TWO-MODE THEORY
OF
BEC INTERFEROMETRY

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INTRODUCTION

♦ Aim

- Develop a theory of BEC interferometry for case of single component BEC - all bosons in same spin state.
- Apply to SUT experiment involving magnetic traps on an atom chip - permanent magnets plus current elements.

♦ BEC Interferometer

- BEC initially at zero temperature with all bosons in lowest orbital $\phi_1(r)$.
- Trapping potential changes from a single well into a double well and back again.
- Asymmetry in double well potential leads to interferometric effects, such as for boson numbers in excited orbital $\phi_2(r)$.
- Interferometer process is depicted in Figure 1. Red squares indicate bosons, trap potential is shown in red, typical orbitals are shown in blue or pink.
Issues

• Does the BEC fragment into two BECs (left well, right well) during the process?

• What happens to the single boson orbitals $\phi_1(r,t), \phi_2(r,t)$ as the trap potential changes?

• What excited BEC states are important in the process?

• How are the interferometric measurements, such as the excited boson probability, related to asymmetry in the trapping potential?

• How does the interferometer sensitivity depend on the number of bosons?

• What is the optimum way to change the trap potential during the process?

• What effect would decoherence, quantum fluctuations, finite temperatures, ... have?

Nature of Orbitals

• Single Well - Possible orbitals are shown in Figure 2a.

• Double Asymmetric Well - Possible delocalised orbitals are shown in Figure 2b.

• Double Asymmetric Well - Possible localised orbitals are shown in Figure 2c.
♦ Full Theory - Future work

- Phase space method (based on Drummond et al, PRA 68, 063822, (2003)).
- Stochastic PDE for condensate wave function.
- Quantum fluctuations around mean field (condensate wave function) treated.
- Decoherence effects due BEC coupling to reservoirs, classical fluctuations in trap potentials, ..included.
- Presence of excited states of BEC (single boson, collective, ..) during process allowed for.
- Multimode and fragmentation effects incorporated.
- Finite temperature effects included.
- Boson number unrestricted.

♦ Simple Theory - Present work

- Variational approach based on two-mode approximation with time dependent orbitals (based on Menotti et al, PRA 63, 023601 (2001)) and using spin operators.
- Self-consistent coupled equations for amplitudes and orbitals - Generalised Gross-Pitaevskii equations.
- Decoherence, thermal, multimode effects ignored.
- Boson number, excitations, fluctuations restricted.
THEORY

♦ Hamiltonian - Kinetic energy, trapping potential, two-body interaction (zero-range approximation)

\[ \hat{H} = \int dr \left( \frac{\hbar^2}{2m} \nabla \hat{\Psi}^\dagger \cdot \nabla \hat{\Psi} + \hat{\Psi}^\dagger \nabla \hat{\Psi} + \frac{g}{2} \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi}^\dagger \hat{\Psi} \right) \]

♦ Field Operators - Bosons

\[ \left[ \hat{\Psi}(r), \hat{\Psi}^\dagger (r') \right] = \delta(r-r') \]

♦ Single Boson Orbitals - Orthogonal and normalised, time dependent in general

\[ \int dr \phi^*_i(r,t) \phi_j(r,t) = \delta_{ij} \]

♦ Annihilation and Creation Operators - Orbital expansion, time dependent creation, annihilation operators

\[ \hat{\Psi}(r) = \sum_i \hat{c}_i(t) \phi_i(r,t) \quad \hat{\Psi}^\dagger (r) = \sum_i \hat{c}_i^\dagger (t) \phi_i^*(r,t) \]

\[ \left[ \hat{c}_i(t), \hat{c}_j^\dagger (t) \right] = \delta_{ij} \quad (i,j = 1,2,\ldots) \]

• Two orbitals only in the sum (two-mode approximation).
♦ **Boson Number Operator** - Conserved quantity

\[ \hat{N} = \int dr \hat{\Psi}^\dagger(r) \hat{\Psi}(r) \]

\[ = \sum_i \hat{c}_i^\dagger \hat{c}_i \]

