Squeezing and superposing many-body states of Bose gases in confining potentials

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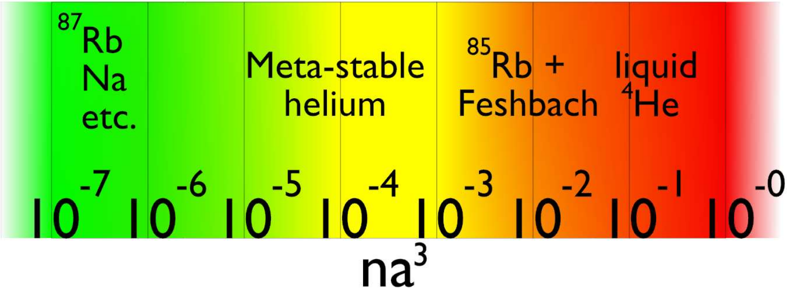
Outline

1. from cold atoms to helium; quantum Monte Carlo methods
2. squeezing trapped cold atoms - repulsive bosons in a double well
3. mesocopic superposition states - attractive bosons and helium

Range of interactions

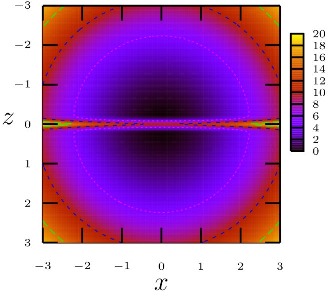
$a > 0$



$a < 0$

^{7}Li, ^{85}Rb + Feshbach, Cs + Feshbach . . .

BEC in a double well



- split condensate
- meso(macro)scopic coherences
- interference
  - squeezing
  - superpositions
- many-body tunneling

$$a > 0: \quad V_{ext}(\mathbf{r}) = x^2 + y^2 + z^2 + V_b((z/l)^2 - 1)^2$$

$$a < 0: \quad V_{ext}(\mathbf{r}) = x^2 + y^2 + z^2 + \frac{V_b}{\sqrt{2\pi l}} e^{-(z/2l)^2}$$

quantum Monte-Carlo Methods

given a general many-body bosonic problem

$$\mathcal{H} = \sum_{i}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + \sum_{i}^{N} V_{ext}(\mathbf{r}_i) + \sum_{i<j}^{N} V_{int}(\mathbf{r}_{ij}) \qquad (1)$$

QMC solves for

- **full many-body** ground state $\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$
- **realistic** interaction potentials $V(|\mathbf{r}_i - \mathbf{r}_j|)$
- **exact** : good for finding unexpected emergent behavior
- **VPI:** ground state energy, densities, $\rho(\mathbf{r}, \mathbf{r}')$ (the OBDM)
- **fixed phase VPI, POITSE:** excited states
- **PIMC, PICF**: finite temperature properties, excited states

the one body density matrix (OBDM)

For a general time dependent N particle many body state

$$\mathbf{\Psi}_N = \sum_i c_i \psi^{(i)}(\mathbf{r}_1, \cdots, \mathbf{r}_N; t)$$

the single particle density matrix is

$$\rho(\mathbf{r}, \mathbf{r}'; t) = \langle \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}', t) \rangle$$

$$= N \sum_i c_i \int d\tilde{\mathbf{R}} \psi^{*(i)}(\mathbf{r}, \tilde{\mathbf{R}}; t) \psi^{(i)}(\mathbf{r}', \tilde{\mathbf{R}}; t)$$

where $\tilde{\mathbf{R}} = \{\mathbf{r}_2, \cdots, \mathbf{r}_N\}$

natural orbitals

The OBDM is Hermitian and so can be diagonalized

$$\rho(\mathbf{r},\mathbf{r}') = \sum_i n_i \phi_i(\mathbf{r}) \phi_i^*(\mathbf{r}')$$

where n_i are real and $\sum_i n_i = N$. $\phi_i(\mathbf{r})$ are the *natural orbitals*.

