ICFP M2 Advanced Quantum Mechanics: Problem #3

D.J. Papoular & F. Chevy

November 19, 2024

1 The Bose–Hubbard Hamiltonian

We consider a collection of cold bosonic atoms (e.g. ^{87}Rb) trapped inside an optical lattice potential. This potential is a (3D, 2D, or 1D) periodic array of wells in which can be either shallow (Fig. 1 left) of deep (Fig. 1 right). This optical potential results from a stationary light wave, obtained e.g. by retro–reflecting a laser in each of the trapping directions.

The simplest description for ultracold bosonic atoms in a spatially periodic potential is the Bose–Hubbard model, which involves two real parameters: the tunnelling amplitude $J > 0$ and the interaction strength U. The corresponding (second–quantised) Hamiltonian reads:

$$H = -J \sum_{<i,j>} a_i^\dagger a_j \quad + \quad \frac{U}{2} \sum_i n_i(n_i - 1)\ . \tag{1}$$

In Eq. (1), the bosonic operator $a_i^\dagger$ creates a particle on the site i, and its conjugate a_i annihilates a particle on the same site. The sum $\sum_{<i,j>}$ is taken over all neighbouring sites $< i, j >$, and the parameter $J > 0$ describes the amplitude for the tunnelling process of a particle from one site to a neighbouring one. The operator $n_i = a_i^\dagger a_i$ counts the number of particles on site i, and the parameter U sets the interaction strength between particles on the same site. Tunnelling between non–neighbouring sites is neglected; the interaction between atoms in different sites is neglected.

Large systems described by the Hamiltonian of Eq. 1 exhibit a quantum phase transition, i.e. a phase transition at zero temperature, because of the competition between *(i)* the tunnelling mechanism proportional to J, which tends to delocalise particles over the whole lattice, and *(ii)* the interaction term proportional to U, which for repulsive interactions ($U > 0$) favours atom numbers on each site satisfying $n_i \leq 1$.

1. What is the criterion on U and J for the system to be *(a)* in the shallow–lattice regime of Fig. 1 left? *(b)* in the deep–lattice regime of Fig. 1 right?

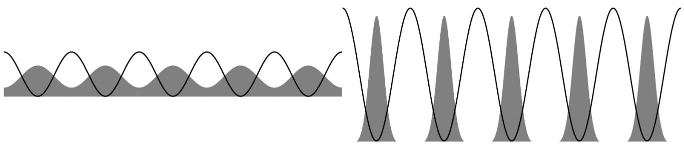

Figure 1 Schematics of the ground state of an ultracold Bose gas trapped in an optical lattice in two different regimes. Left: for a shallow optical lattice, the many–body ground state is a macroscopic coherent wavefunction delocalised over the whole lattice. Right: for a deep optical lattice, each atom is localised at a given site.

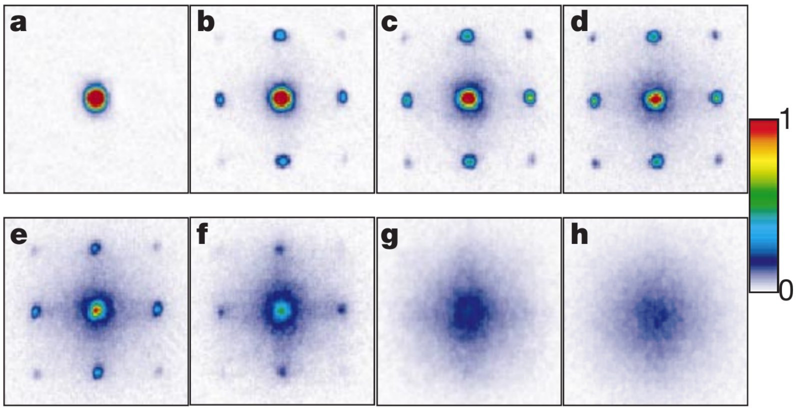

Figure 2 Interference images obtained after switching off the optical lattice potentials. The initial barrier height increases from *(a)* to *(h)*. For low barrier heights *(a)*, the interferogram has a very high visibility; the visibility vanishes for high barriers *(h)*. Reproduced from Ref. [1].

2 The superfluid–to–Mott insulator transition

In this section, we assume that the total number of atoms, N_a, is equal to the total number of sites of the optical lattice potential, $N_l = N_a$, meaning that the filling factor of the lattice is 1.

