Diagrammatic Monte Carlo approach to angular momentum in quantum many-body systems

Main reference: Phys. Rev. Lett. **121**, 165301 (2018).

G. Bighin[1], T.V. Tscherbul[2] and M. Lemeshko[1]

[1]Institute of Science and Technology Austria

[2]University of Nevada, Reno

DPG Frühjahrstagung, Rostock, March 15th, 2019

Quantum impurities

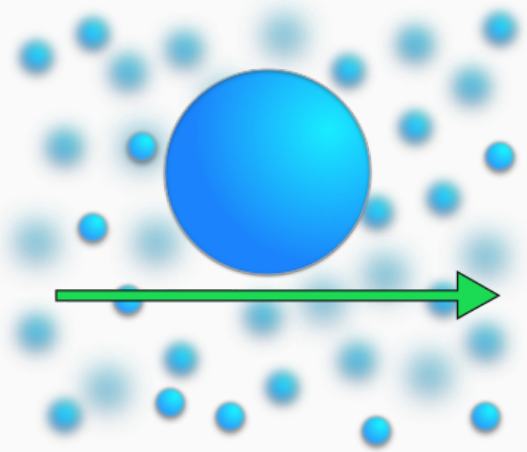
One particle (or a few particles) interacting with a many-body environment.

Quantum impurities

One particle (or a few particles) interacting with a many-body environment.

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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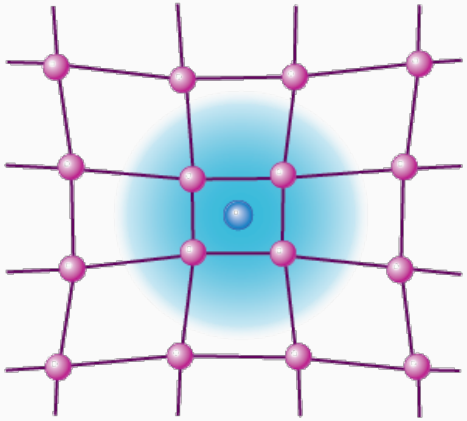

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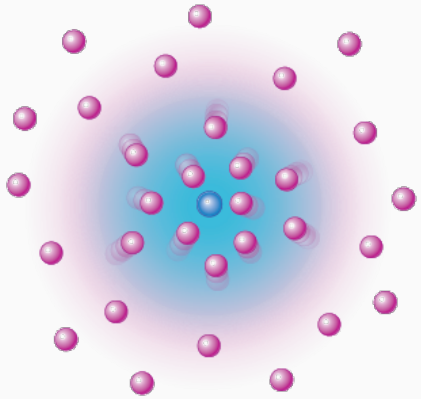

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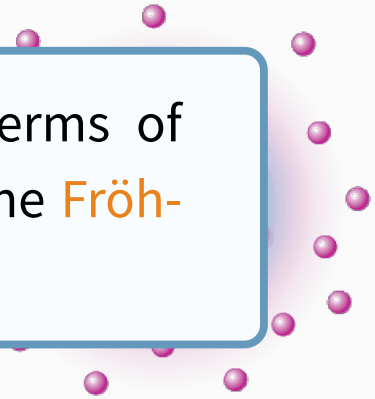
This scenario can be formalized in terms of quasiparticles using the polaron and the Fröhlich Hamiltonian.



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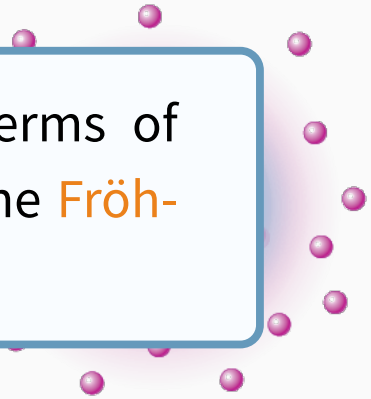

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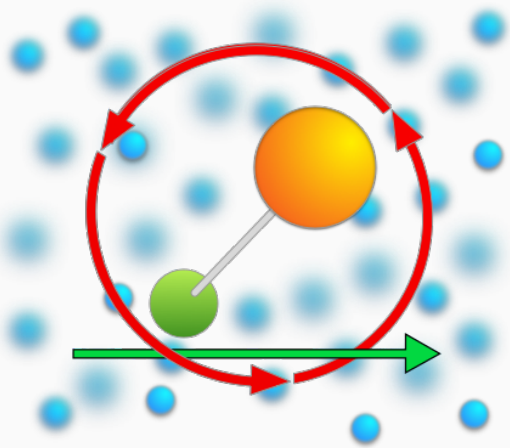

Composite impurity, e.g. a diatomic molecule: translational *and rotational* degrees of freedom/linear and angular momentum exchange.

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Molecules embedded into helium nanodroplets.

Plenary talk: Henrik Stapelfeldt.

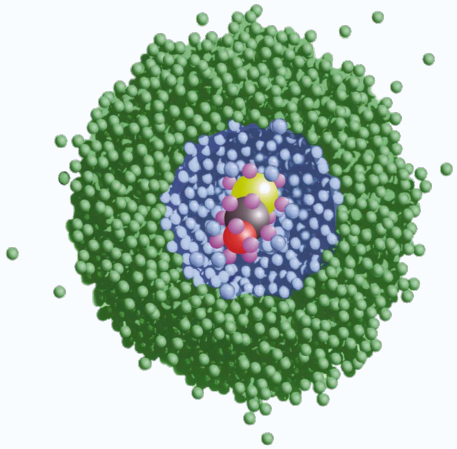

Image from: J. P. Toennies and A. F. Vilesov, Angew. Chem. Int. Ed. **43**, 2622 (2004).

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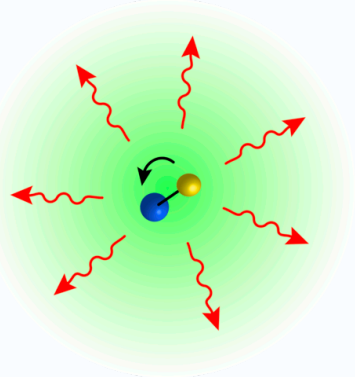
Ultracold molecules and ions.