- simple condensate ::

$$\lim_{N\to\infty} n_0/N \sim 1, \quad n_{\{i>0\}}/N \sim 0$$

- fragmented condensate ::

$$n_{\{0\le i\le k\}}/N \sim 1, \quad n_{\{i>k\}}/N \sim 0$$

fragmentation vs. depletion

- In strongly interacting quantum fluids (e.g. bulk He^4), even when there is only one single particle state with large occupation, the fraction of particles occupying ϕ_0 can be very small $n_0 \lesssim 10\%$ while the rest of the eigenvalues of the OBDM still have essentially zero occupation in the thermodynamic limit.
- large **depletion** implies that the ground state is a *highly entangled* many body state (bulk He $\sim 90\%$ depletion)
- in contrast, a **fragmented** state has more than one single particle state with *large* occupation. Each of these states is a *"real condensate"* and is internally *phase coherent*.

VPI and the one-body density matrix

Variational path integral Monte Carlo (VPI):

- $T = 0$, non-periodic paths in imaginary time. Probability of a path is

$$\mathcal{P} \propto \Psi_T(R_0)\Psi_T(R_{2M}) \left\{ \prod_{m=0}^{2M-1} G_0(R_m, R_{m+1}; \tau) \right\}$$

- At 'center' of the path, distribution is independent of Ψ_T for sufficiently long paths with length $= 2M\tau$
- The one-body reduced density matrix (OBDM) is defined as:

$$\rho(r, r') = \int \psi^*(r, r_2, \ldots, r_N)\psi(r', r_2, \ldots, r_N) dr_2 \ldots dr_N$$

- Diagonalization of the OBDM yields the single-particle eigenfunctions (natural orbitals) and corresponding eigenvalues (occupation numbers)

Interaction potential models for cold atoms

- characterized by s wave scattering length
- $a > 0$

$$V_{int}(r_{ij}) = \begin{cases} 0 & r_{ij} > a \\ \infty & r_{ij} \leq a \end{cases}$$

- $a < 0$

$$V_{int}(r_{ij}) = \epsilon\left((\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6} \right)$$

- semiclassical approximation

(VV Flambaum, GF Gribakin, C Harabati PRA 59, 1998 (1999))

$$a \approx \cos(\frac{\pi}{4})(\frac{\epsilon^{1/2}\sigma^3}{4})^{1/2}[1 - \tan(\frac{\pi}{4})\tan(\gamma\ \sigma\sqrt{2\epsilon} - \frac{\pi}{8})]\frac{\Gamma(3/2)}{\Gamma(5/4)}$$

- choose ϵ, σ to eliminate bound states

Propagators for VPI

$$H = \sum_i^N -\frac{1}{2}\nabla_i^2 + V(R) + \sum_{i<j} V_{int}(r_{ij})$$

spatial configuration

$$R = \mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_N}$$

external potential

$$V(R) = \sum_i \frac{1}{2}(x_i^2 + y_i^2 + V_b\left[(z_i/\ell)^2 - \right]^2)$$

- $a < 0$: 4th order propagator
- $a > 0$: 4th order propagator for $T + V(R)$, modify for hard sphere $V_{int}(r_{ij})$ with image construction

Modified 4th order propagator for hard sphere interactions

$$G(\mathbf{R},\mathbf{R}',\tau) = \int d\mathbf{R}'' e^{-\tau/6V(\mathbf{R})} e^{-\tau/2T(\mathbf{R},\mathbf{R}'')} \times e^{-2\tau/3\tilde{V}(\mathbf{R}'')} e^{-\tau_2 T(\mathbf{R}'',\mathbf{R}')} e^{-\tau/6V(\mathbf{R}')}$$

$$\tilde{V} = V + \frac{\tau^2}{48}[V,[T,V]]$$

- modify to restricted path Green's function $G^r(\mathbf{R},\mathbf{R}',\tau)$, with