2.1 The Mott insulator state

We call $|\mathrm{M}\rangle$ the Mott insulator state, for which each lattice site contains a single atom:

$$|\mathrm{M}\rangle = a_1^\dagger \cdots a_N^\dagger \, |\mathrm{vac}\rangle \quad . \tag{2}$$

2. What are the atom number fluctuations on each site?
   Justify that the one–body density matrix $\rho^{(1)}(i,j) = \langle \mathrm{M}|a_i^\dagger a_j|\mathrm{M}\rangle = 0$ for $i \neq j$.
   Does the system exhibit coherence between two different sites?

3. Show that the energy $\langle \mathrm{M}|H|\mathrm{M}\rangle = 0$.

4. In which of the two limits of Question 1 is $|\mathrm{M}\rangle$ an exact eigenstate of H?

2.2 The superfluid state

We call $|\mathrm{SF}\rangle$ the superfluid state defined as follows:

$$|\mathrm{SF}\rangle = \frac{1}{\sqrt{N_a!}} \, a_{\boldsymbol{k}=\mathbf{0}}^{\dagger N_a} \, |\mathrm{vac}\rangle = \frac{1}{\sqrt{N_a!}} \left(\frac{1}{\sqrt{N_l}} \sum_i a_i^\dagger \right)^{N_a} |\mathrm{vac}\rangle \quad . \tag{3}$$

5. In which of the two limits of Question 1 is $|\mathrm{SF}\rangle$ an exact eigenstate of H?
   Prove it, and show that, for a 1D lattice, the corresponding energy is $-2JN_a$.
   Hint: Apply periodic boundary conditions and use Bloch's theorem.

6. Justify that the average occupation number in the site i is $\langle \mathrm{SF}|a_i^\dagger a_i|\mathrm{SF}\rangle = 1$.
   Show that the off–diagonal one–body density matrix is $\rho^{(1)}(i,j) = \langle \mathrm{SF}|a_i^\dagger a_j|\mathrm{SF}\rangle = 1$.
   Does the system exhibit coherence between two given sites?

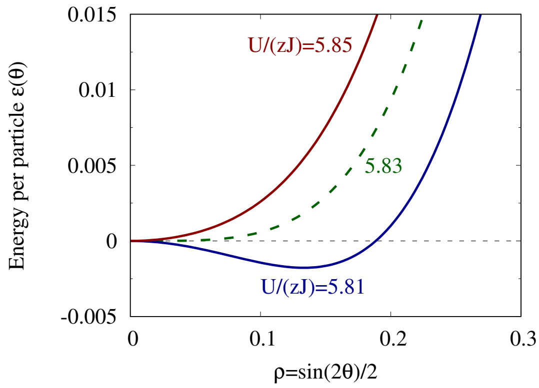

Figure 3 Plot of the function $\epsilon(\theta) = 2\langle\Psi_\theta|H|\Psi_\theta\rangle/(NzJ)$ as a function of $\rho = \sin(2\theta)/2$, for values of $U/(zJ)$ below (blue) and above (red) the critical value $U/(zJ) = 3 + 2\sqrt{2}$ (green).

2.3 The phase transition

In order to approximately determine the critical value of U/J for which the transition occurs, we apply the variational approach to the family of N–body wavefunctions ($|\Psi_\theta\rangle$) defined by:

$$|\Psi_\theta\rangle = \prod_{i=1}^{N_l} \left[\cos\theta\,|n_i = 1\rangle + \sin\theta \frac{|n_i = 0\rangle + |n_i = 2\rangle}{\sqrt{2}}\right] . \tag{4}$$

In the wavefunction of Eq. (4), all sites are in the same quantum state (Hartree–type ansatz).

7. In the many–body state $|\Psi_\theta\rangle$, is the total number of atoms rigorously fixed?
   If not, calculate its mean value $< N >$ and its standard deviation ΔN.

8. Which value of θ leads to $|\Psi_\theta\rangle = |\mathrm{MI}\rangle$?
   For which value of θ does $|\Psi_\theta\rangle$ play the role of $|\mathrm{SF}\rangle$?

9. We call z the number of nearest neighbours for a given site.
   What is z for a 1D lattice? for a 2D square lattice? for a 3D cubic lattice?

10. Show that the expectation value for the energy in the state $|\Psi_\theta\rangle$ reads:

$$\langle\Psi_\theta|\,H\,|\Psi_\theta\rangle = N\,\frac{\sin^2\theta}{2}\left[U - zJ(3 + 2\sqrt{2})\cos^2\theta\right] . \tag{5}$$

11. Deduce from Eq. (5) that, if $U/(zJ) > (3 + 2\sqrt{2})$, the ground state is a Mott insulator, whereas the ground state exhibits coherence for $U/(zJ) < (3 + 2\sqrt{2})$.