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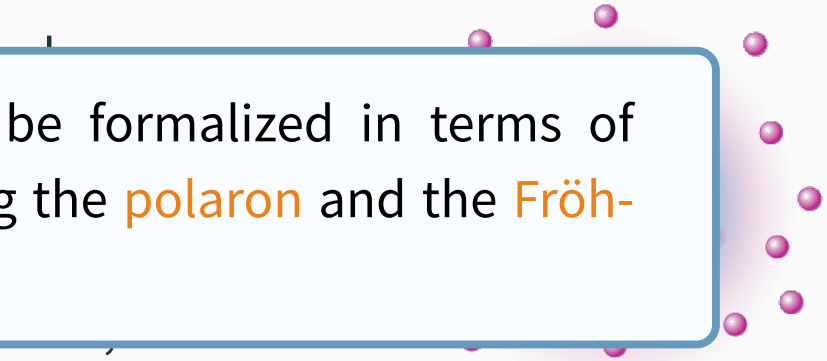
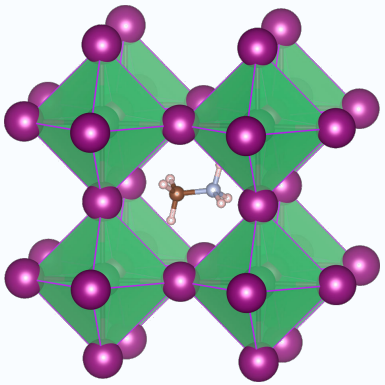


This scenario can be formalized in terms of quasiparticles using the polaron and the Fröhlich Hamiltonian.

Rotating molecules inside a 'cage' in perovskites.



T. Chen et al., PNAS **114**, 7519 (2017).
J. Lahnsteiner et al., Phys. Rev. B **94**, 214114 (2016).
Image from: C. Eames et al, Nat. Comm. **6**, 7497 (2015).

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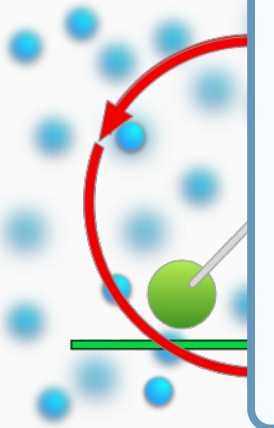

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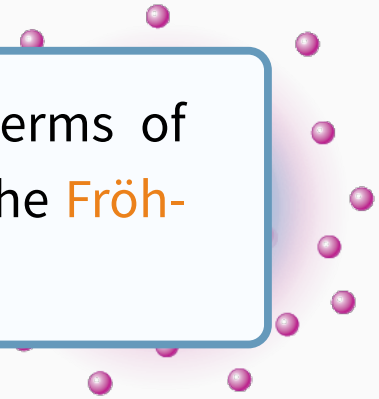

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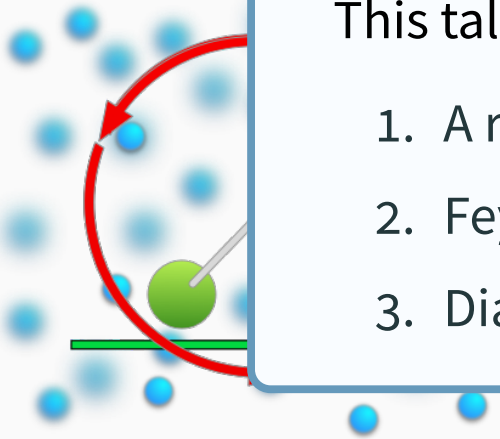

This talk:

1. A rotating impurity as a quasiparticle.
2. Feynman diagrams.
3. Diagrammatic Monte Carlo.

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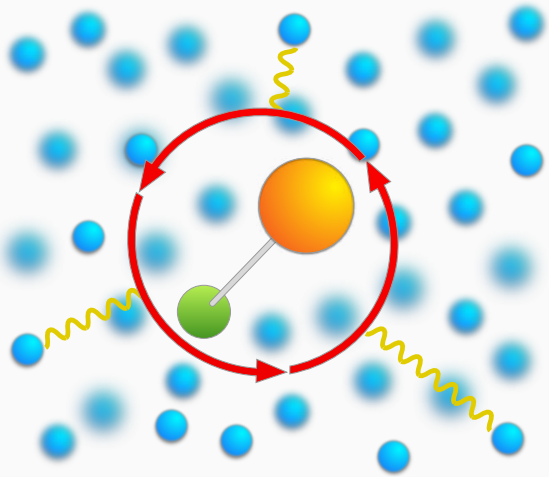
The angulon

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

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

- 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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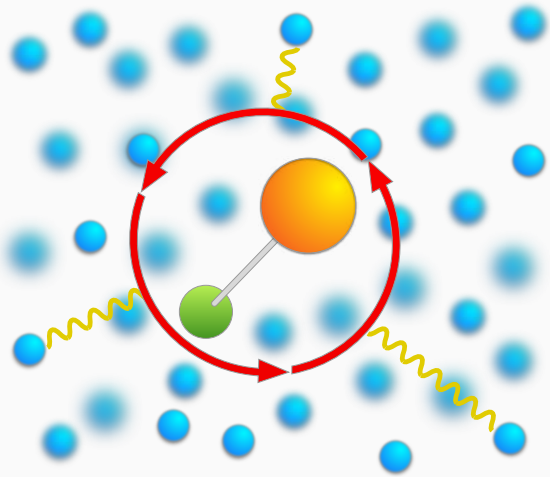
$\lambda = 0$: spherically symmetric part.
$\lambda \geq 1$ anisotropic part.

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

- Phenomenological model for a molecule in any kind of bosonic bath[3].



