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

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Impurities and angular momentum

Motivation for the study of composite impurities, i.e. impurities possessing angular momentum, comes from many different fields. They can be realized as:

- **Molecules** embedded into **helium nanodroplets**.
- **Ultracold molecules** and ions.
- Electronic excitations in **Rydberg atoms**.
- Angular momentum transfer from **electrons** to a **crystal lattice**.

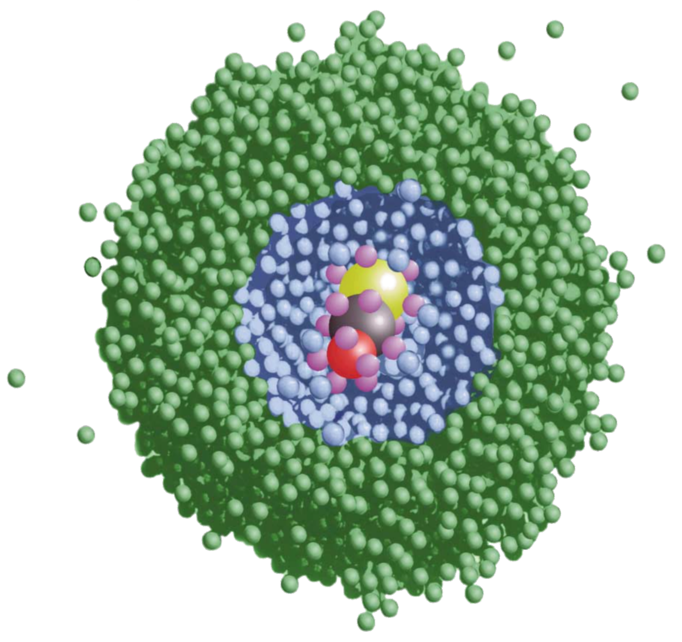


Image from: J. P. Toennies and A. F. Vilesov, Angew. Chem. Int. Ed. **43**, 2622 (2004).

The angulon

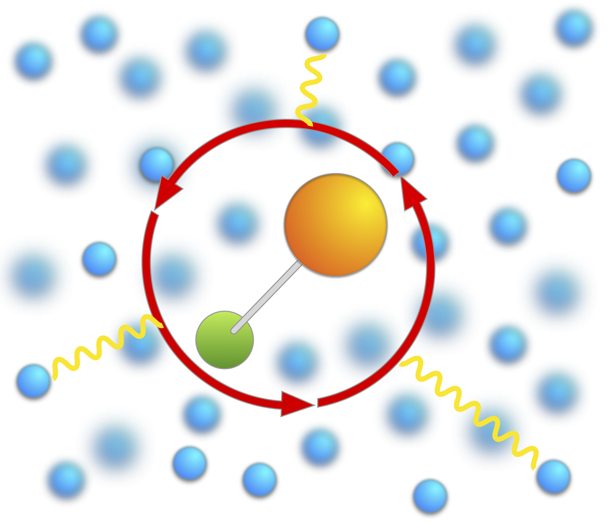
We describe a composite impurity by means of the following Hamiltonian:

$$\hat{H} = \hat{H}_{\text{imp}} + \hat{H}_{\text{bos}} + \hat{H}_{\text{imp-bos}}$$

with

$$\hat{H}_{\text{imp}} = B\hat{\mathbf{J}}^2$$

$$\hat{H}_{\text{bos}} = \sum_{k\lambda\mu} \omega_k \hat{b}^\dagger_{k\lambda\mu}\hat{b}_{k\lambda\mu}$$