12. In the vicinity of the critical point $U/(zJ) = 3 + 2\sqrt{2}$, we let $\rho = \sin(2\theta)/2$.
    a) For $|\rho| \ll 1$, show that Eq. (5) reduces to:

$$\frac{2}{NzJ}\langle\Psi_\theta|H|\Psi_\theta\rangle = \frac{U}{zJ}\rho^4 - \left[(3 + 2\sqrt{2}) - \frac{U}{zJ}\right]\rho^2 . \tag{6}$$

    Hint: Use $\sin^2\theta \approx \rho^2 + \rho^4$.

    b) Using Fig. 3, justify that we are dealing with a second–order phase transition.

    c) What is the order parameter? Which is the broken symmetry?
    Hint: There is a link to Question 19 below.

13. For which geometry is the mean–field approach expected to be most accurate?

14. Use your answers to Questions 2 and 6 to interpret the experimental results of Fig. 2.

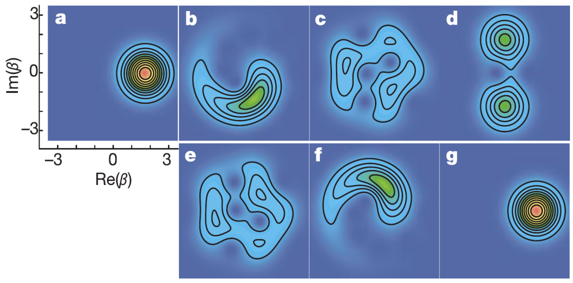

Figure 4 Quantum dynamics of a coherent state of the atoms owing to cold collisions. Here, we consider a single well which initially contains multiple atoms whose wavefunction $|\alpha\rangle$ is a coherent state at $t = 0$ *(a)*. As time evolves *(a–g)*, the wavefunction $|\psi(t)\rangle$ distorts due to the collisions between the atoms. For a given time, the authors plot the overlap $|\langle\beta|\psi(t)\rangle|^2$ of the state $|\psi(t)\rangle$ with an arbitrary coherent state $|\beta\rangle$. Reproduced from Ref. [2].

3 Collapse and revival of the coherent matter–wave field

3.1 Modelling the quantum state of a single site with a coherent state

In this section, we assume that $N_a = \nu N_l$, where the integer ν is the filling factor of the lattice. We assume that the system is initially deep in the superfluid regime, so that its many–body wavefunction is the quantum state $|\mathrm{SF}\rangle$ of Eq. (3).

15. Show that, for N_a large enough, $|\mathrm{SF}\rangle$ practically coincides with the following state:

$$|\Psi_{\mathrm{coh}}\rangle = e^{-N_a/2} \exp\left(\sqrt{N_a}\, a^\dagger_{\boldsymbol{k}=\boldsymbol{0}}\right) |\mathrm{vac}\rangle \quad . \tag{7}$$

Hint: What is the probability distribution for the total number N of particles in the state $|\Psi_{\mathrm{coh}}\rangle$?

16. Show that $|\Psi_{\mathrm{coh}}\rangle$ factorises into a product of quantum states for each lattice site, each site being in the same coherent state $|\alpha\rangle$: $|\Psi_{\mathrm{coh}}\rangle = |\alpha_1\rangle \cdots |\alpha_{N_l}\rangle$. Give the amplitude α of this coherent state, and the corresponding mean particle number and variance.

3.2 Quantum dynamics of the state on a single site

For $t < 0$, the system is deep in the superfluid regime. At $t = 0$, we abruptly increase the height of the potential wells, so that $J = 0$. We focus on a single site of the lattice.

17. Using your answer to Question 16,
determine the initial quantum state $|\psi(t = 0)\rangle$ of the single lattice site.

18. What drives the dynamics of this quantum state?
Justify that, for $t > 0$, the site is in the following state:

$$|\psi(t)\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \exp\left[-iUn(n-1)t/(2\hbar)\right] |n\rangle \quad . \tag{8}$$

19. Show that the average value $\phi(t) = \langle\psi(t)|a|\psi(t)\rangle$ satisfies:

$$\phi(t) = \alpha \exp\left[|\alpha|^2 \left(e^{-iUt/\hbar} - 1\right)\right] \quad . \tag{9}$$

20. Show that the coherent character of the quantum state collapses at short times.
What sets the characteristic time for this collapse?

