Diagrammatic Monte Carlo approach to angular momentum in quantum many-body systems
Giaccomo Bighin\textsuperscript{1}, Timur Tscherbul\textsuperscript{2}, and Mikhail Lemeshko\textsuperscript{1}
\textsuperscript{1}Institute of Science and Technology Austria, \textsuperscript{2}University of Nevada, Reno

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.

Diagrammatic Monte Carlo

DIAGRAMS AND UPDATES
Moving particle: linear momentum circulating on lines.

Rotating particle: angular momentum circulating on lines.

The configuration space is larger than that of the Fröhlich polaron: in the diagram above \( j \) and \( \lambda \) 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)... 

The 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.

REFERENCES


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


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.

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

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