The superfluid density in systems with complex interactions

Presented by

Valéry G. Rousseau

Collaborators:
- Ka-Ming Tam
- Mark Jarrell
- Juana Moreno
- George Batrouni
- Richard Scalettar
What does “complex interactions” stand for?

Examples of Hamiltonians with complex interactions recently studied.

The superfluid density: Avoiding misconceptions.
Particles in interaction are often described by Hamiltonians that take the form

\[ \hat{\mathcal{H}} = - \sum_{s} t_s \sum_{\langle i,j \rangle} \left( a_{i,s}^{\dagger} a_{j,s} + H.c. \right) + \hat{V} \]

where \( i \) and \( j \) run over first-neighboring sites, \( s \) runs over all species of particles, and \( V \) depends only on occupation numbers.

In other words, the non-diagonal part of the Hamiltonian is assumed to be the usual kinetic operator.

But...

**Many Hamiltonians of interest do not fit with this form!**
Particles in interaction are often described by Hamiltonians that take the form

\[ \hat{H} = - \sum \sum t_s \left( a_{i,s}^\dagger a_{j,s} + H.c. \right) + \hat{V} \]

where \( i \) and \( j \) run over first-neighboring sites, \( s \) runs over all species of particles, and \( \hat{V} \) depends only on occupation numbers.

In other words, the non-diagonal part of the Hamiltonian is assumed to be the usual kinetic operator.

But...

Many Hamiltonians...
Particles in interaction are often described by Hamiltonians that take the form

\[ \hat{H} = - \sum_s t_s \sum_{\langle i,j \rangle} \left( a_{i,s}^\dagger a_{j,s} \right) \]

where \( i \) and \( j \) run over first-neighboring sites, \( s \) runs over all species of particles, and \( V \) depends only on occupation numbers.

In other words, the non-diagonal part of the Hamiltonian is assumed to be the usual kinetic operator.

But... Many Hamiltonians of interest do not fit with this form!

What does “complex interactions” stand for?

Example

If we are interested in the BCS-BEC crossover in a lattice, we may consider the following Hamiltonian:

\[ \hat{H} = -t_a \sum_{\langle i,j \rangle} \left( a_i^\dagger a_i + H.c. \right) - t_m \sum_{\langle i,j \rangle} \left( m_i^\dagger m_i + H.c. \right) \]

\[ + U_{aa} \sum_i \hat{n}_i^a (n_i^a - 1) + U_{mm} \sum_i \hat{n}_i^m (n_i^m - 1) + U_{am} \sum_i \hat{n}_i^a \hat{n}_i^m \]

\[ + g \sum_i \left( a_i^\dagger a_i^\dagger m_i + H.c. \right) \]
The superfluid density is an important physical quantity in Condensed Matter Physics. The superfluid density is usually defined as the response of the free energy to boundary phase-twist [1]. For a lattice, the dimensionless superfluid density takes the form:

\[ \hat{\rho}_s = -t \sum \langle \hat{\phi} \rangle \]

The superfluid density is usually measured in QMC simulations via the fluctuations of the winding number [2]:
Two-dimensional Bose-Hubbard model with second-neighbor hopping at half-filling:

This example demonstrates that the well-known formulae that have been used for decades to calculate the superfluid density cannot be applied to all Hamiltonians!

Questions
- What is the condition of validity of the well-known formulae?
- Can we derive a new formula that is valid in all cases?
Experimental detection of superfluidity
Thought experiment and correspondence principle

**Thought experiment:** We idealize the real experiment by taking the limit when the torus’ radius $R$ goes to infinity. The system then becomes equivalent to a fluid enclosed in a cylinder of length $2\pi R$.

**Outcome:** A superfluid does not respond to a Galilean boost.

**Correspondence principle:** The behavior of systems described by Quantum Mechanics must reproduce Classical Physics in the macroscopic limit.
Thought experiment and correspondence principle

Galilean boost operator: \( \hat{U} = e^{-i \frac{m}{\hbar} \vec{v} \cdot \vec{R}} \)

\[
\hat{U}^\dagger \vec{P} \hat{U} = \vec{P} - m \vec{v} \hat{N} \\
\hat{U}^\dagger \vec{R} \hat{U} = \vec{R}
\]

Correspondence principle: The behavior of systems described by Quantum Mechanics must reproduce Classical Physics in the macroscopic limit.