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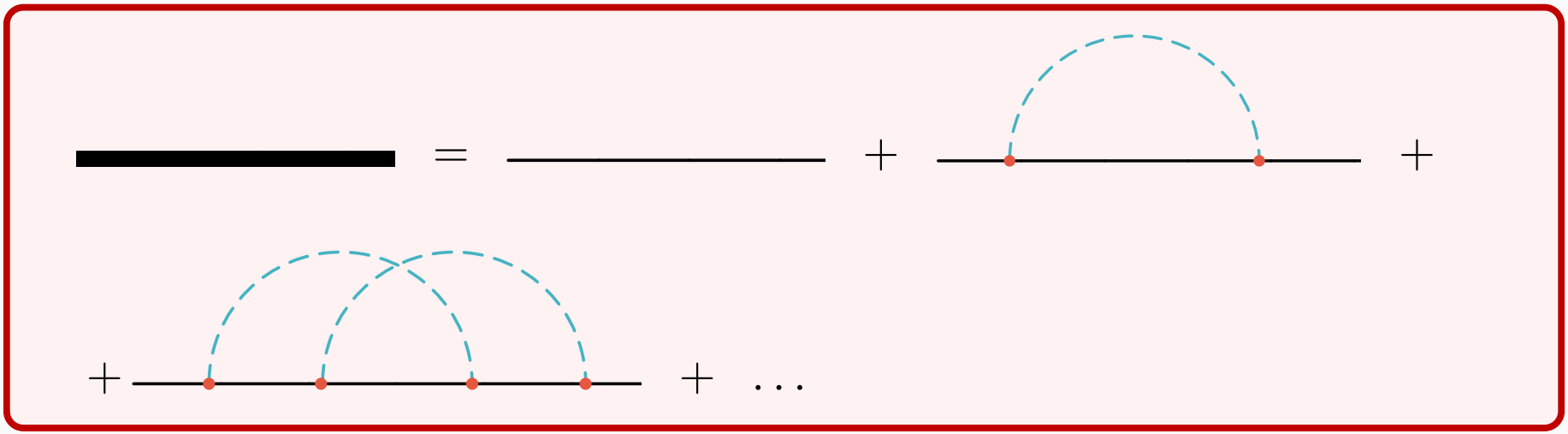
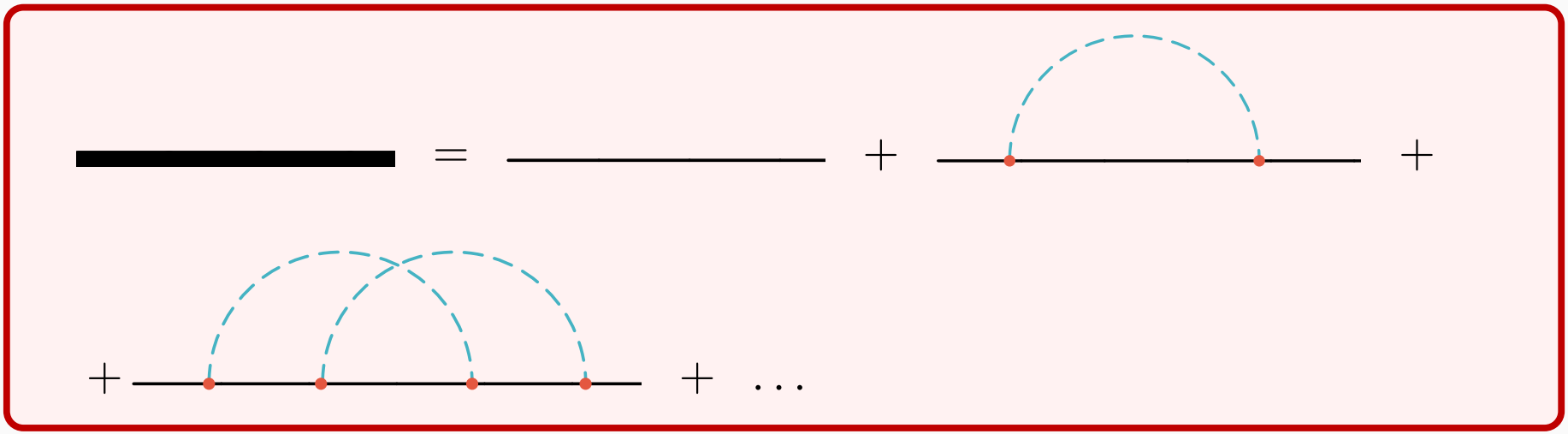
Feynman diagrams



How do we describe **molecular rotations** with Feynman diagrams? How does **angular momentum** enter this picture?

GB and M. Lemeshko, Phys. Rev. B **96**, 419 (2017).

Feynman diagrams



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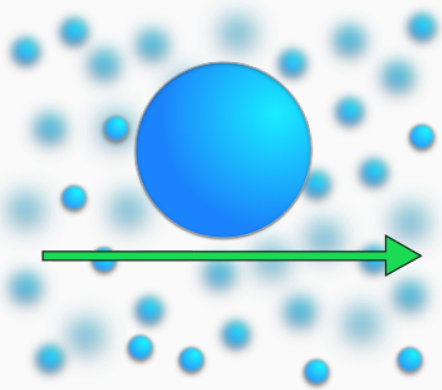
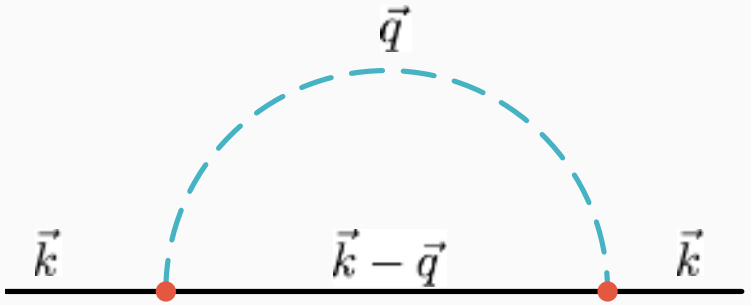
Fröhlich polaron





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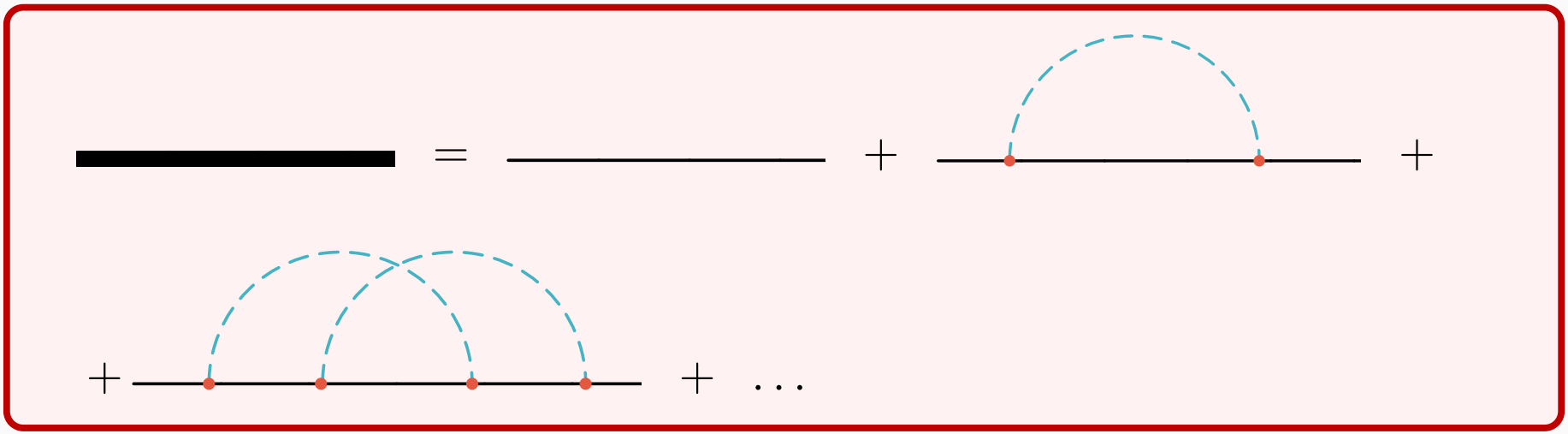