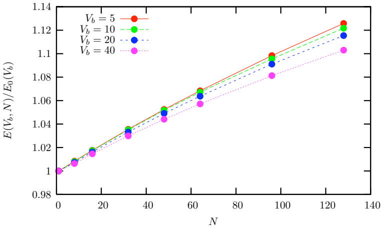
$$G^r(\mathbf{R},\mathbf{R}',\tau) = G(\mathbf{R},\mathbf{R}',\tau) - G(I(\mathbf{R}),\mathbf{R}',\tau)$$

- $I(\mathbf{R})$ is the mirror reflection of R in the plane of the hard wall
- for hard sphere interactions, this gives image correction factor to first kinetic term

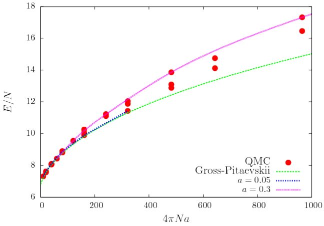
$$G(r,r',\tau) \propto \prod_{i<j} \left[1 - e^{-(r_{ij}-a)(r'_{ij}-a)/\lambda\tau}\right]$$

$a > 0$: Ground state energetics

- energy grows more slowly with higher barriers, suggests increasing fragmentation
- deviations from mean field with increasing N and larger a values



[a]

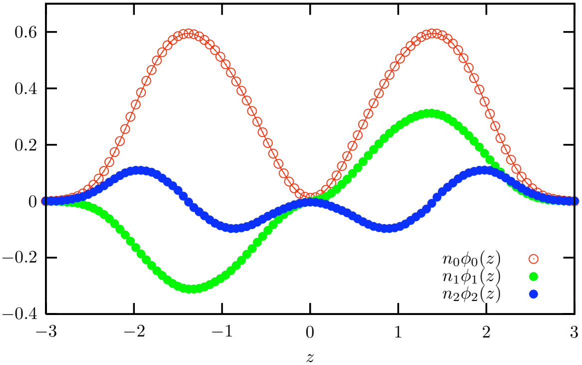


[a]

[a] DMC, a=0.01

[a] VPI

$a > 0$: Natural orbitals



i	n_i/N
0	0.75(4)
1	0.20(0)
2	0.02(5)
3	0.01(2)
4	0.00(2)

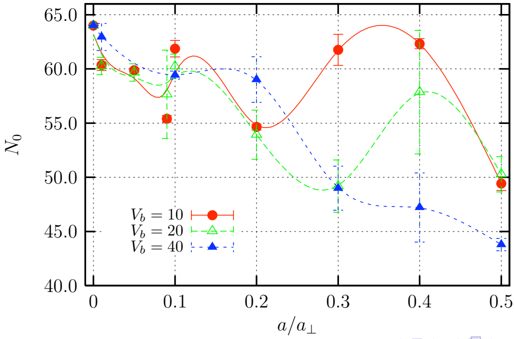
$$N = 40, \quad a/a_{ho} \approx 0.024, \quad Na \approx 0.99, \quad na^3 \approx 3 \times 10^{-4}$$

$$\sigma_{\Delta N} = \langle(\Delta N)^2\rangle - \langle\Delta N\rangle^2 \approx 1.42$$

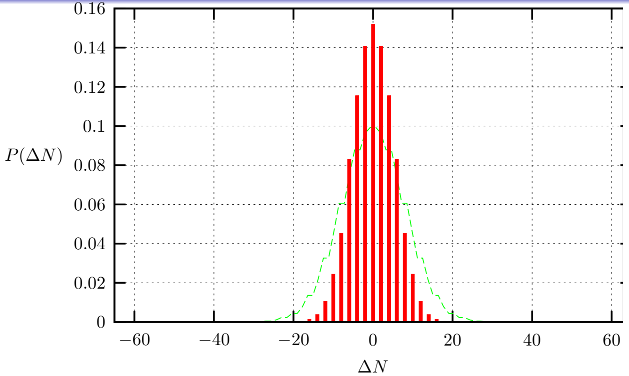
$$\rho(z, z') = \sum_i n_i \phi_i^*(z)\phi_i(z')$$