Limit when the torus' radius goes to infinity
Quantum average of the total momentum in the lab frame:

$$\langle \vec{P} \rangle = \frac{1}{Z_0} \text{Tr} \hat{U} \vec{P} \hat{U}^\dagger e^{-\beta \hat{H}_o}$$

Correspondence principle: The behavior of systems described by Quantum Mechanics must reproduce Classical Physics in the macroscopic limit.
Quantum average of the total momentum in the lab frame:

$$\langle \vec{P} \rangle = \frac{1}{Z_0} \text{Tr} \; \vec{P} e^{-\beta \hat{U}^\dagger \hat{H}_0 \hat{U}}$$

**Correspondence principle:** The behavior of systems described by Quantum Mechanics must reproduce Classical Physics in the macroscopic limit.
Thought experiment and correspondence principle

\[ \frac{1}{Z_0} \text{Tr} \ e^{-\beta \hat{U}^\dagger \hat{H}_0 \hat{U}} = \text{Classical momentum} \]

\( \Rightarrow \)

Correspondence principle

\[ = \rho_n \Omega \hat{v} \]

Thought experiment

Limit when the torus' radius goes to infinity
Thought experiment and correspondence principle

Normal density: \[ \rho_n = -i \frac{m}{\hbar \Omega d} \langle \vec{P} \cdot \int_0^\beta e^{\tau \hat{H}_o} [\vec{R}, \hat{H}_o] e^{-\tau \hat{H}_o} d\tau \rangle \]

Superfluid density: \[ \rho_s = \rho + i \frac{m}{\hbar \Omega d} \langle \vec{P} \cdot \int_0^\beta e^{\tau \hat{H}_o} [\vec{R}, \hat{H}_o] e^{-\tau \hat{H}_o} d\tau \rangle \]

“Superfluid density in continuous and discrete spaces: Avoiding misconceptions”

Limit when the torus’ radius goes to infinity
It can be shown that Fisher et al. and Pollock & Ceperley's formulae can be written in terms of momentum correlations:

$$\rho_s = \rho - \frac{1}{\Omega d} \left\langle \vec{P} \cdot \int_0^\beta e^{\tau \hat{H}_o} \hat{P} e^{-\tau \hat{H}_o} d\tau \right\rangle$$

The new formula,

$$\rho = \rho_s + i \frac{m}{\vec{P}} \left\langle \vec{P} \cdot \int_0^\beta e^{\tau \hat{H}_o} \left[ \vec{P}, \hat{H}_o \right] e^{-\tau \hat{H}_o} d\tau \right\rangle$$

This condition is systematically satisfied for Hamiltonians with no complex interactions.

This is the condition that the Hamiltonian must satisfy for the old formulae to be applicable.

For the model with second-nearest neighbor hopping, we can define the operator:

Then the condition of validity of the old formulae is not satisfied:

Test of the new formula

“Superfluid density in continuous and discrete spaces: Avoiding misconceptions”
Test of the new formula


"Superfluid density in continuous and discrete spaces: Avoiding misconceptions"

The new formula also allows for the calculation of the superfluid density when the winding number is undefined. This is the case for the model of atoms and diatomic molecules interacting via a Feshbach resonance:

\[ t_a = 1 \quad t_m = 0.5 \quad g = 1.5 \]

\[ U_{aa} = 8 \quad U_{mm} = 100 \quad U_{am} = 12 \quad \beta = 10 \]
The superfluid density is an important quantity that allows us to characterize various phases encountered in Condensed Matter physics and in quantum gases. However, the well-known formulae used for the calculation of the superfluid density are not applicable in all cases.

Based on a thought experiment and the Correspondence principle, I derived a general formula for the superfluid density that does not involve any assumption on the form of the Hamiltonian:

$$\rho_s = \rho + i \frac{m}{\hbar \Omega d} \left\langle \vec{P} \cdot \int_0^\beta e^{\tau \hat{H}_0} \left[ \vec{R}, \hat{H}_0 \right] e^{-\tau \hat{H}_0} d\tau \right\rangle$$

I showed that this new formula gives consistent results for a model with second-nearest neighbor hopping, where the old formulae failed. The impact of this new formula on the ongoing research should be important, given the fact that Hamiltonians with complex interactions are currently under intensive investigations.

“Superfluid density in continuous and discrete spaces: Avoiding misconceptions”

All QMC results presented in this talk were obtained with the BGP algorithm.