Cold Atoms and Optical Lattices Problems

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Problem 1: Quasimomentum representation of the Bose-Hubbard model: In one dimension, the relationship between the creation operator for quasimomentum modes, $\hat{a}_k^\dagger$ and the creation operator for Wannier function modes, $\hat{b}_i^\dagger$ is given by

$$\hat{a}_q(x) = \sqrt{\frac{a}{2\pi}} \sum_l \hat{b}_l \mathrm{e}^{-\mathrm{i}x_l q}, \tag{1}$$

where a is the lattice spacing, and $x_l \propto la$ is the position co-ordinate at the centre of site l.

Expressing the system Hamiltonian in terms of quasimomentum operators often aids understanding of basic processes on a lattice, and can be performed in a straight-forward manner with the help of the identity

$$\sum_l \exp[ial(q-q')] = \frac{2\pi}{a}\delta(q - q' + 2\pi N/a), \tag{2}$$

where N is an integer, and remembering that the quasimomentum is always chosen to fall in the first Brillouin zone, $q \in [-\pi/a, \pi/a]$.

1. Kinetic Energy term
   (a) Tight binding Hamiltonian: Show that the kinetic energy term of the Bose-Hubbard model, $H_{KE} = -J\sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j$ can be rewritten using quasimomentum operators as $H_{KE} = \int_{-\pi/a}^{\pi/a} dk E(k) \hat{a}_k^\dagger \hat{a}_k$, with the dispersion relation in the lowest Bloch band given by $E(k) = -2J\cos(ka)$.
   (b) Beyond tight binding: If the shape of the lowest Bloch band is not exactly a cosine, then (as it will be symmetric about $k = 0$) we can write the band shape as a (Fourier) cosine series, $E(k) = \sum_n A_k \cos(nka)$. How would this affect the kinetic energy term written in terms of Wannier function modes?
2. Two-body interation term
   (a) Transform the interaction term $H_I = (U/2)\sum_i \hat{n}_i(\hat{n}_i - 1) = (U/2)\sum_i b_i^\dagger b_i^\dagger \hat{b}_i \hat{b}_i$ into quasimomentum representation.
   (b) In what sense is the quasimomentum conserved in two-body collisions on a lattice?
3. Trapping potential term
   (a) Assume that ε_i corresponds to an additional superlattice potential, where $\varepsilon_l = \cos[(\pi/4)al]$. Transform the corresponding Hamiltonian term $H_T \sum_i \varepsilon_i \hat{b}_i^\dagger \hat{b}_i$ to quasimomentum representation.
   (b) Explain physically what the effect of this term is in quasimomentum space.
4. Linear gradient potential and Introduction to Bloch oscillations:
   (a) Consider a situation where we apply a gradient potential to the lattice (or equivalently, accelerate the lattice), so that $\varepsilon_l = \Omega(t)l$, with $\Omega(t) = \Omega$ for $t \geq 0$, and $\Omega(t) = 0$ for $t < 0$ otherwise. Consider times $t \ll 2\pi/J, t \ll 2\pi/U$, so that other terms in the Hamiltonian do not play an important role. Show that we effectively apply the operator

   $$\Pi_l \exp(-i\Omega t l \hat{n}_l) \tag{3}$$

   to the initial state at $t = 0$. Show that if the initial state is $(b_0^\dagger)^N|vac\rangle$, we will obtain the state $(b_k^\dagger)^N|vac\rangle$, where $k = \Omega t/a + 2\pi N$, and N is chosen so that $k \in [-\pi/a, \pi/a]$. What happens when the quasimomentum reaches $k = \pi/a$?
   (b) Compute the group velocity for free atoms moving in the lowest band, $v(k) = \partial E(k)/\partial k$. What is $v(k = \pm\pi/2)$? Discuss the motion of particles in the system when $J \neq 0$.