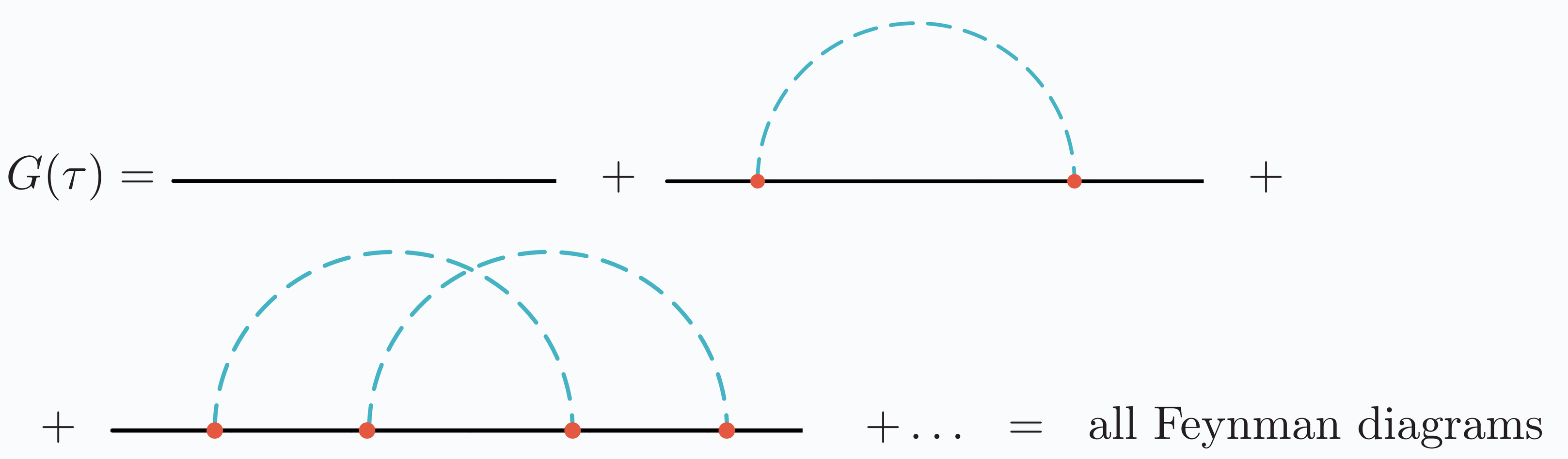
$$\hat{H}_{\text{imp-bos}} = \sum_{k\lambda\mu} U_\lambda(k)\left[Y^*_{\lambda\mu}(\hat{\theta},\hat{\phi})\hat{b}^\dagger_{k\lambda\mu} + Y_{\lambda\mu}(\hat{\theta},\hat{\phi})\hat{b}_{k\lambda\mu}\right]$$

The **angulon quasiparticle**: a quantum rotor dressed by a field of many-body excitations.

Diagrammatic Monte Carlo

General structure of an impurity problem: $\hat{H} = \hat{H}_{\text{imp}} + \hat{H}_{\text{bos}} + \hat{H}_{\text{imp-bos}}$

Green's function



DiagMC idea: set up a stochastic process sampling among all diagrams.
Configuration space: diagram topology, phonons internal variables, times... The number of variables varies with the topology!
How: ergodicity, detailed balance $w_1 p(1 \to 2) = w_2 p(2 \to 1)$, achieved with a two-step update (proposal+acceptance/rejection).
Result: each configuration is visited with probability $\propto$ its weight.

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

For the Fröhlich polaron three updates are enough to explore all possible diagrams:
✓**Add** update: adds a new arc to a diagram.
✓**Remove** update: removes an arc from the diagram.
✓**Change** update: modifies the total length of the diagram.

References

Main references: GB, T.V. Tscherbul and M. Lemeshko, Phys. Rev. Lett. **121**, 165301 (2018). GB and M. Lemeshko, Phys. Rev. B **96**, 085410 (2017).

DiagMC: N. Prokof'ev and B. Svistunov, Phys. Rev. Lett. **81**, 2514 (1998).

Angulon: R. Schmidt and M. Lemeshko, Phys. Rev. X **6**, 011012 (2016).
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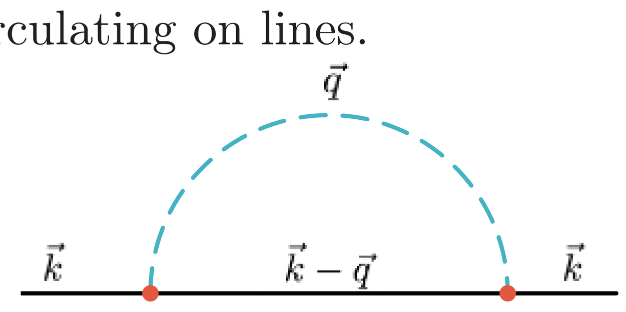
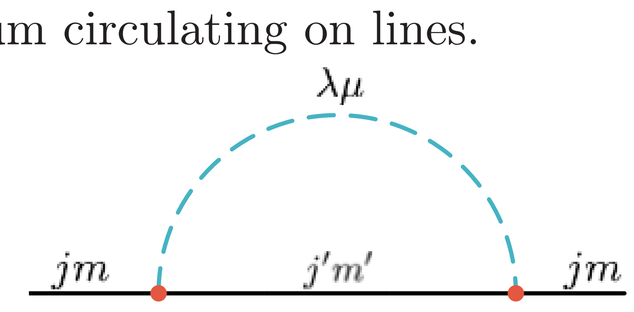
Diagrams and updates

Moving particle: *linear* momentum circulating on lines.

