue of the polaron quasi-particle? The main difficulty: the non-Abelian SO(3) algebra describing rotations.

The angulon

A composite impurity in a bosonic environment can be described by the angulon Hamiltonian[1,2,3,4] (angular momentum basis: $\mathbf{k} \to \{k, \lambda, \mu\}$):

$$\hat{H} = \underbrace{B\hat{\mathbf{J}}^2}_{\text{molecule}} + \underbrace{\sum_{k\lambda\mu} \omega_k \hat{b}^\dagger_{k\lambda\mu} \hat{b}_{k\lambda\mu}}_{\text{phonons}} + \underbrace{\sum_{k\lambda\mu} U_\lambda(k) \left[Y^*_{\lambda\mu}(\hat{\theta}, \hat{\phi}) \hat{b}^\dagger_{k\lambda\mu} + Y_{\lambda\mu}(\hat{\theta}, \hat{\phi}) \hat{b}_{k\lambda\mu} \right]}_{\text{molecule-phonon interaction}}$$

- Linear molecule.
- Derived rigorously for a molecule in a weakly-interacting BEC[1].
- Phenomenological model for a molecule in any kind of bosonic bath[3].



[1] R. Schmidt and M. Lemeshko, Phys. Rev. Lett. **114**, 203001 (2015).
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This talk: toy potential. Can be connected to real PESs[3].

- ...y for a molecule in a weakly-interacting BEC[1].
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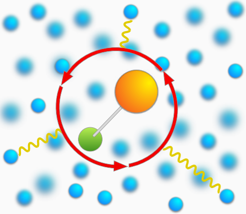

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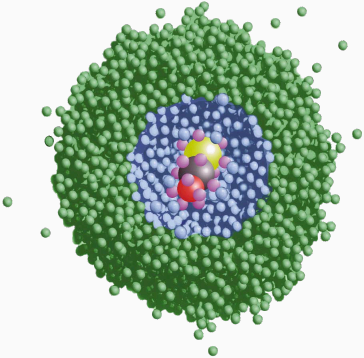
Composite impurities and where to find them

Strong motivation for the theoretical study of composite impurities comes from many different fields. Composite impurities are realized as:

- Molecules embedded into helium nanodroplets (rotational spectra, rotational constant renormalization).



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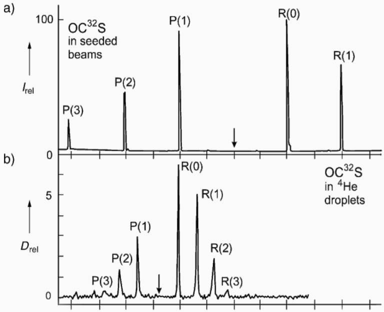

Gas phase

in ^{4}He

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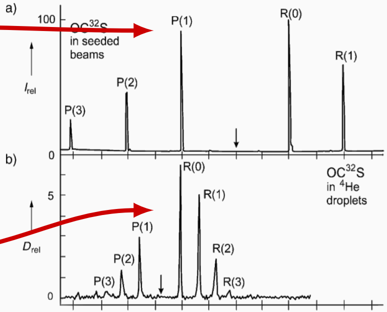
Rotational spectrum

Renormalizated lines (smaller effective B)



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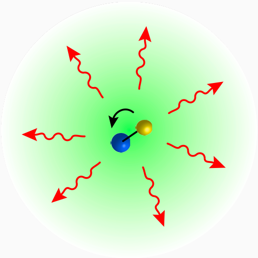

B. Midya, M. Tomza, R. Schmidt, and M. Lemeshko, Phys. Rev. A **94**, 041601(R) (2016).

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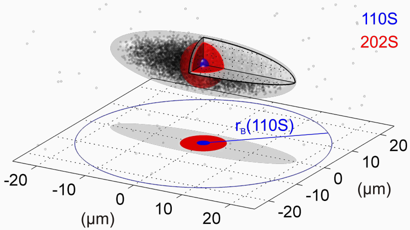

Pfau group, Nature **502**, 664 (2013).