♦ **Spin Operators** - Two-mode case

\[ \hat{S}_x = \left( \hat{c}_2^\dagger \hat{c}_1 + \hat{c}_1^\dagger \hat{c}_2 \right)/2 \]

\[ \hat{S}_y = \left( \hat{c}_2^\dagger \hat{c}_1 - \hat{c}_1^\dagger \hat{c}_2 \right)/2i \]

\[ \hat{S}_z = \left( \hat{c}_2^\dagger \hat{c}_2 - \hat{c}_1^\dagger \hat{c}_1 \right)/2 \]

♦ **Commutation Rules** - Angular momentum theory

\[ \left[ \hat{S}_\alpha, \hat{S}_\beta \right] = i \epsilon_{\alpha \beta \gamma} \hat{S}_\gamma \quad (\alpha, \beta, \gamma = x, y, z) \]

♦ **Angular Momentum Squared** - Conserved quantity

\[ (\hat{S})^2 = \sum_\alpha (\hat{S}_\alpha)^2 \]

\[ = \frac{\hat{N}}{2} \left( \frac{\hat{N}}{2} + 1 \right) \]

• Angular momentum squared related to boson number operator.
Basis States for BEC System - \( N \) bosons

\[
| k \rangle = \frac{\left( \hat{c}_1^\dagger \right)^{\left( \frac{N}{2} - k \right)}}{\left[ \left( \frac{N}{2} - k \right)! \right]^{\frac{1}{2}}} \frac{\left( \hat{c}_2^\dagger \right)^{\left( \frac{N}{2} + k \right)}}{\left[ \left( \frac{N}{2} + k \right)! \right]^{\frac{1}{2}}} | 0 \rangle
\]

- This represents a state with \( \frac{N}{2} - k \) bosons in orbital \( \phi_1(r, t) \) and \( \frac{N}{2} + k \) bosons in orbital \( \phi_2(r, t) \).

- In general, this is a fragmented state of the \( N \) boson system involving two BECs, not just one.

Special State - Single BEC

\[
| -\frac{N}{2} \rangle = \frac{\left( \hat{c}_1^\dagger \right)^{N}}{\left[ N! \right]^{\frac{1}{2}}} | 0 \rangle
\]

- This state is a single unfragmented BEC with all bosons in orbital \( \phi_1(r, t) \).

Giant Spin System - Two-mode approximation

\[
(\hat{S})^2 | k \rangle = \frac{N}{2} \left( \frac{N}{2} + 1 \right) | k \rangle
\]

\[
\hat{S}_z | k \rangle = k | k \rangle
\]

- The BEC behaves as a giant spin system with spin angular momentum quantum number \( j = \frac{N}{2} \) and with spin magnetic quantum number \( k \) \( -\frac{N}{2} \leq k \leq \frac{N}{2} \).
General Quantum State - State amplitudes

\[ | \Phi(t) \rangle = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} b_k(t) | k \rangle \]

- This \( N \) boson state is a quantum superposition of fragmented states.

Normalisation - Conservation of probability

\[ \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} | b_k(t) |^2 = 1 \]

Initial Condition - All bosons in single condensate

\[ | \Phi(0) \rangle = | -\frac{N}{2} \rangle \]

Action - Functional of quantum state \( | \Phi(t) \rangle \)

\[ S = \int dt \left( \frac{\langle \partial_t \Phi | \Phi \rangle - \langle \Phi | \partial_t \Phi \rangle}{2i} - \frac{\langle \Phi | \hat{H} | \Phi \rangle}{\hbar} \right) \]

- Minimisation of action for arbitrary variation of state leads to time-dependent Schrodinger equation (TDSE).

- For restricted variation of state get approximations to TDSE.
Principle of Least Action - Action a functional of amplitudes $b_k(t)$ and orbitals $\phi_i(r, t)$

$$\frac{\delta S[b_k, b_k^*, \phi_i, \phi_i^*]}{\delta b_k^*} = 0$$

$$\frac{\delta S[b_k, b_k^*, \phi_i, \phi_i^*]}{\delta \phi_i^*} = 0$$

- The action is minimised for arbitrary variation of the amplitudes and orbitals. The functional derivatives of the action then are zero.
- The Lagrange multiplier associated with the normalisation constraint can be transformed away.
- Obtain self-consistent coupled equations for amplitudes and orbitals - generalised Gross-Pitaevskii equations.