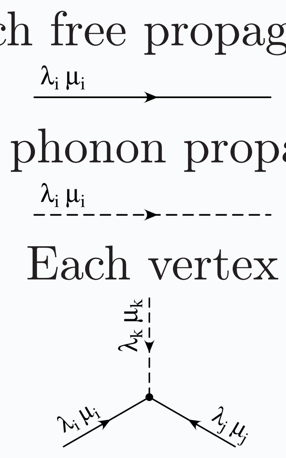


Rotating particle: *angular* momentum circulating on lines.

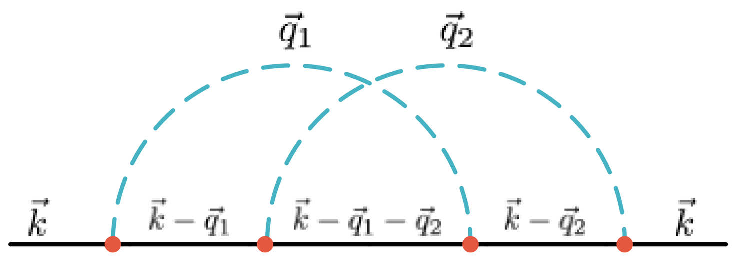


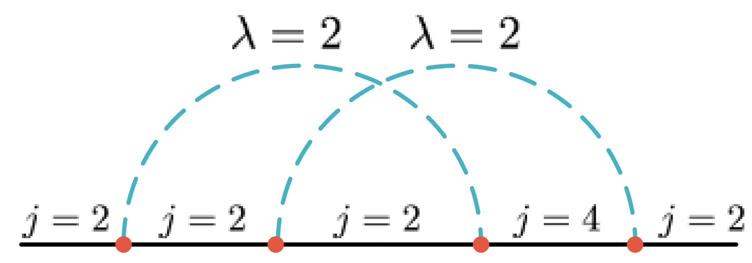
Feynman rules

Each free propagator ($\lambda_i\mu_i$)	$\sum_{\lambda_i\mu_i}(-1)^{\mu_i}G_{0,\lambda_i}$
Each phonon propagator ($\lambda_i\mu_i$)	$\sum_{\lambda_i\mu_i}(-1)^{\mu_i}D_{\lambda_i}$
Each vertex	$(-1)^{\lambda_i}\langle\lambda_i\vert\vert Y^{(\lambda_j)}\vert\vert\lambda_k\rangle\begin{pmatrix}\lambda_i & \lambda_j & \lambda_k\\ \mu_i & \mu_j & \mu_k\end{pmatrix}$

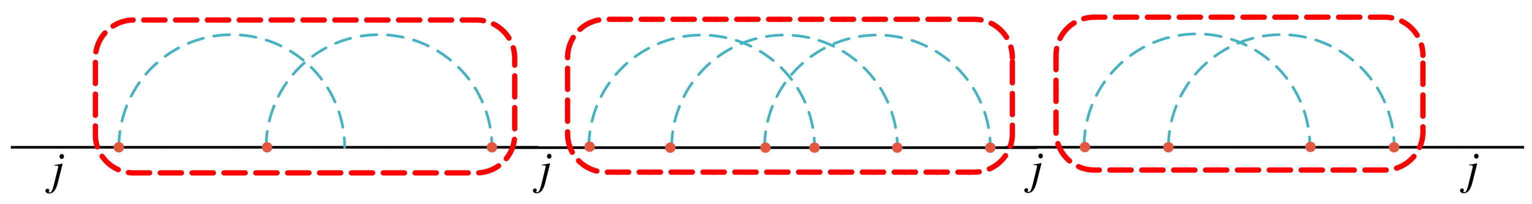


The configuration space is **larger** than that of the Fröhlich polaron: in the diagram above j and λ can couple to give j' in many different ways. The configuration space is also **essentially different**: consider the second diagram below, angular momentum is not conserved on each phonon line (i.e. a phonon line subtracts 0 quanta of angular momentum, but gives back 2)...





