PHYS 635, MBQM

Fall 2019, mid-term

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1. **Bose-Einstein condensates:** Consider N Bosonic atoms of mass m in a 3D isotropic harmonic trap $V(\mathbf{x}) = \frac{1}{2}m\omega^2\mathbf{x}^2$ that undergo Bose-Einstein condensation.
   (a) (2 points) What is the first quantized many body wavefunction at $T = 0$ if we neglect interactions? How do we write this as a Fock state? [max 2 lines]
   (b) (4 points) Now use a field-operator $\hat{\Psi}(\mathbf{x})$ to describe these atoms, take into account contact interactions as discussed in the lecture [no need to justify them] and derive an equation of motion for $\hat{\Psi}(\mathbf{x})$.
   (c) (2 points) Now assume the field-operator acquires a non-vanishing expectation value upon condensation, such that $\langle\hat{\Psi}\rangle \approx \phi_0$, and find an equation from which you can obtain $\phi_0(\mathbf{x}, t)$ if you know its initial state $\phi_0(\mathbf{x}, 0)$. *You may approximate* $\langle\hat{\Psi}^\dagger\hat{\Psi}\hat{\Psi}\rangle \approx \phi_0^*\phi_0\phi_0$.
   (d) (2 points) Discuss all the physical requirements for validity of the equation based on the derivation above. List at least two. [max 6 lines]

Solution:

(a) $\psi(\mathbf{x}) = \prod_k \varphi_0(x_k)$. Fock state $|\, N, 0, 0, 0, 0, 0\,\rangle$.

(b) see solution of assignment 3.

(c) see solution of assignment 3.

(d) (i) For the use of the contact interactions we needed a dilute gas, relative to the range of interactions $\bar{d} \gg R$. We also need low temperature for the s-wave approximation.
   (ii) We need condensation or coherence, in order to make the replacement $\langle\hat{\Psi}\rangle \approx \phi_0$, thus very low T.

2. **Second quantised Hamiltonian:** Consider a 1D Bose gas in a one dimensional optical lattice with a potential $V(x) = V_0 \cos(2\pi x/\lambda)^2$. The single particle Hamiltonian (for $\hbar = m = 1$) is:

$$\hat{H}_0 = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x). \tag{1}$$

Assume any two atoms k, l interact with contact interactions $U(x_k - k_l) = U_0\delta(x_k - x_l)$.

(a) (2 points) From the information above assemble an explicit first-quantized many-body Hamiltonian $\hat{H}$ for N atoms.

(b) (2 points) Identify the location of all local minima of the optical lattice potential, number these with a site-index m, with minima location x_m. For sufficiently strong potential (large V_0), we can assume atoms are always trapped in harmonic oscillator ground-states localized at each minimum, with wave-function $\varphi_m(x) = \exp\left[-(x - x_m)^2/2/\sigma^2\right]/(\pi\sigma^2)^{1/4}$. This wave function is called (approximate) Wannier state. Make a sketch of $V(x)$ and two adjacent $\varphi_m(x)$, for this assume $\sigma \approx \lambda/2$, so that adjacent Wannier functions overlapp a bit in the tails, but not much.

(c) (8 points) For each Wannier state $\varphi_m(x)$, we define an associated pair of creation and destruction operators $\hat{a}_m^\dagger$, $\hat{a}_m$. Assuming the Wannier states are the only required single particle states, convert the first-quantized Hamiltonian from (a) into second quantized form with explicit steps. Show

$$\hat{H} = \sum_m \left\{ \bar{E}\hat{a}_m^\dagger \hat{a}_m + \bar{J}[\hat{a}_{m+1}^\dagger \hat{a}_m + \hat{a}_{m-1}^\dagger \hat{a}_m] + \bar{U}\hat{n}_m(\hat{n}_m - 1) \right\}, \tag{2}$$

with $\hat{n}_m = \hat{a}_m^\dagger \hat{a}_m$, by using the simplifications:

(i) $\int dx\ \varphi_n^*(x)\hat{H}_0\varphi_n(x) = \hbar\omega/2$, where ω matches the trap frequency of a second order taylor expansion of $V(x)$ around x_n.

(ii) $\int dx\ \varphi_n^*(x)\hat{H}_0\varphi_{n\pm k}(x) \neq 0$, if $k = 1$ but vanishes for $k > 1$.

(iii) $\int dx\ \varphi_n^*(x)\varphi_m^*(x)\varphi_k(x)\varphi_l(x) \neq 0$, only if $k = l = m = n$.

Determine the integrals that define $\bar{E}$, $\bar{J}$, $\bar{U}$, without trying to evaluate them.