Application of Least Action Principle

- Hamiltonian can be written in terms of spin operators and its matrix elements calculated from previous expressions plus

$$\hat{S}_\pm \left| \frac{N}{2}, k \right\rangle = \left\{ \frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k \pm 1) \right\}^{1/2} \left| \frac{N}{2}, k \pm 1 \right\rangle$$

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$$

- Angular momentum theory method involving step-up and step-down operators.
Functions of Orbitals - \((i, j, m, n = 1, 2)\)

\[
\widetilde{W}_{ij}(r, t) = \frac{\hbar^2}{2m} \sum_{\mu=x,y,z} \partial_\mu \phi_i^* \partial_\mu \phi_j + \phi_i^* V \phi_j
\]

\[
\widetilde{V}_{ijmn}(r, t) = \frac{g}{2} \phi_i^* \phi_j^* \phi_m \phi_n
\]

\[
\widetilde{T}_{ij}(r, t) = \frac{1}{2i} (\partial_t \phi_i^* \phi_j - \phi_i^* \partial_t \phi_j)
\]

Rotation Matrix - \((-\frac{N}{2} \leq k, l \leq +\frac{N}{2}\))

\[
U_{kl} = \frac{1}{2i} \left[ (\partial_t \langle k|) |l \rangle - \langle k| (\partial_t |l \rangle) \right]
\]

\[
= \int dr \widetilde{U}_{kl}(\phi_i, \phi_i^*, \partial_t \phi_i, \partial_t \phi_i^*)
\]

\[
\widetilde{U}_{kl} = \bar{T}_{11}(\frac{N}{2} - k) \delta_{kl} + \bar{T}_{22}(\frac{N}{2} + k) \delta_{kl}
\]

\[
+ \bar{T}_{12} \left\{ (\frac{N}{2} - k)(\frac{N}{2} + l) \right\} \frac{1}{2} \delta_{k,l+1}
\]

\[
+ \bar{T}_{21} \left\{ (\frac{N}{2} - l)(\frac{N}{2} + k) \right\} \frac{1}{2} \delta_{l,k+1}
\]

- Space integrals of orbitals and their time derivatives.

Hamiltonian Matrix - \((-\frac{N}{2} \leq k, l \leq +\frac{N}{2}\))

\[
H_{kl} = \langle k| \hat{H} |l \rangle
\]

\[
= \int dr \widetilde{H}_{kl}(\phi_i, \phi_i^*, \partial_\mu \phi_i, \partial_\mu \phi_i^*)
\]

- Space integrals of orbitals and their spatial derivatives.
Hamiltonian density

\[ \tilde{H}_{kl} = \tilde{W}_{11}(\frac{N}{2} - k)\delta_{kl} + \tilde{W}_{22}(\frac{N}{2} + k)\delta_{kl} \]

\[ + \tilde{W}_{12} \left\{ (\frac{N}{2} - k)(\frac{N}{2} + l) \right\}^{\frac{1}{2}} \delta_{k,l+1} \]

\[ + \tilde{W}_{21} \left\{ (\frac{N}{2} - l)(\frac{N}{2} + k) \right\}^{\frac{1}{2}} \delta_{l,k+1} \]

\[ + \tilde{V}_{1111}(\frac{N}{2} - k)(\frac{N}{2} - k - 1)\delta_{kl} \]

\[ + (\tilde{V}_{1212} + \tilde{V}_{1221} + \tilde{V}_{2121} + \tilde{V}_{2112})(\frac{N^2}{4} - k^2)\delta_{kl} \]

\[ + \tilde{V}_{2222}(\frac{N}{2} + k)(\frac{N}{2} + k - 1)\delta_{kl} \]

\[ + (\tilde{V}_{1112} + \tilde{V}_{1121})(\frac{N}{2} - l)\left\{ (\frac{N}{2} - k)(\frac{N}{2} + l) \right\}^{\frac{1}{2}} \delta_{k,l+1} \]

\[ + (\tilde{V}_{1222} + \tilde{V}_{2122})(\frac{N}{2} + k)\left\{ (\frac{N}{2} - k)(\frac{N}{2} + l) \right\}^{\frac{1}{2}} \delta_{k,l+1} \]