Finite Size Effects on Fragmentation

- occupation of lowest symmetric natural orbital as function of $a/a_\perp$
- $a_\perp$ is perpendicular trap length, $0.1 \le a/a_{ho} \le 0.5$, $N = 64$
- expect more fragmentation as a increases
- see non-monotonic dependence because a approaches length scale of trapping potential

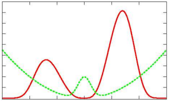


$a > 0$: squeezed states



$$P(\Delta N) = 2\langle\delta(\sum_i \Theta(z_i) - N_R)\rangle - N$$

$N = 64$, $a/a_{ho} = 0.01$, $na^3 \approx 1.5 \times 10^{-4}$, $V_b = 5$



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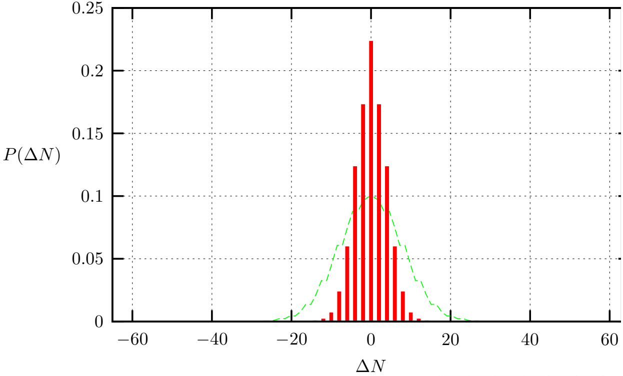
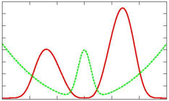


$N = 64, \quad a/a_{ho} = 0.01, \quad na^3 \approx 1.7 \times 10^{-4}, \quad V_b = 10$



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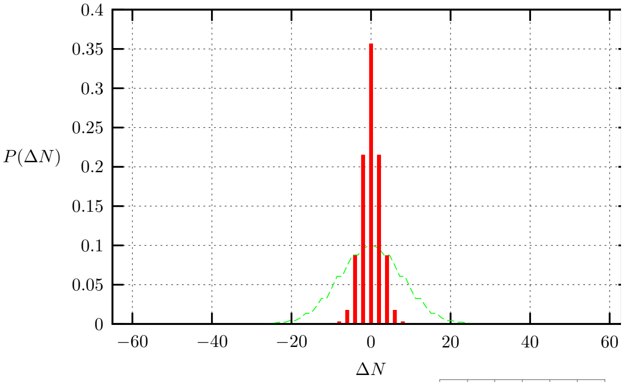
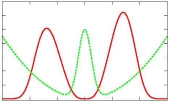
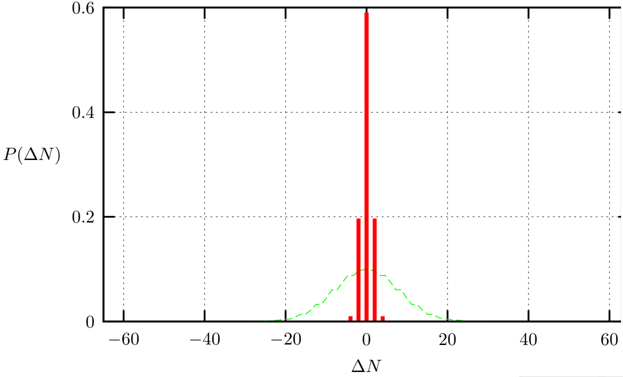
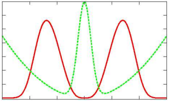


$N = 64, \quad a/a_{ho} = 0.01, \quad na^3 \approx 1.8 \times 10^{-4}, \quad V_b = 20$



$a > 0$: squeezed states

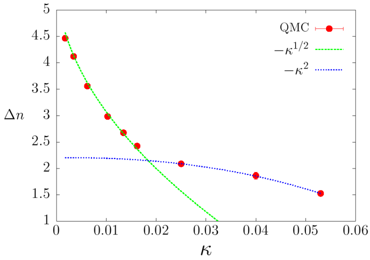




$$\Psi \approx |N/2, N/2\rangle$$

$N = 64, \quad a/a_{ho} = 0.01, \quad na^3 \approx 2.7 \times 10^{-4}, \quad V_b = 40$