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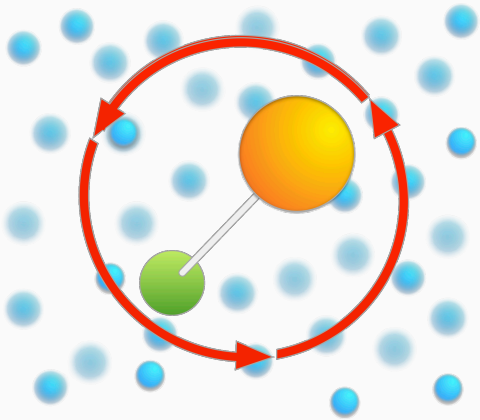

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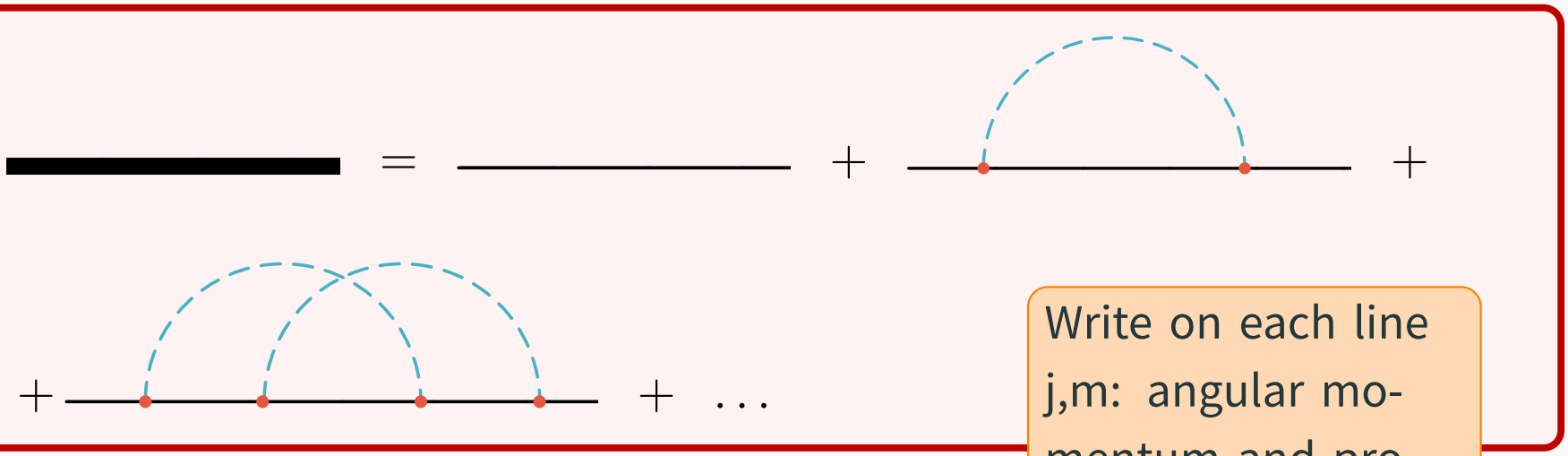

Write on each line j,m: angular momentum and projection along z axis.

How do we describe **molecular rotations** with Feynma s **angular momentum** enter this picture?

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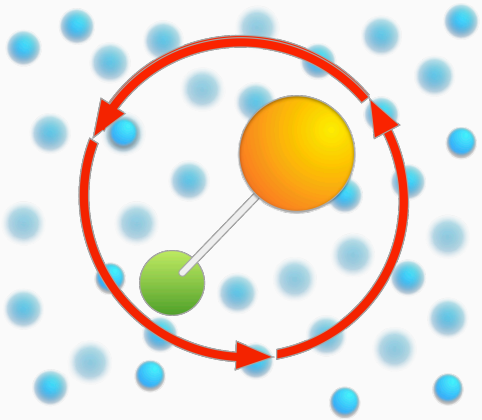

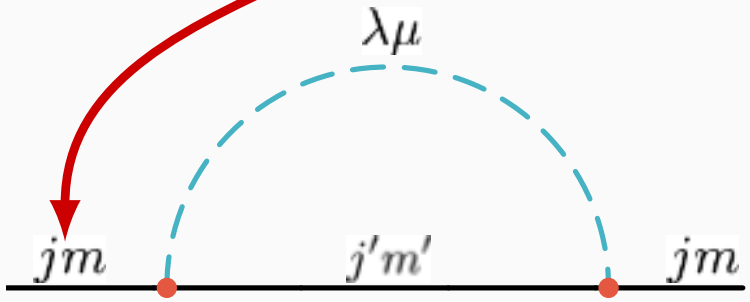

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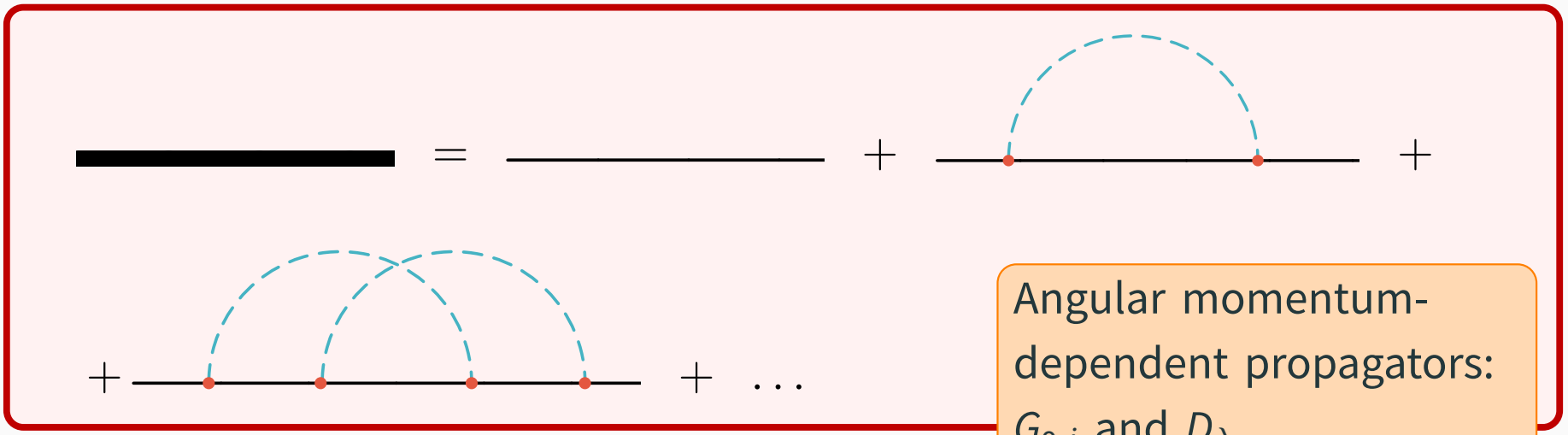