(d) (4 points) [max 6 lines] Discuss the physical meaning of each term in the Hamiltonian above.

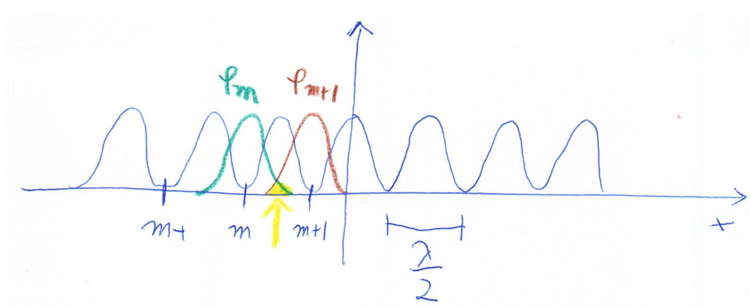

Figure 1: Sketch for (2b).

Solution:

(a) The many body Hamiltonian reads $\hat{H} = \sum_k^N \left[-\frac{1}{2}\frac{\partial^2}{\partial x_k^2} + V(x_k) + \frac{1}{2}\sum_l U_0\delta(|x_k - x_l|)\right]$.

(b) Minima of $\cos^2$ are at $x_m = \lambda/2(\pm m + 1/2)$ $m \in \mathbb{I}$. See sketch Fig. 1. Adjacent Wannier fct in green and brown, overlapp in yellow.

(c) From lecture (2.21) $\hat{H} = \sum_{nm} A_{nm}\hat{a}_n^\dagger \hat{a}_m + \sum_{nm;kl} B_{nm,kl}\hat{a}_n^\dagger \hat{a}_m^\dagger \hat{a}_k \hat{a}_l$, with $A_{nm} = \langle \varphi_n | \hat{A} | \varphi_m \rangle$ and $B_{nm,kl} = \langle \varphi_n\varphi_m | \hat{B} | \varphi_k\varphi_l \rangle$. Since we said Wannier states more than two sites away do not overlapp, $A_{nm} = 2$ for $|n-m| \gtrsim 2$, leaving the three terms with $\bar{E} = \int dx \varphi_0^*(x)[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)]\varphi_0(x)$ and $\bar{J} = \int dx \varphi_0^*(x)[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)]\varphi_1(x)$ in the single body sector. [*optional statement:* For tightly trapped atoms you can approximate the cosine by a parabola whereever $\varphi_0(x)$ is significant, thus $\bar{E} \approx \hbar\omega/2$, where ω can be found from a Taylor expansion of the cosine.]

$B_{nm,kl} = \int dxdy \varphi_n^*(x)\varphi_m^*(y)[U_0/2]\delta(x-y)\varphi_k(x)\varphi_l(y) = U_0/2 \int dx \varphi_n^*(x)\varphi_m^*(x)\varphi_k(x)\varphi_l(x) \overset{hint(iii)}{=} \delta_{nm}\delta_{mk}\delta_{kl}U_0/2 \int dx |\varphi_n(x)|^4$. Thus $\bar{U} = U_0/2 \int dx\; \varphi_0^*(x)\varphi_0^*(x)\varphi_0(x)\varphi_0(x)$.

(d) Term $\sim \bar{E}$ is single particle ground state energy on site m (oscillator ground state energy). Term $\sim \bar{J}$ describes quantum tunneling of an atom from one site to the next. Term $\sim \bar{U}$ describes collisional interactions when more than one atom share the same site.

3. **Ideal Bose gas, density fluctuations:** Consider N Bosonic atoms in a 1D harmonic trap. To measure local density, we count atoms in a small region of size L, which corresponds to the operator

$$\hat{n}_{\text{loc}}(x_0) = \int_{x_0}^{x_0+L} dx\;\; \hat{\Psi}^\dagger(x)\hat{\Psi}(x), \tag{3}$$

and then use $\hat{\rho} = n_{\text{loc}}(x_0)/L$ to get a density.

Let us define the local number uncertainty

$$\Delta n_{\text{loc}}(x_0)^2 = \langle \hat{n}_{\text{loc}}(x_0)^2 \rangle - \langle \hat{n}_{\text{loc}}(x_0) \rangle^2. \tag{4}$$

We also define

$$p_{\text{loc}} = \int_{x_0}^{x_0+L} dx |\varphi_0(x)|^2, \tag{5}$$

which is the local probability to find an individual atom near x_0 in state 0.

(a) (5 points) Assume the many-body quantum state is $\psi = |N, 0, 0, 0\cdots\rangle$, i.e. all N atoms are in the ground state. Show that the mean local number in that state is $\langle \hat{n}_{\text{loc}}(x_0) \rangle = N p_{\text{loc}}$.