Scaling of number fluctuations with interaction strength



- large N analytic two mode invalid
  - $N = 128$ is too few particles - compare exact diagonalization
  - or two mode Hamiltonian is not valid in this regime $\delta = 5\text{x}10^{-4}$, $10^{-2} < a/a_{ho} < 0.3$

Analytic two mode (based on harmonic analysis in large N limit):

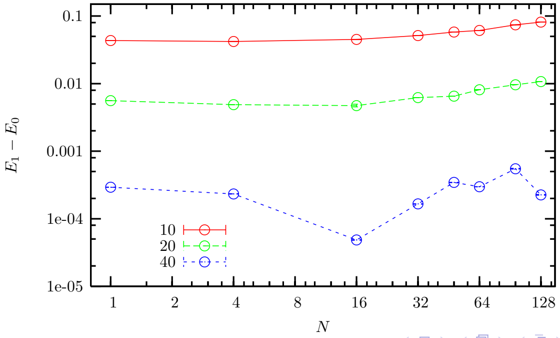
$$\Delta n = \sqrt{N/4}(\delta/(\delta + 4N\kappa))^{1/4}$$

for $\kappa > N\delta/2^{8/3} \approx 0.01$

$$\Delta n = \delta N/(8\sqrt{2}\kappa)$$

$a > 0$: Tunneling energetics

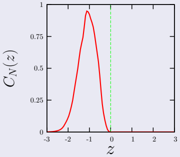
- excited state energy gives effective tunneling which decreases for higher barrier
- tunneling depends on N and a
- strong finite size effects for high barrier



$a < 0$: cat states possible

ideal cat

$|N, 0\rangle + |0, N\rangle$:



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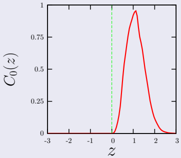
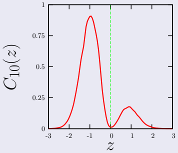


non-ideal cat

$\sum_k c_k |k, N - k\rangle$:



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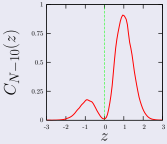


$+ \ldots$

Distinguishability Measure of Cat State Size

consider 2-branch cat state $|A\rangle + |B\rangle$

- define cat size as *the largest number of partitions, such that branches can be distinguished with probability* $1-\delta$ *by measuring any one of the partitions*
- or, if all particles are equivalent: N/n_{min}, where n_{min} is the smallest number of particles that must be measured
- $\rightarrow$ branch distinguishability problem: determine which of two possible states, $|A\rangle$ or $|B\rangle$, a given unknown state is
- motivated by recognition that $\frac{1}{\sqrt{2}}(|0000\cdots\rangle + |1111\cdots\rangle)$ requires only 1 measurement if $\langle 0|1\rangle = 0$ but more if $\langle 0|1\rangle \neq 0$ [Korsbakken, Whaley, DuBois, Cirac PRA (2007)]

How to distinguish branches

How do we describe a measurement to distinguish branches of cat-like state $|A\rangle + |B\rangle$?

- Outcomes of measurement associated with POVM elements E_A and E_B

Positive Operator Valued Measurements

Generalization of projective measurements. Set $\{E_i\}$ of non-negative Hermitian operators satisfying $\sum_i E_i = \mathbb{I}$. Probability of outcome i for density matrix ρ is $P_i = \text{tr}\,(\rho E_i)$.