Angular momentum-dependent propagators: $G_{0,j}$ and D_λ

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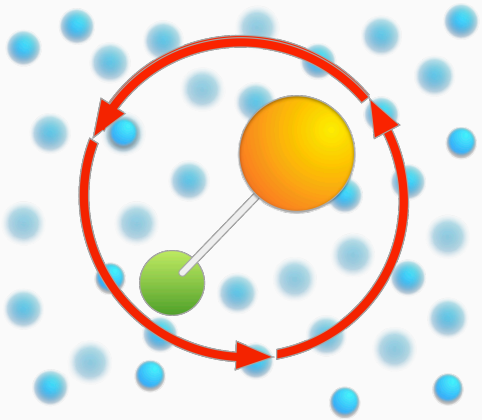

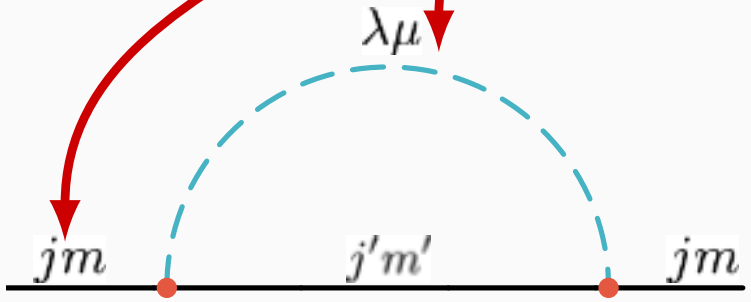

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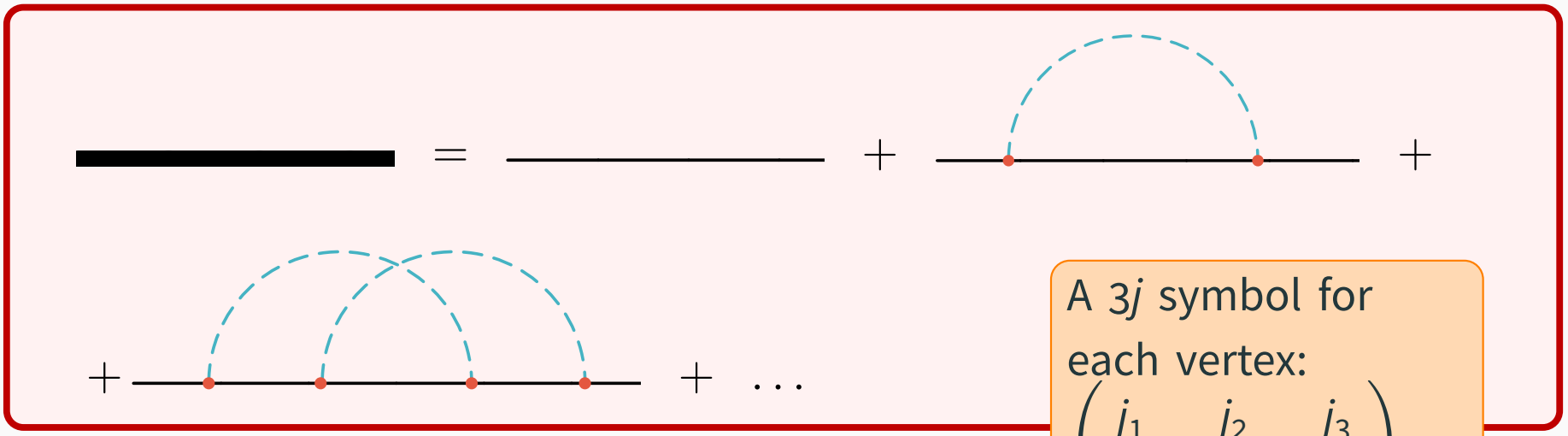

A $3j$ symbol for each vertex:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

How do we describe **molecular rotations** with Feynma s **angular momentum** enter this picture?

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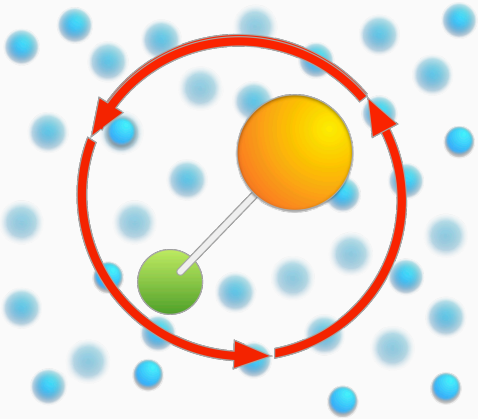