(b) (5 points) Then show that the local number uncertainty in Eq. 4 is $N(p_{\text{loc}} - p_{\text{loc}}^2)$.

Solution:

(a) see solution of assignment 2.

(b) see solution of assignment 2.

4. **Quantum fields:** Consider a Bose gas of atoms with spin $s = 1$. The field operator is $\hat{\Psi}_k(\mathbf{x})$, where k indicates the *Spin* of the atom $k = m_s$ with $k \in \{-1, 0, 1\}$. Then the Hamiltonian is:

$$\hat{H} = \int d^3\mathbf{x} \Big\{ \sum_k \hat{\Psi}_k^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 + V_k(\mathbf{x}) \right) \hat{\Psi}_k(\mathbf{x}) + \sum_{kk'} \frac{c_0}{2} \hat{\Psi}_k^\dagger(\mathbf{x}) \hat{\Psi}_{k'}^\dagger(\mathbf{x}) \hat{\Psi}_{k'}(\mathbf{x}) \hat{\Psi}_k(\mathbf{x})$$
$$+ \sum_{kk'\ell\ell'} \frac{c_2}{2} \hat{\Psi}_k^\dagger(\mathbf{x}) \hat{\Psi}_{k'}^\dagger(\mathbf{x}) \mathbf{F}_{k\ell} \cdot \mathbf{F}_{k'\ell'} \hat{\Psi}_{\ell'}(\mathbf{x}) \hat{\Psi}_\ell(\mathbf{x}), \Big\} \quad (6)$$

where $\mathbf{F}$ is a vector of spin matrices ($\mathbf{F} = [F_x, F_y, F_z]^T$, where each F_k is a 3×3 matrix). The fields obey the commutation relation $\left[\hat{\Psi}_k(\mathbf{x}), \hat{\Psi}_{k'}^\dagger(\mathbf{x}')\right] = \delta_{kk'}\delta(\mathbf{x} - \mathbf{x}')$, where $\delta_{kk'}$ is the Kronecker delta.

(a) (4 points) Discuss the physical meaning of each term in the Hamiltonian (also discuss the difference between items within the sum). [max 6 lines].

(b) (6 points) Derive the Heisenberg equations for $\hat{\Psi}_k(\mathbf{x})$.

Solution:

(a) The first two are kinetic energy and some external potential, where the external potential may depend on the spin. The second are interactions between an atom of spin k with atoms in all other spin-states k'. The last terms include spin-changing interactions.

(b)

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}_k(\mathbf{x}) = \left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 + V_k(\mathbf{x}) \right) \hat{\Psi}_k(\mathbf{x}) + c_0 \sum_{k'} \hat{\Psi}_{k'}^\dagger(\mathbf{x}) \hat{\Psi}_{k'}(\mathbf{x}) \hat{\Psi}_k(\mathbf{x})$$
$$+ c_2 \sum_{k'll'} \hat{\Psi}_{k'}^\dagger(\mathbf{x}) \mathbf{F}_{k\ell} \mathbf{F}_{k'\ell'} \hat{\Psi}_{\ell'}(\mathbf{x}) \hat{\Psi}_\ell(\mathbf{x}) \quad (7)$$

5. (7 points) **Second quantisation I** Consider a non-linear oscillator with an external driving $E(t)$, the Hamiltonian of which is given by

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}) + \frac{\chi}{2}\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a} + E(t)(\hat{a}^\dagger + \hat{a}). \tag{8}$$

Within the restricted Fock space $|\,0\,\rangle \cdots |\,5\,\rangle$, write the Hamiltonian in matrix form.

Solution: $$\begin{bmatrix} \hbar\omega\frac{1}{2} & E(t) & 0 & 0 & 0 & 0 \\ E(t) & \hbar\omega\frac{3}{2} & \sqrt{2}E(t) & 0 & 0 & 0 \\ 0 & \sqrt{2}E(t) & \hbar\omega\frac{5}{2}+\chi & \sqrt{3}E(t) & 0 & 0 \\ 0 & 0 & \sqrt{3}E(t) & \hbar\omega\frac{7}{2}+3\chi & 2E(t) & 0 \\ 0 & 0 & 0 & 2E(t) & \hbar\omega\frac{9}{2}+6\chi & \sqrt{5}E(t) \\ 0 & 0 & 0 & 0 & \sqrt{5}E(t) & \hbar\omega\frac{11}{2}+10\chi \end{bmatrix}.$$

6. (7 points) **Coherent states** Show that the action of the destruction operator on a coherent state is $\hat{b}|\,\alpha\,\rangle = \alpha|\,\alpha\,\rangle$.

Solution:

(a) see lecture notes page 29.