- Success probability given by

$$P = \frac{1}{2}\text{tr}\,(|A\rangle\langle A|E_A) + \frac{1}{2}\text{tr}\,(|B\rangle\langle B|E_B)$$

- For an n-particle measurement, this reduces to

$$P = \frac{1}{2}\,\mathrm{tr}\left(\rho_A^{(n)} E_A^{(n)}\right) + \frac{1}{2}\,\mathrm{tr}\left(\rho_B^{(n)} E_B^{(n)}\right), \qquad E_{A,B} \equiv E_{A,B}^{(n)} \otimes \mathbb{I}^{(N-n)}$$

where $\rho_{A,B}^{(n)}$ are n-particle reduced density matrices

- Optimal measurement is projective measurement in the basis where $\rho_A^{(n)} - \rho_B^{(n)}$ is diagonal
- Corresponding success probability is (Helstrom 1976):

$$P = \frac{1}{2} + \frac{1}{4}\,\mathrm{tr}\left\|\rho_A^{(n)} - \rho_B^{(n)}\right\|$$

- If each branch is a separable state, same success probability is obtained with an adaptive scheme using only one-particle non-entangled measurements (PRA **75** 042106 (2007))

- fit QMC fluctuation number distribution $P(\Delta N)$ to form obtained from 2-state model

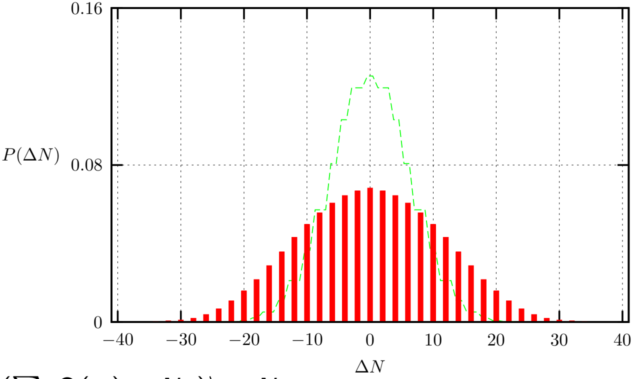
$$\int \mathrm{d}\theta\, f(\theta) \left[\left(\hat{a}^\dagger \cos\theta + \hat{b}^\dagger \sin\theta \right)^N + \left(\hat{a}^\dagger \sin\theta + \hat{b}^\dagger \cos\theta \right)^N \right] |0\rangle$$

$$f(\theta) = C_{\mathcal{N}} \exp\left(\frac{-(\theta - \theta_0)^2}{2\sigma^2}\right)$$

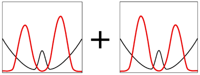
  - orthogonal branches for $\theta_0 = 0$
  - completely overlapping branches for $\theta_0 = \pm\pi/4$
  - σ measures spread of branches (also causes overlap)

- n-RDM calculations possible with this form, yields cat size C_δ
- Korsbakken, DuBois, Cirac, Whaley, PRA 2007

$a < 0$: Number distribution



$$P(\Delta N) = 2\langle \delta(\sum_i \Theta(z_i) - N_R)\rangle - N$$



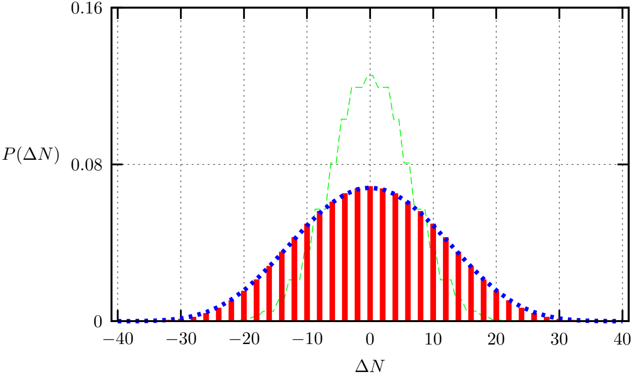
N$= 40$, N$|a|/a_{ho} = 0.11$, $V_b = 10\hbar\omega$