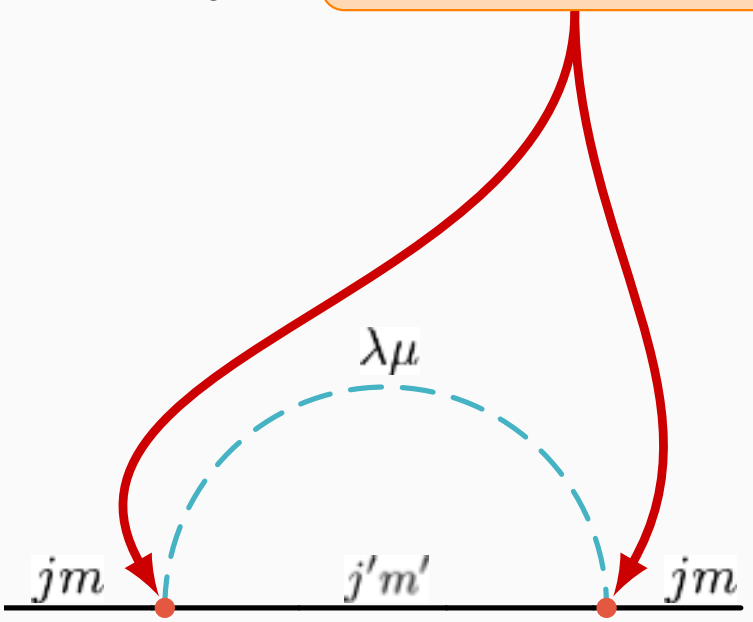

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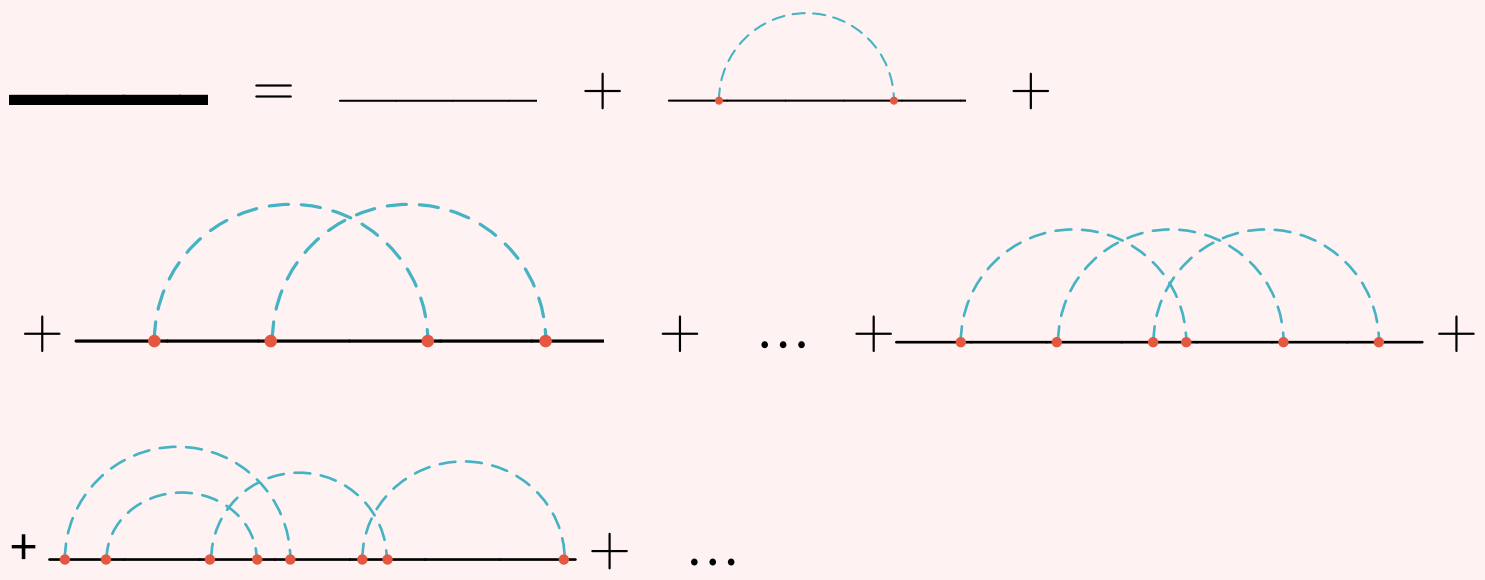
Diagrammatic Monte Carlo

Numerical technique for sampling over all Feynman diagrams[1].



Up to now: structureless particles (Fröhlich polaron, Holstein polaron), or particles with a very simple internal structure (e.g. spin $1/2$).

This talk: molecules[2].

[1] N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. Lett. **81**, 2514 (1998).
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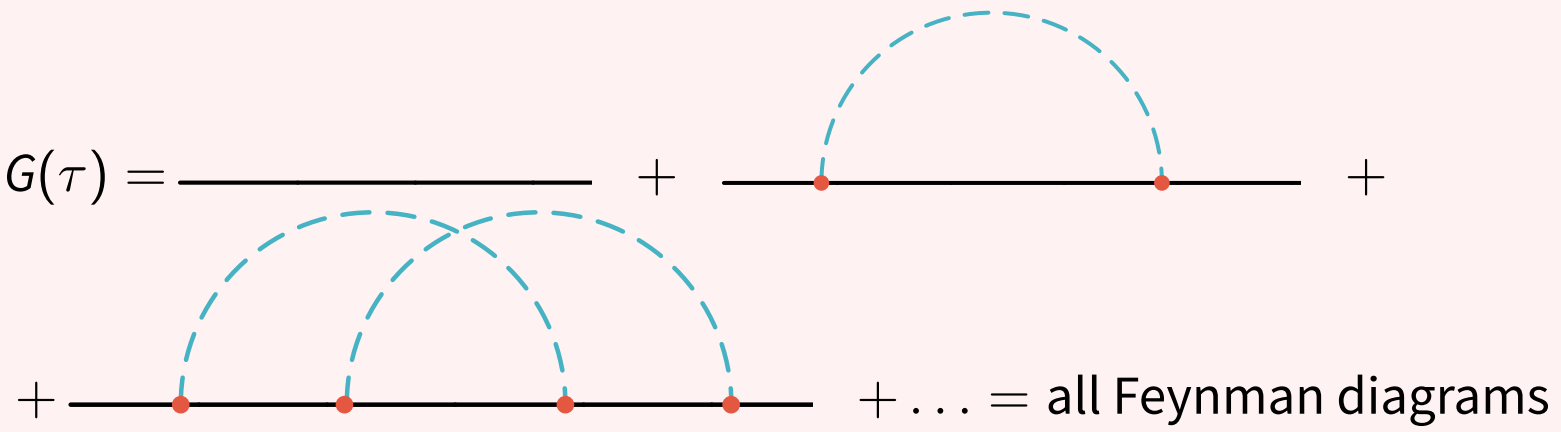
Diagrammatic Monte Carlo for a quantum impurity

Green's function



DiagMC idea: set up a stochastic process sampling among all diagrams[1].

Configuration space: diagram topology, phonons internal variables, times, etc... Number of variables varies with the topology!

How: ergodicity, detailed balance $w_1 p(1 \to 2) = w_2 p(2 \to 1)$

Result: each configuration is visited with probability $\propto$ its weight.

[1] N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. Lett. **81**, 2514 (1998).

