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

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Workshop on *"Polarons in the 21st century"*, ESI, Vienna, December 10th, 2019

Rotations in a many-body environment

Rotations in a many-body environment and rotating impurities:

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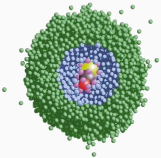
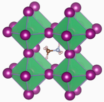
Molecular physics/chemistry: molecules embedded into helium nanodroplets.



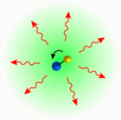
J. P. Toennies and A. F. Vilesov, Angew. Chem. Int. Ed. **43**, 2622 (2004).

Condensed matter: rotating molecules inside a 'cage' in perovskites.



C. Eames et al, Nat. Comm. **6**, 7497 (2015).

Ultracold matter: molecules and ions in a BEC.



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

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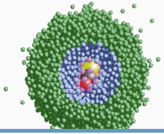


d. **43**, 2622 (2004).

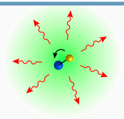
Condensed
molecules in
perovskites.

m. **6**, 7497 (2015).

Questions:

- How to describe rotations in a many-body environment in terms of Feynman diagrams?
- How to sample these diagrams at all orders using Diagrammatic Monte Carlo?

Ultracold matter: molecules and ions in a BEC.



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Feynman diagrams

The angulon Hamiltonian:

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

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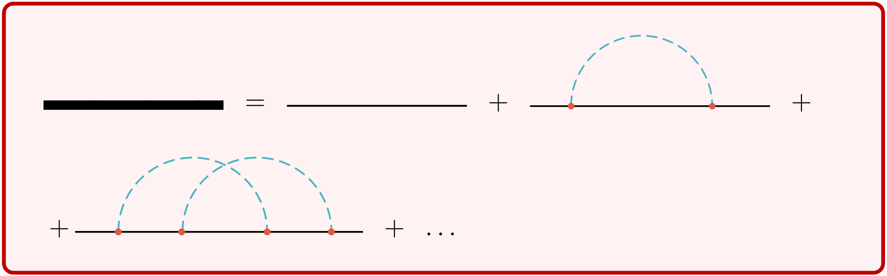
Feynman diagrams and perturbation theory:



How does **angular momentum** enter this picture?

Feynman diagrams

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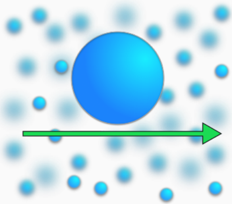
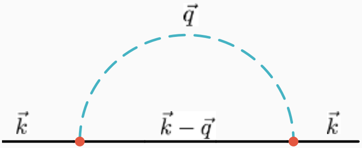
Feynman diagrams and perturbation theory:

Fröhlich polaron





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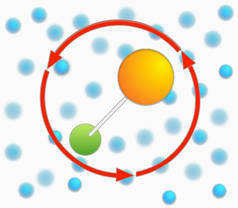
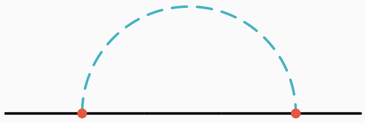
Feynman diagrams and perturbation theory:

Angulon





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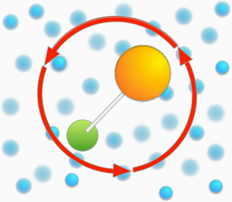
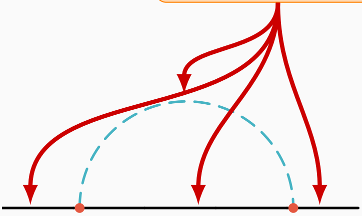


How does **angular momentum** enter here?



