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 $\phi_1(\mathbf{r})$.
- 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 $\phi_2(\mathbf{r})$.
- 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 $\phi_1(\mathbf{r},t), \phi_2(\mathbf{r},t), ..$ 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)

$$\hat{H} = \int d\mathbf{r}\left(\frac{\hbar^2}{2m}\nabla\hat{\Psi}^{\dagger} \cdot \nabla\hat{\Psi} + \hat{\Psi}^{\dagger} V\hat{\Psi} + \frac{g}{2}\hat{\Psi}^{\dagger}\hat{\Psi}^{\dagger}\hat{\Psi}\hat{\Psi} \right)$$

♦ **Field Operators** - Bosons

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

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

$$\int d\mathbf{r}\, \phi_i^*(\mathbf{r},t)\, \phi_j(\mathbf{r},t) = \delta_{ij}$$

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

$$\hat{\Psi}(\mathbf{r}) = \sum_i \hat{c}_i(t)\, \phi_i(\mathbf{r},t) \qquad \hat{\Psi}^{\dagger}(\mathbf{r}) = \sum_i \hat{c}_i^{\dagger}(t)\, \phi_i^*(\mathbf{r},t)$$

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

- Two orbitals only in the sum (two-mode approximation).

♦ **Boson Number Operator** - Conserved quantity

$$\hat{N} = \int d\mathbf{r}\, \hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r})$$

$$= \sum_{i} \hat{c}_i^{\dagger}\hat{c}_i$$

♦ **Spin Operators** - Two-mode case

$$\hat{S}_x = (\hat{c}_2^{\dagger}\hat{c}_1 + \hat{c}_1^{\dagger}\hat{c}_2)/2$$

$$\hat{S}_y = (\hat{c}_2^{\dagger}\hat{c}_1 - \hat{c}_1^{\dagger}\hat{c}_2)/2i$$

$$\hat{S}_z = (\hat{c}_2^{\dagger}\hat{c}_2 - \hat{c}_1^{\dagger}\hat{c}_1)/2$$

♦ **Commutation Rules** - Angular momentum theory

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

♦ **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

$$|k\rangle = \frac{(\widehat{c_1}^{\dagger})^{(\frac{N}{2}-k)}}{[(\frac{N}{2}-k)!]^{\frac{1}{2}}} \frac{(\widehat{c_2}^{\dagger})^{(\frac{N}{2}+k)}}{[(\frac{N}{2}+k)!]^{\frac{1}{2}}} |0\rangle$$

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

• In general, this is a *fragmented state* of the N boson system involving two BECs, not just one.

♦ Special State - Single BEC

$$\left|-\frac{N}{2}\right\rangle = \frac{(\widehat{c_1}^{\dagger})^{N}}{[N!]^{\frac{1}{2}}} |0\rangle$$

• This state is a single *unfragmented* BEC with all bosons in orbital $\phi_1(\mathbf{r}, t)$.

♦ Giant Spin System - Two-mode approximation

$$(\widehat{S})^2 |k\rangle = \frac{N}{2}(\frac{N}{2} + 1) |k\rangle$$

$$\widehat{S}_z |k\rangle = k |k\rangle$$

• 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 $(-\frac{N}{2} \le k \le \frac{N}{2})$.

♦ 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

$$|\Phi(0)\rangle = \left|-\frac{N}{2}\right\rangle$$

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

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

• 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 $\phi_i(\mathbf{r}, t)$

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

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

- 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

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

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

- Angular momentum theory method involving step-up and step-down operators.

♦ Functions of Orbitals - $(i, j, m, n = 1, 2)$

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

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

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

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

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

$$= \int d\mathbf{r}\,\widetilde{U}_{kl}(\phi_i,\phi_i^*,\partial_t\phi_i,\partial_t\phi_i^*)$$

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

$$+\ \widetilde{T}_{12}\,\{(\frac{N}{2}-k)(\frac{N}{2}+l)\}^{\frac{1}{2}}\,\delta_{k,l+1}$$

$$+\ \widetilde{T}_{21}\,\{(\frac{N}{2}-l)(\frac{N}{2}+k)\}^{\frac{1}{2}}\,\delta_{l,k+1}$$

- Space integrals of orbitals and their time derivatives.

