Week 13

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
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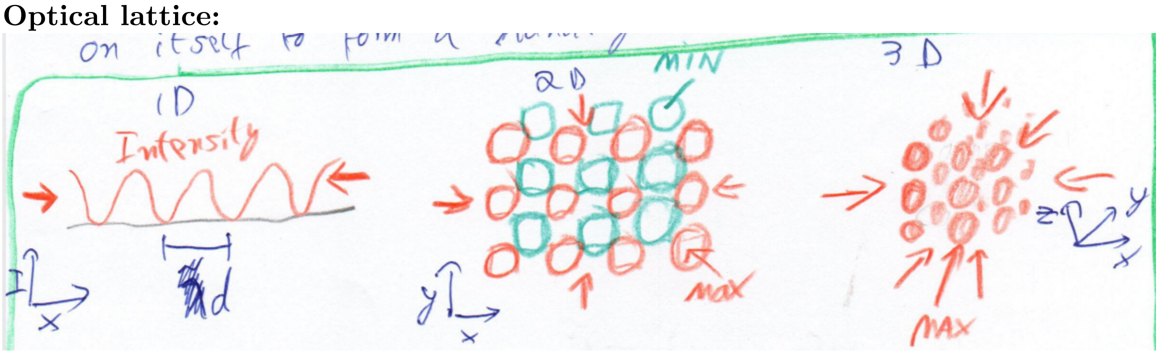
5.4 Lattice Models

We have mentioned few times, the similarities between an electron gas in a crystal lattice and a cold atomic gas in an optical lattice. Now few more details on the latter:

5.4.1 Optical lattices

Consider a coherent laser beam which is back-reflected on itself to form a standing wave in

Optical lattice:



- We obtain an intensity pattern for the light that can be written as,

$$I(x) = I_0 \cos^2(k_L x) \tag{5.8}$$

where $d = \frac{\lambda_L}{2}$ is the distance between adjacent sites, λ_L is laser wavelength and $k_L = \frac{2\pi}{\lambda_L}$.

We can calculate the energy shift of an atom due to exposure to the rapidly varying E-field of the laser (AC Stark shift). This shifts turns I(x) into a spatial potential

$$V(x) = -\frac{1}{2}\alpha(\omega) \underbrace{\langle \epsilon(t)^2 \rangle_t}_{\substack{\text{time avg of} \\ \text{light intensity}}} \tag{5.9}$$

where α is the atomic polarizability and ω is the laser frequency.

We find $\alpha(\omega) < 0$, just above an atomic resonance (blue detuned) $\implies V > 0$.

$\cdots\ \cdots\ \alpha(\omega) > 0$, just below $\cdots\ \cdots\ \cdots\ \cdots\ \cdots$ (red detuned) $\implies V < 0$.

(See PHY 402, Assignment 4, also c.f. section 5.1 and Mid-sem exam). We thus have an

Optical lattice potential

$$V(x) = V_0 \cos^2(k_L x), \tag{5.10}$$

where V_0 can be positive or negative dependent on light detuning.

5.4.2 Bose-Hubbard Model

You had shown in the mid-term exam how starting from Eq. (3.37) [$\hat{H}$ for Bose gas in form with $\hat{\Psi}$], we can derive

Bose-Hubbard Hamiltonian

$$\hat{K} = \hat{H} - \mu\hat{N} = \sum_m \left[J(\hat{a}^\dagger_{m+1}\hat{a}_m + \hat{a}^\dagger_{m-1}\hat{a}_m) + \frac{U}{2}\hat{n}_m(\hat{n}_m - 1) - \tilde{\mu}\hat{n}_m \right] \tag{5.11}$$

- $\hat{a}^\dagger_m$ creates an atom "on site m". 

- J allows <u>tunneling/hopping</u> from site to site.
- U are repulsive <u>on-site interactions</u> $\hat{n}_m = \hat{a}^\dagger_m\hat{a}_m$
- $\tilde{\mu} = \mu - E$ ($E \to$ on site energy) is the chemical potential.