Feynman rules

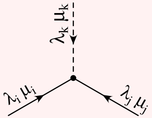
Each free propagator

$\sum_{\lambda_i \mu_i} (-1)^{\mu_i} G_{0,\lambda_i}$

Each phonon propagator

$\sum_{\lambda_i \mu_i} (-1)^{\mu_i} D_{\lambda_i}$

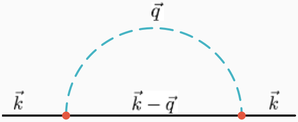
Each vertex



$(-1)^{\lambda_i} \langle \lambda_i || Y^{(\lambda_j)} || \lambda_k \rangle \begin{pmatrix} \lambda_i & \lambda_j & \lambda_k \\ \mu_i & \mu_j & \mu_k \end{pmatrix}$

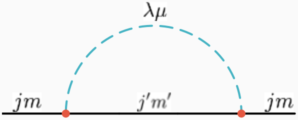
GB and M. Lemeshko, Phys. Rev. B **96**, 419 (2017).

Usually momentum conservation is enforced by an appropriate labeling.



Not the same for angular momentum, j and λ couple to $|j - \lambda|, \ldots, j + \lambda$.

$\sum_{j'm'}$



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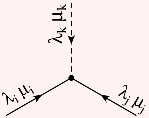

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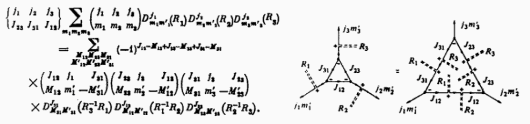
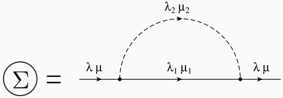
Diagrammatic theory of angular momentum (developed in the context of theoretical atomic spectroscopy)

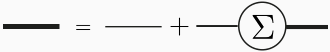


from D. A. Varshalovich, A. N. Moskalev, V. K. Khersonskii, *"Quantum Theory of Angular Momentum"*.

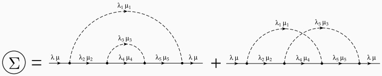
Self-energy (first order)

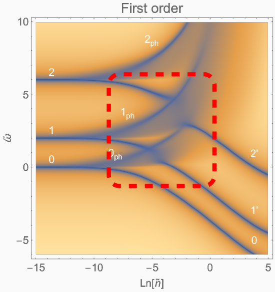


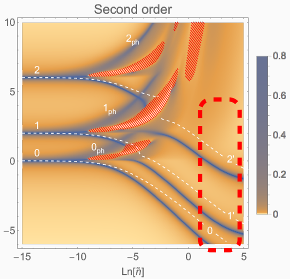
Dyson equation



Self-energy (second order)







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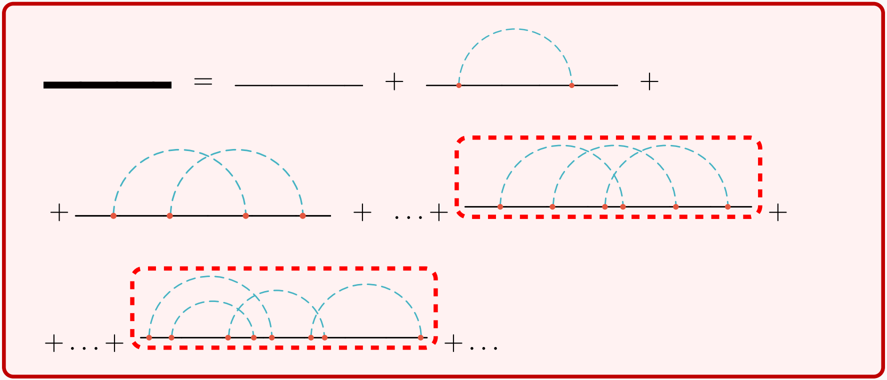
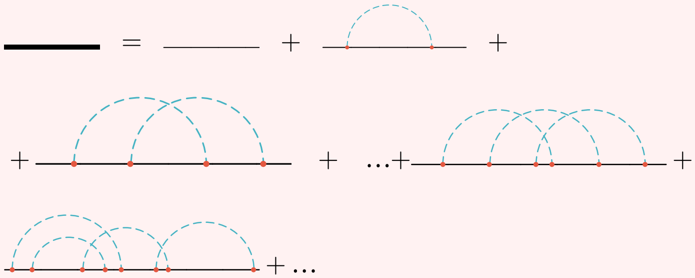
What about higher orders?