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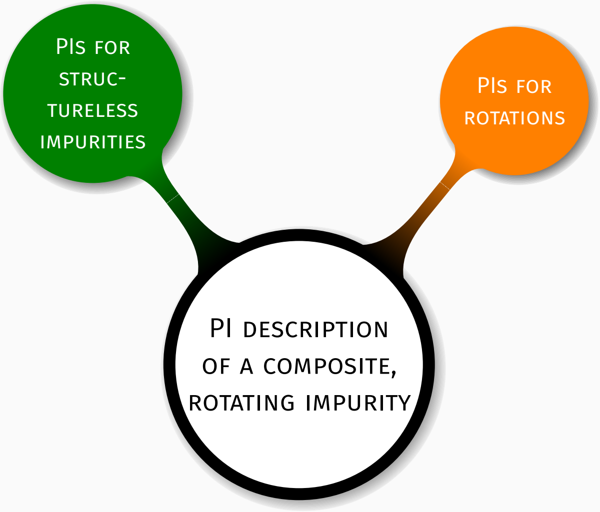
- Molecules embedded into helium nanodroplets (rotational spectra, rotational constant renormalization).
- Ultracold molecules and ions.
- Electronic excitations in Rydberg atoms.
- Angular momentum transfer from the electrons to a crystal lattice.

Path integral description for the angulon

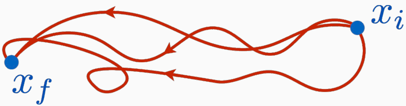


Main reference: GB and M. Lemeshko, arXiv:1704.02616

Path integral description for the angulon

The path integral in QM describes the transition amplitude between two states with a weighted average over all trajectories, S is the classical action.

$$G(x_i, x_f; t_f - t_i) = \langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}x \; e^{iS[x(t)]}$$



Path integral description for the angulon

The angulon's Green function is calculated in the same way. We need

- Molecular coordinates: two angles (θ, ϕ) describing the orientation of the molecule.
- An infinite number of harmonic oscillators $b_{k\lambda\mu}$ to describe the bosonic bath.

$$G(\theta_i, \phi_i \to \theta_f, \phi_f; T) = \int \mathcal{D}\theta \mathcal{D}\phi \prod_{k\lambda\mu} \mathcal{D}b_{k\lambda\mu}\, e^{\mathrm{i}(S_{\text{mol}} + S_{\text{bos}} + S_{\text{mol-bos}})}$$

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Derived from the Hamiltonian

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Critically the environment $(b_{k\lambda\mu})$ can be integrated out exactly

$$G(\theta_i, \phi_i \to \theta_f, \phi_f; T) = \int \mathcal{D}\theta \mathcal{D}\phi \, e^{\mathrm{i}S_{\text{eff}}[\theta(t), \phi(t)]}$$

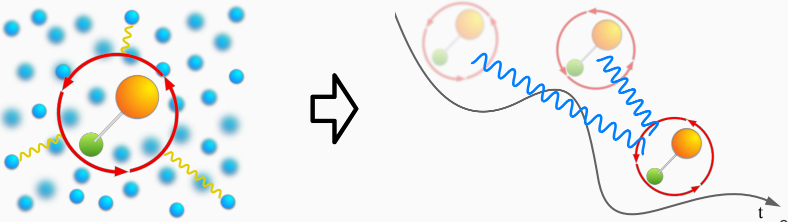
and included in an effective action S_{eff}.

Path integral description for the angulon

A closer look at the effective action:

$$S_{\text{eff}} = \underbrace{\int_0^T \mathrm{d}t\, B\mathbf{J}^2}_{S_0} + \underbrace{\frac{\mathrm{i}}{2}\int_0^T \mathrm{d}t \int_0^T \mathrm{d}s \sum_\lambda P_\lambda(\cos\gamma(t,s))\mathcal{M}_\lambda(|t-s|)}_{S_{\text{int}}}$$

- A term describing a free molecule $\sim B\mathbf{J}^2$.
- A memory term accounting for the many-body environment, a function of the angle $\gamma(t,s)$ between the angulon position at different times.



Path integral description for the angulon

A closer look at the effective action:

Legendre polynomials → P_λ

Memory kernel → $\mathcal{M}_\lambda$

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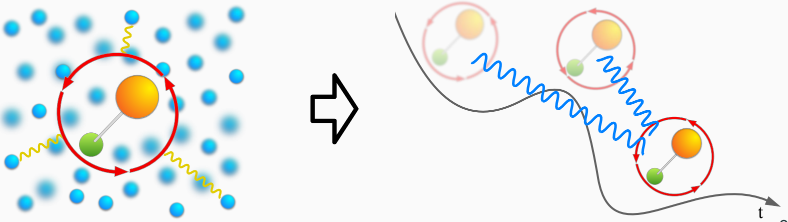