Updates

Usually (e.g. Fröhich polaron) three updates are enough to span the whole configuration space:

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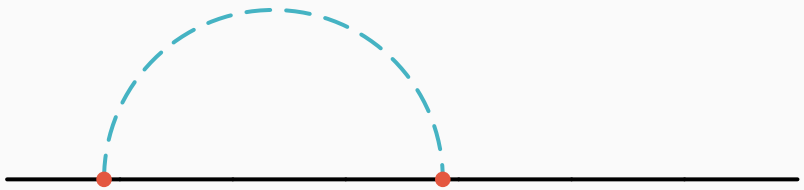

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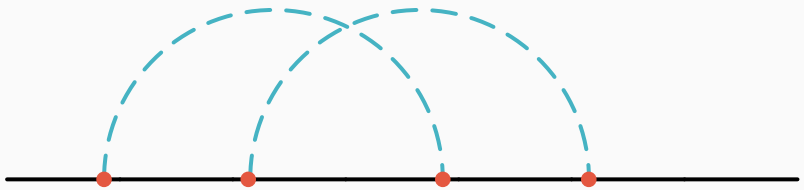

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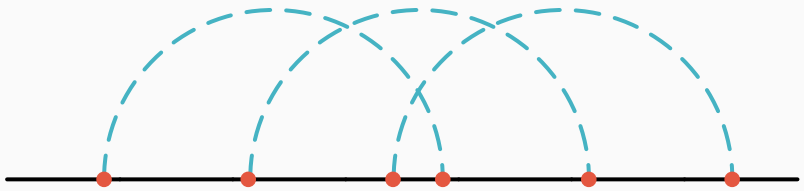

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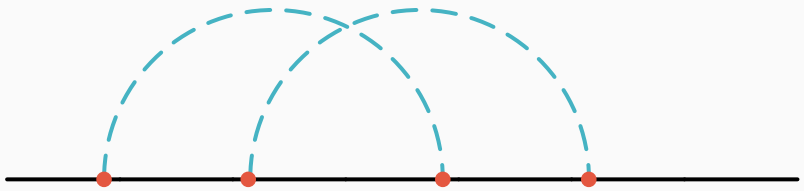

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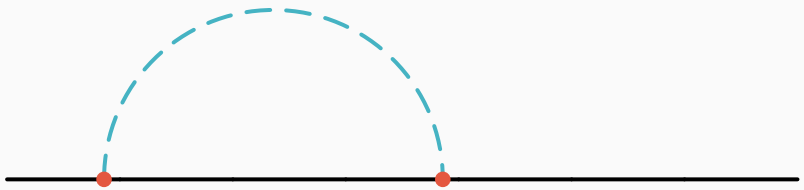

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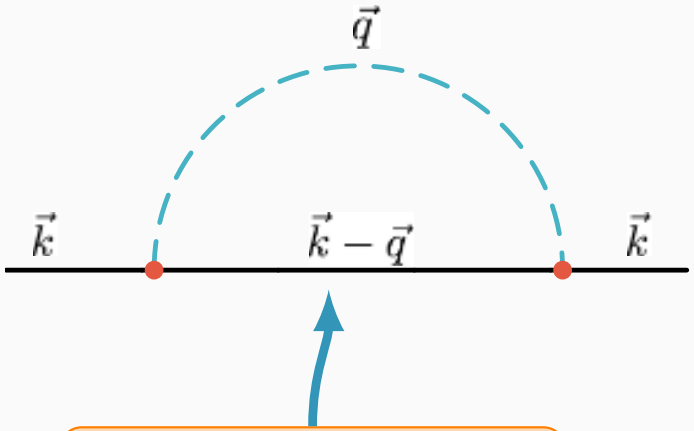
Are these three updates enough for a molecular rotations?

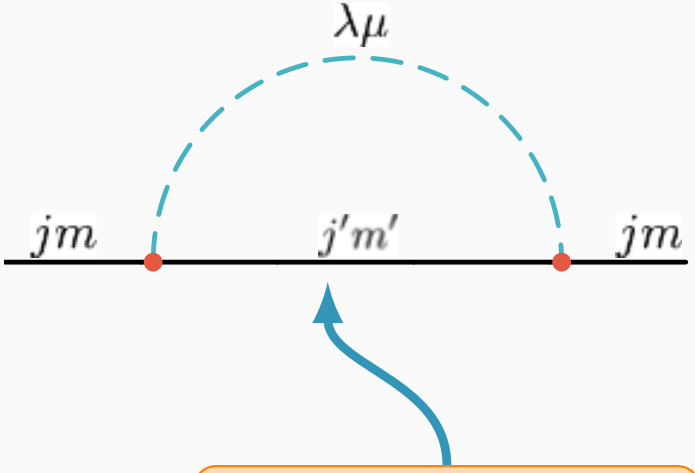
Are three updates enough for molecular rotations?

Moving particle: linear momentum circulating on lines.



$\vec{k}$ and $\vec{q}$ fully determine $\vec{k}-\vec{q}$

Rotating particle: angular momentum circulating on lines.



j and λ can sum in many different ways: $|j-\lambda|, \ldots j+\lambda$

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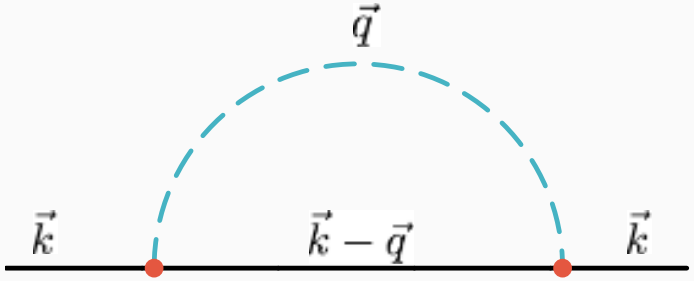

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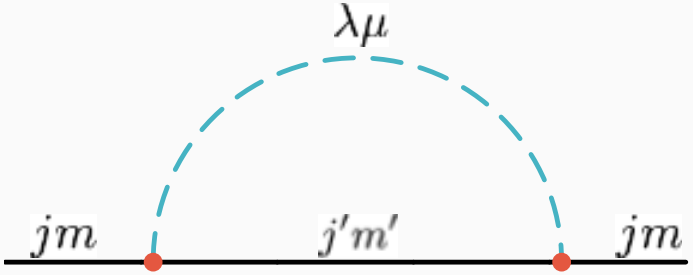

At higher orders the problem gets worse!

