Ultracold Atoms and Quantum Simulators

Problem set 5

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Derivation of the bosonic Hubbard Hamiltonian

The purpose of this problem set is to show how the bosonic Hubbard Hamiltonian can be derived from a simple microscopic model of particles moving in a sinusoidal potential. We thus consider a system of identical bosonic particles constrained to move in along a single axis x and subject to the external potential

$$V(x) = V_0 \sin^2(kx) = V_0(1 - \cos(\pi x/a))$$

and interacting through a contact interaction potential

$$U(x, x') = g\,\delta(x - x')\ .$$

We describe the problem in the framework of second-quantization and introduce the field operator $\hat{\Psi}(\mathbf{r})$. We remind you that the field operator 'destroys' a particle at a position $\mathbf{r}$ and that it can be decomposed on any single-particle basis $\{\lambda\}$ following:

$$\hat{\Psi}(\mathbf{r}) = \sum_{\lambda} \varphi_\lambda(x)\,\hat{a}_\lambda\ , \tag{1}$$

where $\varphi_\lambda(x)$ is the wavefunction of a single-particle state λ and $\hat{a}_\lambda$ is the annihilation operator in the same state.

The many-body Hamiltonian thus reads:

$$\hat{H} = \int \mathrm{d}x \left[\frac{\hbar^2}{2m}\boldsymbol{\nabla}\hat{\Psi}^\dagger(x)\cdot\boldsymbol{\nabla}\hat{\Psi}(x) + V(x)\hat{\Psi}^\dagger(x)\hat{\Psi}(x) + \frac{g}{2}\hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(x)\hat{\Psi}(x)\hat{\Psi}(x)\right]\ . \tag{2}$$

1. Separate the Hamiltonian (2) in a 'non-interacting' term, denoted $\hat{H}^{\mathrm{ni}}$ and gathering the kinetic and potential energies, and an 'interaction' term, denoted $\hat{H}^{\mathrm{i}}$, with the interaction energy. We will treat both terms separately.

2. What are the single-particle eigenstates of the non-interacting term? What are their quantum numbers and what is their physical meaning?

3. We now introduce the basis of Wannier states, whose wavefunctions $w_{n,j}(x)$ are localised around the potential minima $x = ja$. Write the non-interacting term of the Hamiltonian in the basis of Wannier states using the decomposition (1).

4. The Wannier states are related to the non-interacting eigenstates $\varphi_n(q)$ by the relations

$$|w_{n,j}\rangle = \left(\frac{a}{2\pi}\right)^{1/2}\int_{-k}^{+k}\mathrm{d}q\ e^{-ijaq}\,|\varphi_n(q)\rangle\ . \tag{3}$$

Based on this relation, justify why the non-interacting part of the Hamiltonian only couples Wannier states with the same quantum number n. From now on we will consider only the sector $n = 0$.

5. Knowing that the Wannier wavefunctions decrease exponentially fast away from their centres when the lattice potential is deep, justify why we can neglect the coupling induced by the non-interacting term of the Hamiltonian between Wannier states centred on lattice sites distant by more than one lattice period. This limit is known as the *tight-binding limit*. In the following we will write

$$\langle w_{j'}|\hat{H}^{\rm ni}|w_j\rangle \equiv J < 0 \, .$$

6. We now turn to the interaction term in the Hamiltonian. Decompose this term in the Wannier state basis using again equation (1). Is this term diagonal or not in the Wannier state basis?

7. In the tight-binding limit, show that the interaction Hamiltonian can be approximated by

$$\hat{H}^{\rm i} \simeq \frac{g}{2}\sum_j \left[\int {\rm d}x\, |w_j(x)|^4\right] \hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_j \, , \tag{4}$$

where $\hat{a}_j$ and $\hat{a}_j^\dagger$ are the annihilation and creation operators in the Wannier state centred on the lattice site j.

8. Since the Wannier wavefunctions are all identical up to a translation in space, the integral in the above equation turns out to be independent of j. Rewrite equation (4) as

$$\hat{H}^{\rm i} \simeq \frac{U}{2}\sum_j \hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_j \tag{5}$$

and give the expression of the interaction strength U. Comment on the value of U as a function of the lattice depth V_0.

9. Using the commutation relations of the annihilation and creation operators, show that the interaction term can be put in the form

$$\hat{H}^{\rm i} \simeq \frac{U}{2}\sum_j \hat{n}_j(\hat{n}_j - 1) \, .$$

We have finally shown how we can derive the bosonic Hubbard Hamiltonian from the many-body Hamiltonian (2) in the tight-binding limit. Note that the Hubbard Hamiltonian was initially proposed as a heuristic model to describe the dynamics of identical quantum particles moving in a deep lattice potential, like electrons in a crystal. The fact that it can be derived accurately and from first principles in ultracold gases illustrates the usefulness of these experimental systems.