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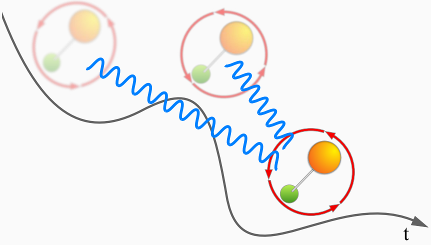


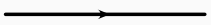
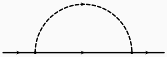
- The many-body problem is reformulated in terms of a self-interacting free molecule.
- Time-non-local interaction (cf. Caldeira-Leggett, polaron, more generally: open quantum systems)
- The interaction term is very difficult to treat: it encodes exactly the many-body nature of the problem.

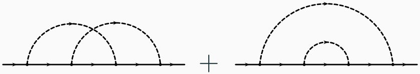
Diagrammatic theory of angular momentum in a many-body bath

We treat the interaction as a perturbation

$$G = \int \mathcal{D}\theta\mathcal{D}\phi\, e^{iS_0+iS_{int}} = \int \mathcal{D}\theta\mathcal{D}\phi\, e^{iS_0}\left(1+iS_{int}-\frac{1}{2}S_{int}^2+\dots\right) = G^{(0)}+G^{(1)}+G^{(2)}+\dots$$

The result can be interpreted as a diagrammatic expansion (solid lines represent a free rotor, dashed lines are the interaction)

- $G^{(0)}(\theta_i,\phi_i \to \theta_f,\phi_f;T)$ is the Green's function for a free rotor 
- $G^{(1)}(\theta_i,\phi_i \to \theta_f,\phi_f;T)$ is the one-loop correction 
- $G^{(2)}(\theta_i,\phi_i \to \theta_f,\phi_f;T)$ is the two-loop correction



- and so on...

Angulon spectral function

Let us use the theory! The plan is simple:

1. Self-energy (Σ)
2. Dyson equation to obtain the angulon Green's function (G)
3. Spectral function ($\mathcal{A}$)

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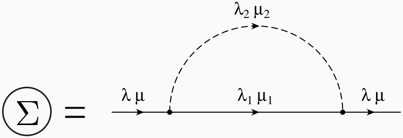
First order:



Equivalent to a simple, 1-phonon variational Ansatz (cf. Chevy Ansatz for the polaron)

$$|\psi\rangle = Z_{LM}^{1/2} |0\rangle\ |LM\rangle + \sum_{\substack{k\lambda\mu \\ jm}} \beta_{k\lambda j} C_{jm,\lambda\mu}^{LM} b_{k\lambda\mu}^{\dagger} |0\rangle\ |jm\rangle$$

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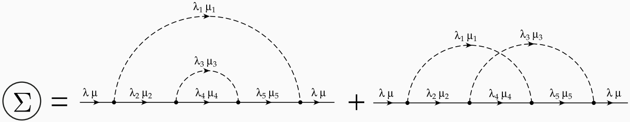
Second order:



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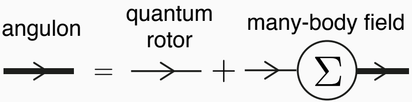
Dyson equation



Angulon spectral function

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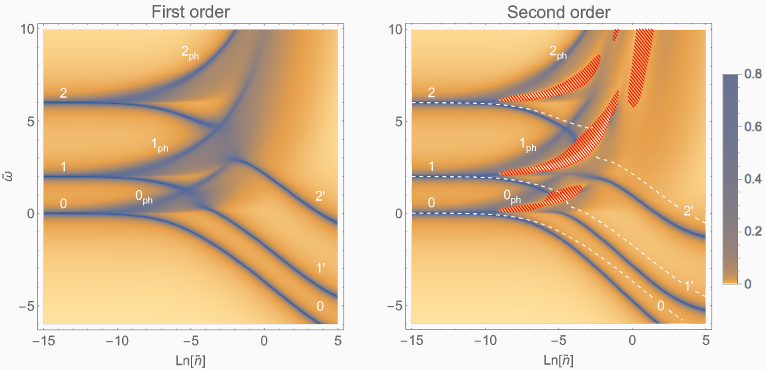
Finally the spectral function allows for a study the whole excitation spectrum of the system:

$$\mathcal{A}_\lambda(E) = -\frac{1}{\pi} \operatorname{Im} G_\lambda(E + \mathrm{i}0^+)$$