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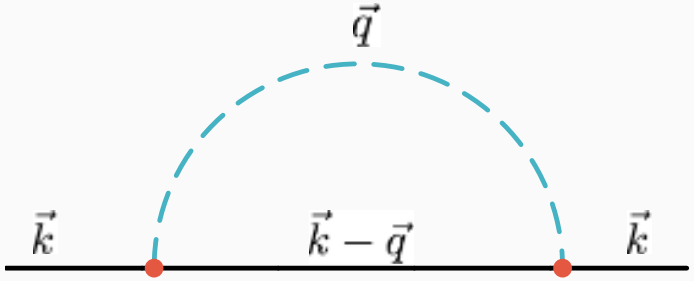

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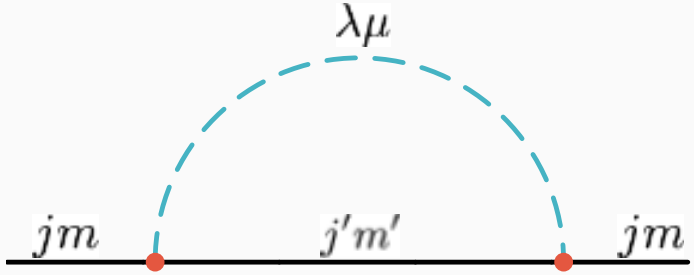
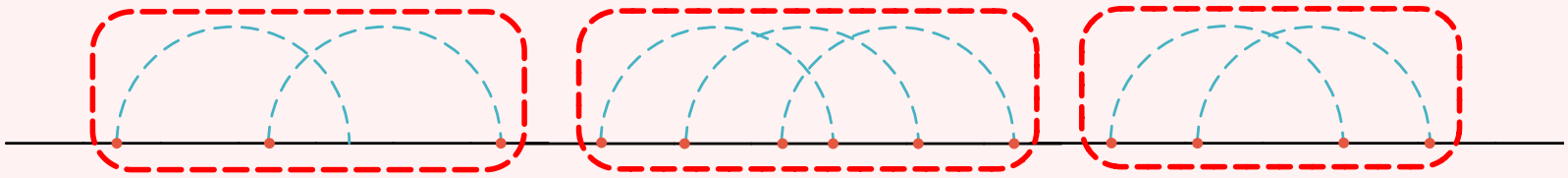


At higher orders the problem gets worse!

The configuration space is bigger! Another update is needed to cover it.



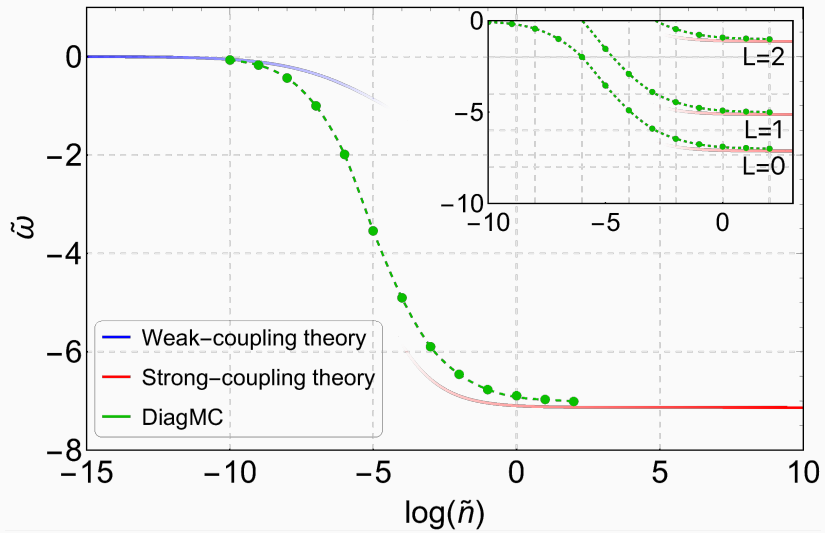
Shuffle update: select one 1-particle-irreducible component, shuffle the momenta couplings to another allowed configuration.

Results

The ground-state energy of the angulon Hamiltonian obtained using DiagMC[1] as a function of the dimensionless bath density, $\tilde{n}$, in comparison with the weak-coupling theory[2] and the strong-coupling theory[3].

The energy is obtained by fitting the long-imaginary-time behaviour of G_j with $G_j(\tau) = Z_j \exp(-E_j\,\tau)$.

Inset: energy of the $L = 0, 1, 2$ states.



[1] GB, T.V. Tscherbul, M. Lemeshko, Phys. Rev. Lett. **121**, 165301 (2018).
[2] R. Schmidt and M. Lemeshko, Phys. Rev. Lett. **114**, 203001 (2015).
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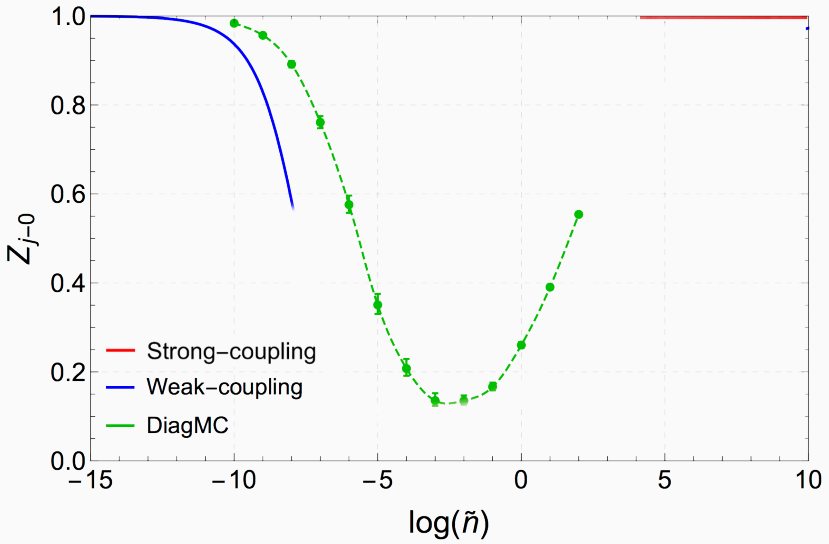

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Conclusions

- A numerically-exact approach to quantum many-body systems involving coupled angular momenta.
- Works in continuous time and in the thermodynamic limit: no finite-size effects or systematic errors.
- Future perspectives:
  - More advanced schemes (e.g. Σ, bold).
  - More realistic systems, such as molecules and molecular clusters in superfluid helium nanodroplets.
  - Hybridisation of translational and rotational motion.
  - Real-time dynamics?

Thank you for your attention.

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Institute of Science and Technology

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Der Wissenschaftsfonds.

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Backup slide # 1

Free rotor propagator

$$G_{0,\lambda}(E) = \frac{1}{E - B\lambda(\lambda+1) + \mathrm{i}\delta}$$

Interaction propagator

$$\chi_\lambda(E) = \sum_k \frac{|U_\lambda(k)|^2}{E - \omega_k + \mathrm{i}\delta}$$

Backup slide # 2

Backup slide # 3