\[ + (\tilde{V}_{1211} + \tilde{V}_{2111})(\frac{N}{2} - k)\left\{ (\frac{N}{2} - l)(\frac{N}{2} + k) \right\}^{\frac{1}{2}} \delta_{l,k+1} \]

\[ + (\tilde{V}_{2212} + \tilde{V}_{2221})(\frac{N}{2} + l)\left\{ (\frac{N}{2} - l)(\frac{N}{2} + k) \right\}^{\frac{1}{2}} \delta_{l,k+1} \]

\[ + \tilde{V}_{1122} \left\{ (\frac{N}{2} - l + 1)(\frac{N}{2} - k)(\frac{N}{2} + l)(\frac{N}{2} + k + 1) \right\}^{\frac{1}{2}} \delta_{k,l+2} \]

\[ + \tilde{V}_{2211} \left\{ (\frac{N}{2} - k + 1)(\frac{N}{2} - l)(\frac{N}{2} + k)(\frac{N}{2} + l + 1) \right\}^{\frac{1}{2}} \delta_{l,k+2} \]
Quadratic Functions of Amplitudes
(i, j, m, n = 1, 2), \((-\frac{N}{2} \leq k, l \leq +\frac{N}{2}\))

\[ X_{ij} = \sum_{k,l} b_k^* X_{kl}^{ij} b_l \]

\[ Y_{ijmn} = \sum_{k,l} b_k^* Y_{kl}^{ijmn} b_l \]

\[ X_{kl}^{11} = (\frac{N}{2} - k)\delta_{kl} \quad X_{kl}^{12} = (\frac{N}{2} - k)(\frac{N}{2} + l) \frac{1}{2} \delta_{k,l+1} \]

\[ X_{kl}^{21} = (\frac{N}{2} - l)(\frac{N}{2} + k) \frac{1}{2} \delta_{l,k+1} \quad X_{kl}^{22} = (\frac{N}{2} + k)\delta_{kl} \]

\[ Y_{kl}^{1111} = (\frac{N}{2} - k)(\frac{N}{2} - k - 1)\delta_{kl} \]

\[ Y_{kl}^{2222} = (\frac{N}{2} + k)(\frac{N}{2} + k - 1)\delta_{kl} \]

\[ Y_{kl}^{1212} = Y_{kl}^{1221} = Y_{kl}^{2112} = Y_{kl}^{2121} = (\frac{N}{2} - k)(\frac{N}{2} + k)\delta_{kl} \]

\[ Y_{kl}^{1112} = Y_{kl}^{1121} = (\frac{N}{2} - l)(\frac{N}{2} - k)(\frac{N}{2} + l) \frac{1}{2} \delta_{k,l+1} \]

\[ Y_{kl}^{1222} = Y_{kl}^{2122} = (\frac{N}{2} + k)(\frac{N}{2} - k)(\frac{N}{2} + l) \frac{1}{2} \delta_{k,l+1} \]

\[ Y_{kl}^{1211} = Y_{kl}^{2111} = (\frac{N}{2} - k)(\frac{N}{2} - l)(\frac{N}{2} + k) \frac{1}{2} \delta_{l,k+1} \]

\[ Y_{kl}^{2212} = Y_{kl}^{2221} = (\frac{N}{2} + l)(\frac{N}{2} - k)(\frac{N}{2} + k) \frac{1}{2} \delta_{l,k+1} \]

\[ Y_{kl}^{1122} = (\frac{N}{2} - l + 1)(\frac{N}{2} - k)(\frac{N}{2} + l)(\frac{N}{2} + k + 1) \frac{1}{2} \delta_{k,l+2} \]

\[ Y_{kl}^{2211} = (\frac{N}{2} - k + 1)(\frac{N}{2} - l)(\frac{N}{2} + k)(\frac{N}{2} + l + 1) \frac{1}{2} \delta_{l,k+2} \]
Coupled Amplitude Equations

\[ i\hbar \frac{\partial b_k}{\partial t} = \sum_l (H_{kl} - \hbar U_{kl}) b_l \]

- Matrix elements depend on orbitals \( \phi_i(r, t) \).