$a < 0$: Number distribution

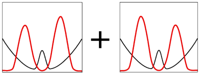
size

$C_\delta = 0$

$\delta = 10^{-2}$



N= 40, $N|a|/a_{ho} = 0.11$, $V_b = 10\hbar\omega$



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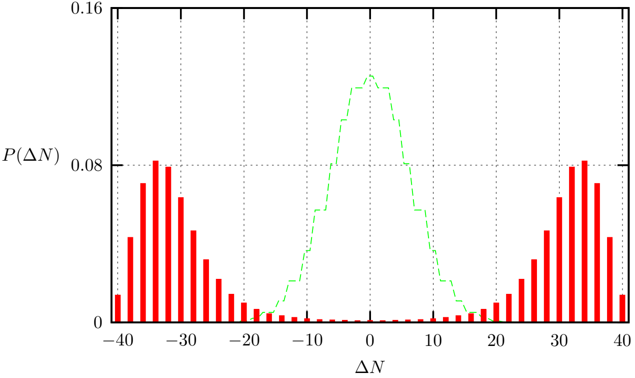
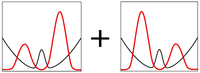


N= 40, $N|a|/a_{ho} = 0.11$, $V_b = 15\hbar\omega$

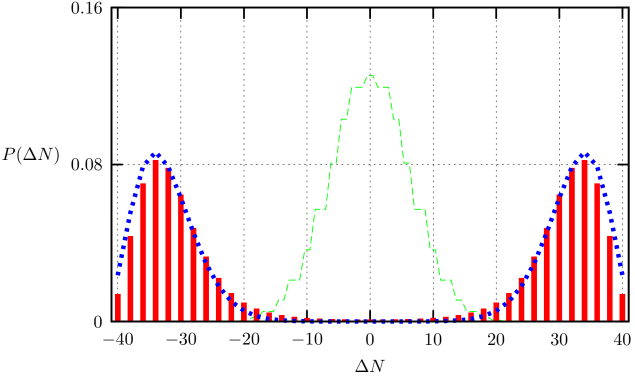


$a < 0$: Number distribution

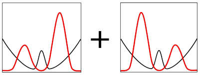
size

$C_\delta = 10$

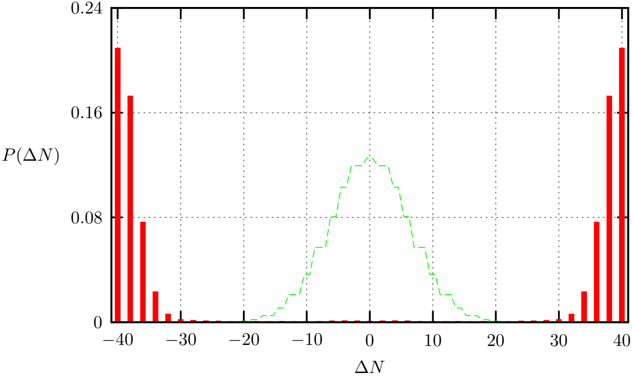
$\delta = 10^{-2}$



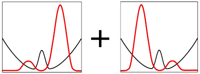
N= 40, $N|a|/a_{ho} = 0.11$, $V_b = 15\hbar\omega$