<u>Let us try to find ground-states of $\hat{K}$ in two simple cases</u>

[A] <u>$J = 0$</u>, no tunelling:

No tunneling, $[\hat{K}, \hat{n}_m] = 0 \implies$ We can write eigenstates as Fock-states $|\,\mathbf{N}\,\rangle$. Since all sites are equivalent, we pick $|\,\mathbf{N}_0\,\rangle = |\,M, M, \cdots, M\,\rangle$, i.e. a state with exactly <u>M bosons</u> per site. Its energy is

$$\langle\,\mathbf{N}_0\,|\mathbf{K}|\,\mathbf{N}_0\,\rangle = N_{\text{sites}}[\frac{U}{2}M(M-1) - \tilde{\mu}M]. \tag{5.12}$$

This is minimized by $M = \frac{\tilde{\mu}}{U} + \frac{1}{2}$. Since M has to be an integer, for parameters $\tilde{\mu}$, U in the range $M - 1 < \frac{\tilde{\mu}}{U} < M$ we have exactly M bosons per site. This is called the

Mott-insulating state

$$| \psi_{\text{Mott}} \rangle = \sum_m \frac{(\hat{a}_m^\dagger)^M}{\sqrt{M!}} | 0 \rangle, \tag{5.13}$$

- The sum here runs over the lattice sites.
- Mott-insulator in condensed matter: A material that should conduct from band-theory (i.e. based on single particle physics), but does not due to $e^- - e^-$ interactions (i.e. due to many-body physics).

[B] $\underline{U = 0}$ **no interactions:** This becomes a single particle problem

Find eigen-states of the single-particle Hamiltonian, lowest state

$$| \varphi_0 \rangle = \frac{1}{\sqrt{N_{\text{states}}}} \sum_m \hat{a}_m^\dagger | 0 \rangle \tag{5.14}$$

(particle fully de-localized on lattice)

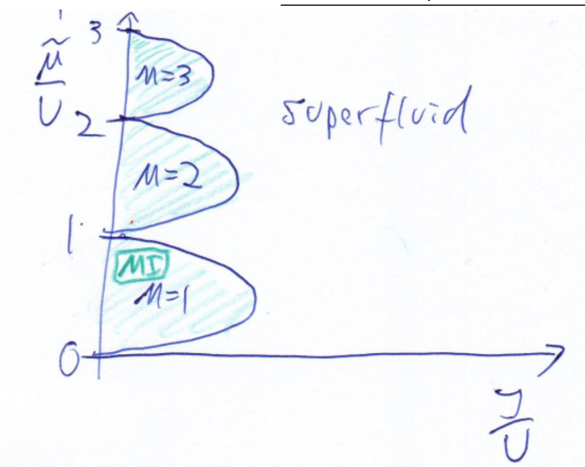
- We know at $T = 0$ we will have a BEC condensed in $| \varphi_0 \rangle$ and can use mean-field theory.

Super-fluid state

$$| \psi_{\text{BEC}} \rangle = \mathcal{N} \left(\sum_m \hat{a}_m^\dagger \right)^M | 0 \rangle \qquad \mathcal{N} \text{ is a Normalization factor,} \tag{5.15}$$

[C] For both, non-vanishing interactions and hopping, $U \neq 0, J = 0$, we require a more complicated analysis. The result of that would be:

Phase-diagram for superfluid/Mott-insulator Quantum phase transition:



left:

- Mott insulating phase is shown in green.
- Transitions between green and white are called quantum phase transition, because they can happen due to change of parameters in the Hamiltonian, but at zero temperature $T = 0$.

From Eq. (5.13) and Eq. (5.15) we can calculate the inter-site coherence

$$g_{m,m+1} = \langle \hat{a}_m^\dagger \hat{a}_{m+1} \rangle \tag{5.16}$$

We find $g = 0$ for the Mott insulator (5.13) and $g \neq 0$ for the superfluid (5.15) (Exercise).

This means atoms from different sites interfere in a superfluid state after time-of-flight expansion, but not in the Mott-insulator $\implies$ clear experimental signature, see Greiner *et. al*, Nature **415** 39 (2002).

The End

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