Coupled Generalised Gross-Pitaevskii Equations for Orbitals

\[ i\hbar \sum_j X_{ij} \frac{\partial \phi_j}{\partial t} = \sum_j X_{ij} \left( -\frac{\hbar^2}{2m} \sum_{\mu=x,y,z} \partial^2_{\mu} \phi_j + V \phi_j \right) + g \sum_{jmn} Y_{ijmn} \phi_j^* \phi_m \phi_n \]

- Coefficients depend quadratically on amplitudes \( b_k(t) \).
- The combined set of equations for the amplitudes and orbitals form a self-consistent set.

Interferometer Measurement - Boson number in orbital \( \phi_2(r, t) \)

\[ N_2 = \langle \Phi | \hat{c}_2^\dagger \hat{c}_2 | \Phi \rangle = \frac{N}{2} + \sum_k k |b_k|^2 \]

- Measurement of \( N_2 \) at end of process depends on asymmetry and exhibits interferometric effects.
Initial Conditions

\[ b_k(0) = \delta_{k,-\frac{N}{2}} \]

- In this case only non-zero coefficients are
  \[ X_{11}(0) = N \quad Y_{1111}(0) = N(N - 1) \]
- Orbital \( \phi_1(r, t) \) satisfies single GPE as \( t \to 0 \)

\[ i\hbar \frac{\partial \phi_1}{\partial t} = -\frac{\hbar^2}{2m} \sum_{\mu=x,y,z} \partial^2_{\mu} \phi_1 + V \phi_1 + g(N - 1) |\phi_1|^2 \phi_1 \]

which is consistent with initial condition of all bosons occupying this orbital.

- Orbital \( \phi_2(r, t) \) is chosen by orthogonality.

Iterative Method of Solution

- First Step: * Assume know amplitudes \( b_k \)
  * Calculate the \( X_{ij} \) and \( Y_{ijmn} \)
  * Solve generalised GPE for orbitals \( \phi_i \)

- Second Step: * Calculate the \( H_{kl} \) and \( U_{kl} \)
  * Solve for amplitudes \( b_k \)

- Third Step: * Repeat process until solutions converge.

Direct Method of Solution

- Solution of coupled set of equations via XMDS.
Regime of Validity - Two-mode theory

- Mean field energy $Ng|\phi|^2$ and thermal energy quantum $k_B T$ both small compared to trap phonon energy $\hbar \omega_0$ gives

$$N \ll \frac{a_0}{a_s} \quad T \ll \frac{\hbar \omega_0}{k_B},$$

with scattering length $a_s$ and vibrational amplitude $a_0 = \sqrt{\frac{\hbar}{2m \omega_0}}$ (Milburn et al, PRA 55, 4318 (1997)).

- For $^{87}\text{Rb}$ with $a_s = 5 \text{ nm}$, $a_0 = 1 \mu\text{m}$, $\omega_0 = 2\pi \cdot 5.8 \text{ s}^{-1}$, find $N \ll 2 \cdot 10^2$ and $T \ll 2.8 \text{ nK}$.

Related Work - Two-mode theory

- Menotti et al, PRA 63, 023601 (2001) write orbitals and state amplitudes in terms of Gaussian forms with a total of four variational functions. Coupled self-consistent equations are derived for these. Dynamical BEC splitting, fragmentation, collapses and revivals treated.

- Spekkens et al, PRA 59, 3868 (1999) use variational principle and spin operator methods for static, symmetrical potential cases to derive self-consistent coupled equations for state amplitudes and orbitals - generalised time independent GPE. Static BEC fragmentation found.

Numerous papers exist treating BEC dynamics in a double well potential assuming fixed orbitals or assuming that no BEC fragmentation occurs. Spin operators based on fixed orbitals are also widely used.
SUMMARY

• Using the two-mode approximation and treating the $N$ bosons as a giant spin system, a theory of BEC interferometry has been developed based on applying the Principle of Least Action to a variational form for the quantum state which allows for a possible fragmentation of the BEC.

• Self-consistent coupled equations are obtained for the state amplitudes and the orbitals, the latter being a generalisation of the Gross-Pitaevskii equations.

• Numerical studies of these equations are planned with the aim of applying the results to future BEC interferometry experiments at Swinburne University of Technology involving a double well interferometer based on an atom chip.