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

$$H_{kl} = \left\langle k\right|\widehat{H}\left|l\right\rangle$$

$$= \int d\mathbf{r}\,\widetilde{H}_{kl}(\phi_i,\phi_i^*,\partial_\mu\phi_i,\partial_\mu\phi_i^*)$$

- Space integrals of orbitals and their spatial derivatives.

- Hamiltonian density

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

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

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

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

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

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

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

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

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

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

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

$$+\tilde{V}_{2211}\{(\frac{N}{2}-k+1)(\frac{N}{2}-l)(\frac{N}{2}+k)(\frac{N}{2}+l+1)\}^{\frac{1}{2}}\delta_{l,k+2}$$

♦ Quadratic Functions of Amplitudes

$(i, j, m, n = 1, 2)$, $(-\frac{N}{2} \leq k, l \leq +\frac{N}{2})$

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

$$Y_{ij\,mn} = \sum_{k,l} b_k^* Y_{kl}^{ij\,mn} b_l$$

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

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

$$Y_{kl}^{11\,11} = (\frac{N}{2} - k)(\frac{N}{2} - k - 1)\delta_{kl}$$

$$Y_{kl}^{22\,22} = (\frac{N}{2} + k)(\frac{N}{2} + k - 1)\delta_{kl}$$

$$Y_{kl}^{12\,12} = Y_{kl}^{12\,21} = Y_{kl}^{21\,12} = Y_{kl}^{21\,21} = (\frac{N}{2} - k)(\frac{N}{2} + k)\delta_{kl}$$

$$Y_{kl}^{11\,12} = Y_{kl}^{11\,21} = (\frac{N}{2} - l)\{(\frac{N}{2} - k)(\frac{N}{2} + l)\}^{\frac{1}{2}} \delta_{k,l+1}$$

$$Y_{kl}^{12\,22} = Y_{kl}^{21\,22} = (\frac{N}{2} + k)\{(\frac{N}{2} - k)(\frac{N}{2} + l)\}^{\frac{1}{2}} \delta_{k,l+1}$$

$$Y_{kl}^{12\,11} = Y_{kl}^{21\,11} = (\frac{N}{2} - k)\{(\frac{N}{2} - l)(\frac{N}{2} + k)\}^{\frac{1}{2}} \delta_{l,k+1}$$

$$Y_{kl}^{22\,12} = Y_{kl}^{22\,21} = (\frac{N}{2} + l)\{(\frac{N}{2} - l)(\frac{N}{2} + k)\}^{\frac{1}{2}} \delta_{l,k+1}$$

$$Y_{kl}^{11\,22} = \{(\frac{N}{2} - l + 1)(\frac{N}{2} - k)(\frac{N}{2} + l)(\frac{N}{2} + k + 1)\}^{\frac{1}{2}} \delta_{k,l+2}$$

$$Y_{kl}^{22\,11} = \{(\frac{N}{2} - k + 1)(\frac{N}{2} - l)(\frac{N}{2} + k)(\frac{N}{2} + l + 1)\}^{\frac{1}{2}} \delta_{l,k+2}$$

♦ 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 $\phi_i(\mathbf{r}, t)$.

♦ Coupled Generalised Gross-Pitaevskii Equations for Orbitals

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

- 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 $\phi_2(\mathbf{r}, t)$

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

- 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

$$X_{11}(0) = N \qquad Y_{1111}(0) = N(N-1)$$

- Orbital $\phi_1(\mathbf{r}, t)$ satisfies single GPE as $t \to 0$

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

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

- Orbital $\phi_2(\mathbf{r}, t)$ 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 ϕ_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

$$N \ll \frac{a_0}{a_S} \qquad T \ll \frac{\hbar\omega_0}{k_B},$$

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

• For Rb^{87} with $a_S = 5$ nm, $a_0 = 1$ μm, $\omega_0 = 2\pi.58$ s^{-1}, find $N \ll 2.10^2$ and $T \ll 2.8$ 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.

• Cederbaum et al, PRA 70, 023610 (2004) predict fragmented excited BEC states in the static case using generalised time independent GPE derived using variational methods.

- 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.