$a < 0$: Number distribution



N= 40, $N|a|/a_{ho} = 0.11$, $V_b = 20\hbar\omega$

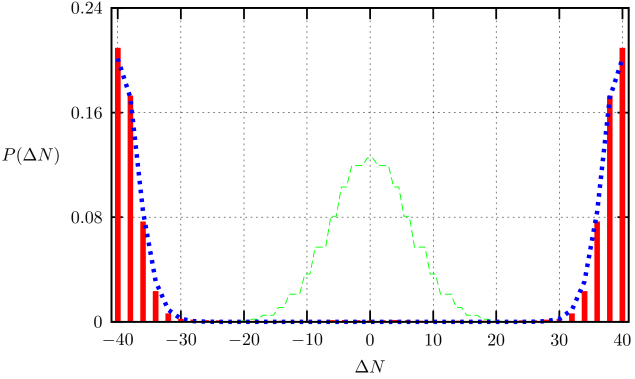


$a < 0$: Number distribution

size

$C_\delta = 20$

$\delta = 10^{-2}$



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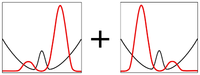
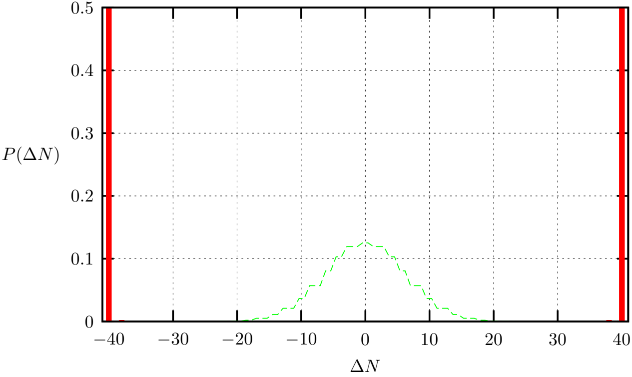
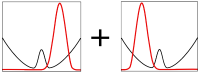


$a < 0$: Number distribution "MEOW!!"



N$= 40$, N$|a|/a_{ho} = 0.22$, $V_b = 120\hbar\omega$



$a < 0$: Number distribution "MEOW!!"

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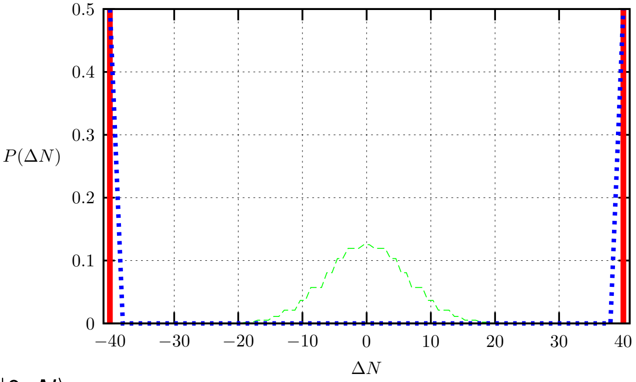
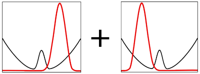
$C_\delta = 40$

$\delta = 10^{-2}$



$\Psi \approx |N, 0\rangle + |0, N\rangle$



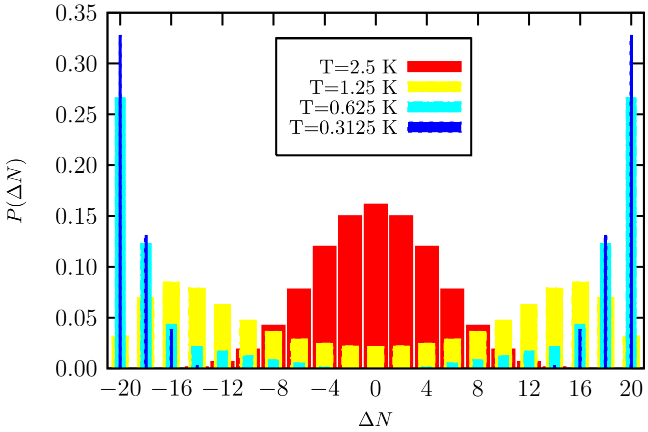
$N = 40,\ N|a|/a_{ho} = 0.22,\ V_b = 120\hbar\omega$

liquid ^{4}He in a double well potential

^{4}He in a double well : parameters

- Aziz-1992 potential
- $N = 20$
- barrier width $a_b = 0.15$ Å
- barrier height 10 K
- trap frequency $\omega = 0.1$ Hz

Cats in liquid ^{4}He: N=20



cattiness at T=0.31 K (cold cat)

for $\delta = 0.01$, $C_\delta = 10$; *for* $\delta = 10^{-5}$, $C_\delta = 5$

Summary

- VPI for strongly interacting bosons in double well potential
- repulsive bosons - finite size effects on squeezing
- attractive bosons - cat states, also for helium
- validity of two mode approximations
- excitations...