At order n: n integrals, and higher angular momentum couplings (3n-j symbols).

Diagrammatic Monte Carlo

Numerical technique for summing all Feynman diagrams[1].



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

Molecules[2]? Connecting DiagMC and molecular simulations!

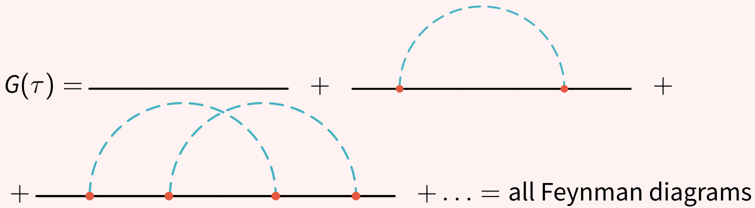
[1] N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. Lett. **81**, 2514 (1998).

[2] GB, T.V. Tscherbul, M. Lemeshko, Phys. Rev. Lett. **121**, 165301 (2018).

Diagrammatic Monte Carlo

Hamiltonian for an impurity problem: $\hat{H} = \hat{H}_{\text{imp}} + \hat{H}_{\text{bath}} + \hat{H}_{\text{int}}$

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).

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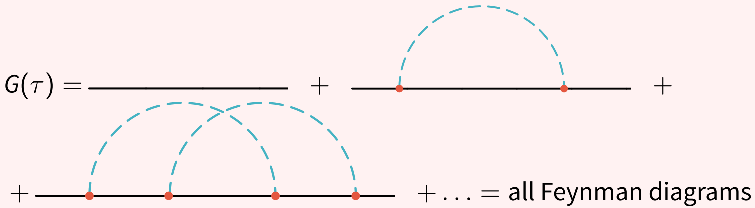

DiagMC idea ... ms[1].

Configuratio ... , times, etc... Numbe

How: ergodi

Result: each

A Monte Carlo technique that works in second quantization.

Works in continuous time and in the thermodynamic limit: no finite-size effects or systematic errors.

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

Updates

We need updates spanning the whole configuration space:

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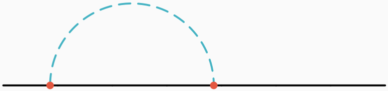

Add update: a new arc is added to a diagram.

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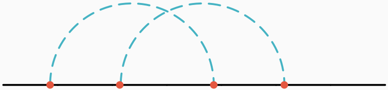

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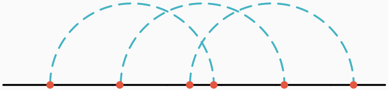

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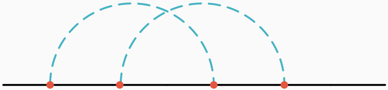

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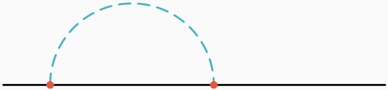

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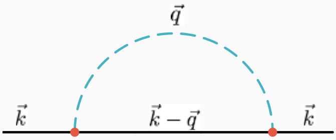
Change update: modifies the total length of the diagram.

Result: the time the stochastic process spends with diagrams of length τ will be proportional to $G(\tau)$. One can fill a histogram after each update and get the Green's function.

Diagrammatics for a rotating impurity

Moving particle: linear momentum circulating on lines.