Angulon spectral function

Angulon spectral function as a function of the density:



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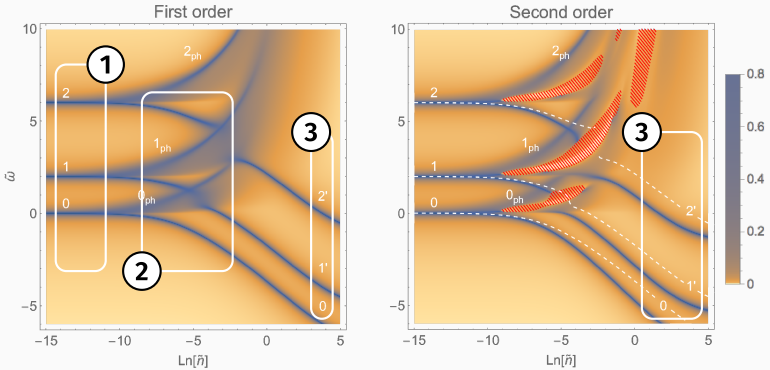
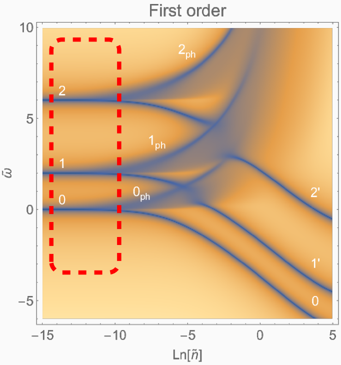


Key features:

1. Low density
2. Intermediate instability
3. High density

Angulon spectral function: low density

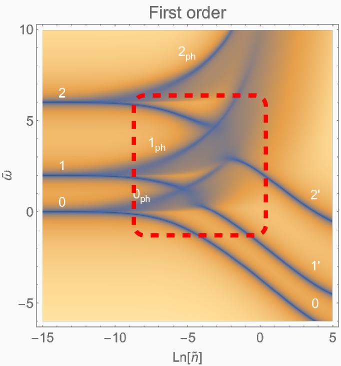


Density range: from ultra-cold atoms to superfluid helium.

Low density: free rotor spectrum, $E \sim L(L+1)$.

Many-body-induced fine structure: upper phonon wing (one phonon with $\lambda = 0$, isotropic interaction).

Angulon spectral function: instability

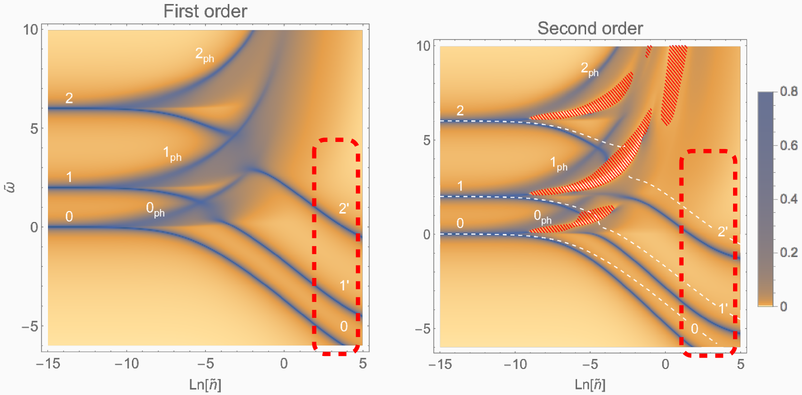


Intermediate region: angulon instability.

Corresponding to the emission of a phonon with $\lambda = 1$ (due to anisotropic interaction).

Experimental observation: I. N. Cherepanov, M. Lemeshko, "*Fingerprints of angulon instabilities in the spectra of matrix-isolated molecules*", arXiv:1705.09220.

Angulon spectral function: high density



High density: the two-loop corrections start to be relevant.

Conclusions

- The problem of angular momentum redistribution in a many-body environment has been treated through the path integral formalism and reformulated in terms of diagrams.
- It allows for a simple, compact derivation of angulon properties, including higher order terms.
- Future perspectives:
    - Dynamics.
    - Diagrammatic Monte Carlo.

Thank you for your attention.

Der Wissenschaftsfonds.

This work was supported by the Austrian Science Fund (FWF), project Nr. P29902-N27.

Backup slide # 1

Backup slide # 2

Backup slide # 3