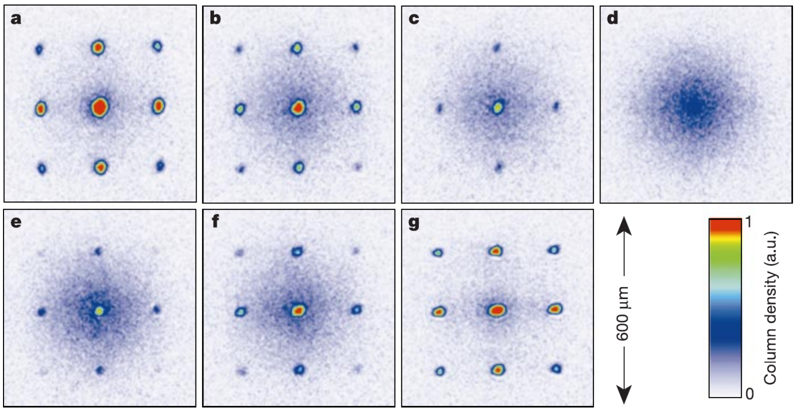

Figure 5 Interference images demonstrating the collapse and revival of quantum coherence. Initially, the gas is prepared in a superfluid state in a shallow lattice. At time $t = 0$, the height of the potential barriers is suddenly increased so as to isolate each site of the optical lattice. The gas is held in this deep lattice for a variable time t, which increases from *(a)* to *(g)*. Finally, the optical potential is turned off and the gas expands, leading to the various interferograms. Reproduced from Ref. [2].

21. The time evolution of the state $|\psi(t)\rangle$ is illustrated on Fig. 4.
Argue why the dynamics of $|\psi(t)\rangle$ is richer than that of $\phi(t)$. Justify that the characteristic phase washout time is different for $|\psi(t)\rangle$ and $\phi(t)$.
Does the phase washout signal a complete loss of coherence?

22. Show that, for times that are integer multiples of $t_R = h/U = 2\pi\hbar/U$, the state $|\psi(t)\rangle$ exactly coincides with the initial state, i.e. the system exhibits a revival of the initial coherence.

23. Show that, at the time $t = t_R/2$, the system is in a "Schrödinger cat" state, i.e. a superposition of two coherent states $|i\alpha\rangle$ and $|-i\alpha\rangle$, with the amplitudes $i\alpha$ and $-i\alpha$:
$$|\psi(t_R/2)\rangle = \frac{1}{\sqrt{2}}\left(e^{-i\pi/4}\,|i\alpha\rangle + e^{i\pi/4}\,|-i\alpha\rangle\right) \ . \tag{10}$$
What is the average value $\phi(t_R/2)$?
Hint for the calculation of $|\psi(t_R/2)\rangle$: For any integer n, $e^{-i\pi n(n-1)/2} = [e^{-i\pi/4}e^{in\pi/2} + e^{i\pi/4}e^{-in\pi/2}]/\sqrt{2}$.

24. Use your answers to Questions 17– 23 to interpret the experimental results shown in Fig. 5.

Further reading

Introductory

- Coherent states play a key role in Quantum Optics. A detailed description of their experimental production and manipulation is given in Ref. [3, chaps. 3 & 8].
- Section 20.4 of Ref. [4] provides an introduction to the Poisson distribution applied to classical gases.
- An accessible introduction to the physics of ultracold atoms in optical lattices may be found in §7.4.5 and §14.4.3 of Ref. [5]. Section 26.3 of the same book provides simple ideas concerning the superfluid–to–Mott insulator phase transition.

More advanced

- Broken symmetries and phase transitions are introduced in simple terms in Ref. [6, chap. 5]. Landau's approach for the description of critical phenomena is reviewed in Ref. [7, chap. 17].
- The collapse and revival of quantum coherence were first observed in a Cavity Quantum ElectroDynamics (CQED) experiment [8]. There, the cavity was initially prepared to contain a coherent state of the electromagnetic field. A single atom crossing the cavity underwent Rabi oscillations involving many frequencies corresponding to each of the Fock–state components of the coherent state. Their Fig. 2 on p. 3 is particularly eloquent: it presents the collapse and revival of the Rabi oscillations and shows how these signals can be analysed to reconstruct the initial photon number distribution.

References

[1] M. Greiner, O. Mandel, T. W. Hänsch, I. Bloch, Nature **419**, 51 (2002).

[2] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, I. Bloch, Nature **415**, 39 (2002).

[3] S. Haroche, J. Raimond, *Exploring the quantum*, Oxford University Press (2006).

[4] W. Appel, *Mathematics for Physics and Physicists*, Princeton University Press (2007).

[5] C. Cohen-Tannoudji, D. Guéry-Odelin, *Advances in atomic physics: an overview*, World Scientific (2011).

[6] J. Iliopoulos, *The origin of mass*, Oxford University Press (2017).

[7] K. Huang, *Statistical Mechanics*, Wiley, 2nd ed. (1987).

[8] M. Brune, et al., Phys. Rev. Lett. **76**, 1800 (1996).