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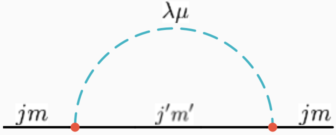

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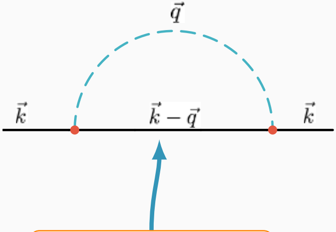

$\vec{k}$ and $\vec{q}$ fully determine $\vec{k}-\vec{q}$

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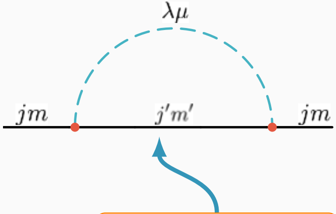

j and λ can sum in many different ways: $|j-\lambda|, \ldots j+\lambda$

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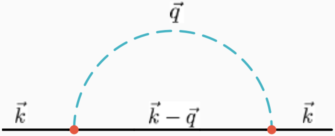

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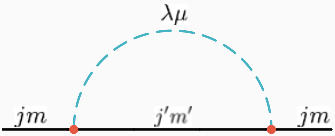
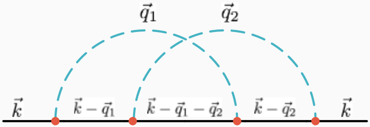
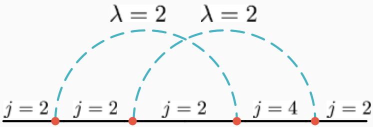


Higher order angular momentum composition!





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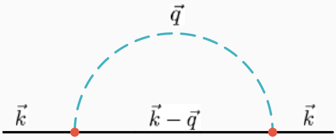

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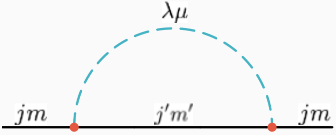

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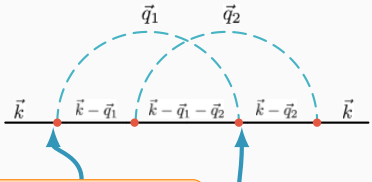
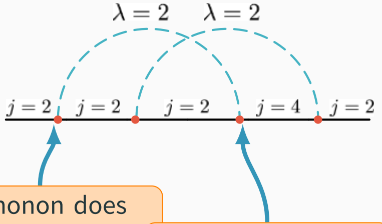




The phonon takes away $\vec{q}_1$ momentum...

...and gives back $\vec{q}_1$ momentum

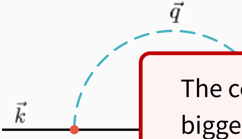
The phonon does not subtract angular momentum from the impurity...

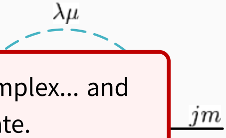
...but gives back two quanta!

Diagrammatics for a rotating impurity

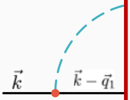
Moving particle: linear momentum circulating on lines.

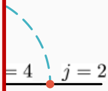
Rotating particle: angular momentum circulating on lines.



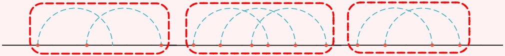


Higher order





The configuration space is more complex... and bigger! We need an additional update.



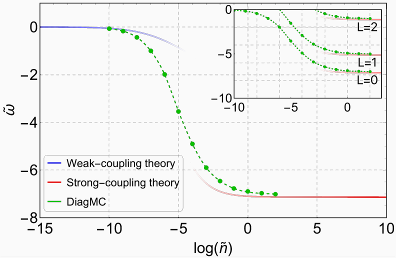
Shuffle update: select one 1-particle-irreducible component, shuffle the momenta couplings to another allowed configuration.

DiagMC: 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 and quasiparticle weight are 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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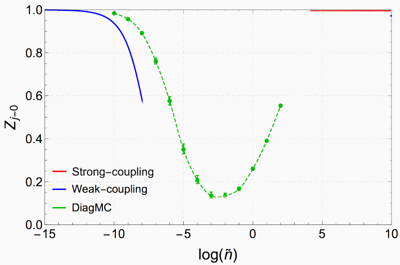

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Conclusions

- A description of rotations in a many-body environment in terms of Feynman diagrams and a numerically-exact approach to rotations in quantum many-body systems.
- 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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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