RPTU KAISERSLAUTERN-LANDAU | Winter Term 2023/2024
Department of Physics | Priv.-Doz. Dr. Axel Pelster

Quantum Mechanics II — Problem Sheet 3

Problem 7: Bosons in Optical Lattice (16 points)

A system of bosons in a d-dimensional cubic lattice is described in mean-field theory by the Hamilton operator of an anharmonic oscillator:

$$\hat{H} = -Jz\left(\psi^*\hat{a} + \psi\hat{a}^\dagger - \psi^*\psi\right) + \frac{U}{2}\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a} - \mu\hat{a}^\dagger\hat{a}\,. \tag{1}$$

Here $\hat{a}$ and $\hat{a}^\dagger$ describe annihilation and creation operators of bosons at some lattice site, which fulfill the commutation relations of the ladder operators of a harmonic oscillator, see **Problem 1**: $[\hat{a},\hat{a}] = \left[\hat{a}^\dagger,\hat{a}^\dagger\right] = 0$, $\left[\hat{a},\hat{a}^\dagger\right] = 1$. Furthermore, the expectation values $\psi = \langle\hat{a}\rangle$, $\psi^* = \langle\hat{a}^\dagger\rangle$ denote a macroscopic occupation of bosons at some lattice site. And J represents the hopping energy, U is the on-site two-particle interaction energy, μ stands for the chemical potential, and $z = 2d$ abbreviates the number of neighbouring lattice sites.

a) Summarize concisely the physics of bosons in an optical lattice as discovered experimentally in the seminal paper M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, *Quantum Phase Transition from a Superfluid to a Mott Insulator in a Gas of Ultracold Atoms*, Nature **415**, 39 (2002).

b) Determine the eigenstates of the unperturbed Hamiltonian

$$\hat{H}_0 = Jz\psi^*\psi + \frac{U}{2}\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a} - \mu\hat{a}^\dagger\hat{a}\,. \tag{2}$$

Sketch the energy eigenvalues $E_n^{(0)}$ as functions of the chemical potential μ and confirm that within the interval $U(n-1) < \mu < Un$ the state with n bosons has the lowest energy.

c) Determine the non-vanishing matrix elements of the perburbation operator $\hat{V} = -Jz\left(\psi^*\hat{a} + \psi\hat{a}^\dagger\right)$ and show within perturbation theory that the ground-state energy E_n has the form of a Landau expansion:

$$E_n = a_0 + a_2|\psi|^2 + a_4|\psi|^4 + \ldots\,. \tag{3}$$

Calculate with the help of **Problem 6** the Landau coefficients a_0, a_2, a_4 and show that $a_4 > 0$.

d) Determine from the condition $a_2 = 0$ the equation for the quantum phase boundary and sketch the result in the $(zJ/U, \mu/U)$-plane. Determine the maximal value of zJ/U, where one could cross the quantum phase boundary. Which result do you obtain for the compressibility $\kappa = \partial n/\partial\mu$ in the Mott-Isolator phase, where $\psi = 0$, and in the superfluid phase, where $\psi \neq 0$, respectively?

Problem 8: Particle in a Square (8 points)

Calculate the energy eigenfunctions and eigenvalues for a particle of mass M confined in a square with side length L, i.e. $0 \le x \le L$, $0 \le y \le L$. Introduce the perturbation $\hat{V} = gxy$ and find the corrections up to the first order in both the ground level and the first excited level.

Drop the solutions in the post box on the 5th floor of building 46 or, in case of illness/quarantine, send them via email to jkrauss@rhrk.uni-kl.de until November 20 at 11.45.