....but it must be conserved on each 1-particle-irreducible component.



Solution

Shuffle update: select one 1-particle-irreducible component, then shuffle the momenta couplings to another allowed configuration, keeping phonon momenta fixed but including configurations in which a phonon arc subtracts/gives back a different number of quanta.
The **Add** and **Remove** updates now only act on phonon lines which add/subtract the same number of quanta of angular momentum.

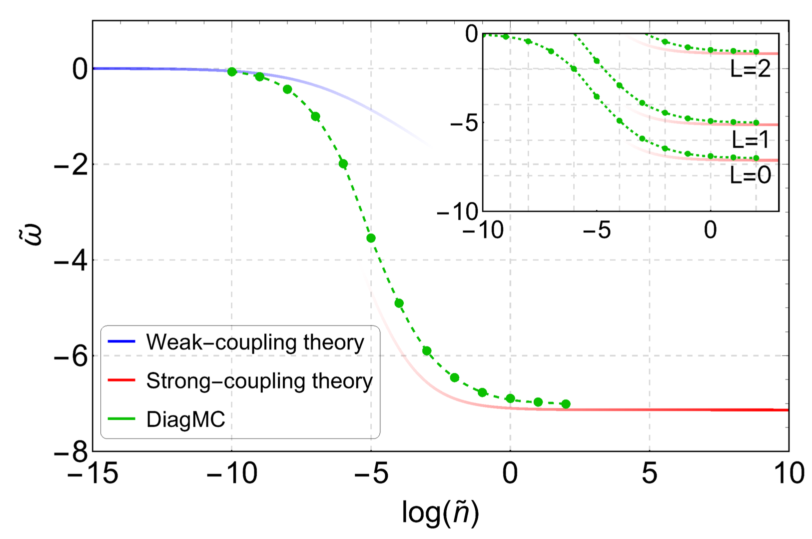
This scheme allows us to **visit all diagrams**.

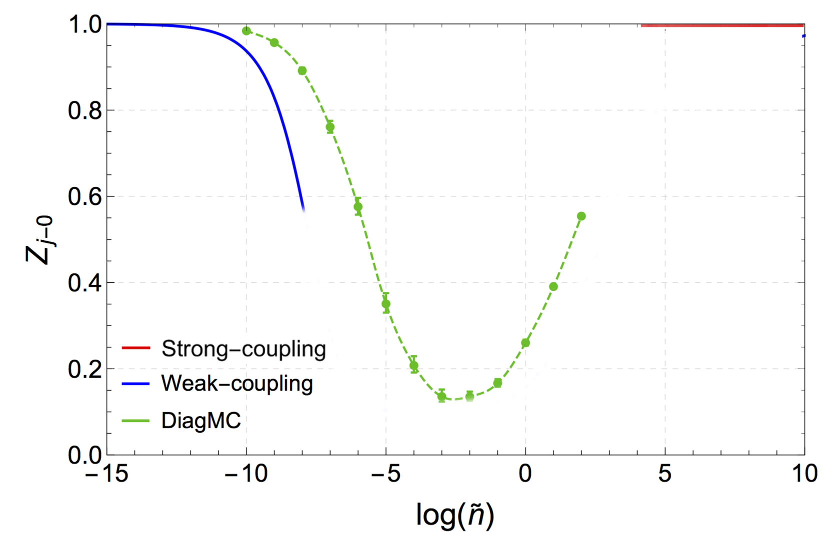
Results

The **ground-state** energy, the energy of the **first two excited states** and the **quasiparticle weight** for the angulon are obtained by fitting the long-imaginary-time behaviour of G_j with

$$G_j(\tau) = Z_j \exp(-E_j\,\tau)$$

as a function of the dimensionless bath density $\tilde{n}$. They are compared with the weak- and strong-coupling theories.





Conclusions

- A technique for **molecular simulations** using the DiagMC framework.
- **Angular momentum** and **rotations** can be described with DiagMC. The configuration space is bigger, and an **additional update** is needed.
- Works naturally in the **thermodynamic limit** and in **continuous time**: no finite-size effect, no systematic errors.
- Straightforward access to the **Green's function** and to angular momentum properties: they are encoded in the formalism.