Problem 2: Particle pairs on a Lattice: We would like to solve the Schrödinger equation for particles moving in an optical lattice along one dimension, described by the Bose-Hubbard model:

$$H = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \sum_i \varepsilon_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1). \quad (4)$$

1. Consider a single particle on a lattice, described by the kinetic energy part of the Bose-Hubbard Hamiltonian, with no external trapping potential, $\varepsilon_i = 0$ (and no interactions!). If we expand the wavefunction in terms of Wannier functions as

$$\psi(x) = \sum_i \psi_i w_0(x - x_i), \quad (5)$$

then we obtain the time-independent Schrödinger equation

$$-J\psi_{i+1} - J\psi_{i-1} = E\psi_i. \quad (6)$$

This takes the form of a difference equation, with E the energy, and J the tunnelling amplitude for particles moving between neighbouring sites.

   (a) Solve this equation, by substituting the discrete wavefunction $\psi_x = A\exp(-\mathrm{i}kax) + B\exp(+\mathrm{i}kax)$, where x is an integer, and a is a lattice spacing, or otherwise.

   (b) Determine $E(k)$, and identify k with the lattice quasimomentum.

2. Consider a single particle on a lattice, described by the kinetic energy part of the Bose Hubbard model, but with an additional energy shift on site 0, $\varepsilon_0 = V_0$, $V_0 < 0$, with $\varepsilon_{i\neq 0} = 0$. This corresponds to the with time-independent Schrödinger equation

$$-J\psi_{i+1} - J\psi_{i-1} + V_0\delta_{i,0}\psi_i = E\psi_i, \quad (7)$$

where $\delta_{i,j}$ is a Kronecker delta. This difference equation is the discrete analog to the problem of a δ-potential in continuous space.

   (a) Write down the general solution to this difference equation for ψ_x in the regions $x \leq 0$ and $x \geq 0$ for the case that the solution is bound ($E < -2J$). [Hint: Similarly to the analogous problem of a single δ potential in continuous space, the solutions will decay here].

   (b) Derive a condition for the relationship between the wavefunction to the left and the right of the boundary, $\psi_{x<0}$, and $\psi_{x>0}$ from the Schrödinger equation with $i = 0$ (i.e., including a non-zero contribution from the Kronecker delta).

   (c) Using this, and the condition of continuity, write the full solution to the Schrödinger equation for $E < -2J$. What is the energy of the bound state?

   (d) Show that solutions also exist for $-2J < E < 2J$.

3. Now consider two particles moving on a uniform lattice, with interaction energy U, $U < 0$, when the two particles are on the same site. The Schrödinger equation is given by

$$\left[-J\left(\tilde{\Delta}_x + \tilde{\Delta}_y\right) + U\delta_{x,y}\right]\Psi(x,y) = E\,\Psi(\mathbf{x},\mathbf{y}), \quad (8)$$

where the operator

$$\tilde{\Delta}_x\Psi(x,y) = \left[\Psi(x+1,y) + \Psi(x-1,\mathbf{y})\right]. \quad (9)$$

   (a) Rewrite this equation using relative and centre of mass coordinates $r = x - y$, $R = (x+y)/2$, and show that using the ansatz

$$\Psi(x,y) = \exp(iKR)\psi_K(r), \quad (10)$$

   that the equation can be reduced to a Schrödinger equation in the relative co-ordinate. Here, K denotes the centre of mass quasi-momentum.

   (b) Show that this model reduces to the same as that in (2), but with a tunneling parameter dependent on K. Deduce from the solution in (2) the bound state energy $E_b(K)$ as a function of K. Sketch the form of the full energy spectrum of the solutions (bound and unbound) as a function of K, and explain what they mean physically.

   (c) Using the result from 2c, compute the form of the bound state energy $E_b(K)$ solution for $U \gg J$. How does this form compare to the energy of a single particle from (1)? Can you find an effective tunnelling parameter for bound pairs moving through the lattice in this limit?