

Instructions: Answer all questions for full marks. All necessary formulae are given. Hand in question paper together with your answer script. Put your name and roll no. on both Question paper as well as the Answer script. Total marks: 30.

Name:

Roll No.:

1. The Hubbard Dimer: a toy model for the Mott Insulator. (20 marks)

Consider the problem of a two-site lattice with $N = 2$ electrons (half-filling), nearest neighbour hopping ($-t$) and an on-site Hubbard repulsion ($U > 0$)

$$H_{Hubbard} = -t \sum_{\sigma} (c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow}). \quad (1)$$

(i) Show that the above Hamiltonian commutes with the total particle number operator $N = \sum_{j,\sigma} n_{j\sigma}$, the magnetisation operator $S_{Tot}^z = \frac{1}{2} \sum_{j=1,2} (n_{j\uparrow} - n_{j\downarrow})$ and the two-site permutation/parity operator \hat{P} : $\hat{P}(\text{site 1}) = (\text{site 2})$, $\hat{P}(\text{site 2}) = (\text{site 1})$. (3 marks)

(ii) Use (i) to show that the 6 eigenstates of the Hubbard dimer at half-filling (i.e., $N = 2$) are particular linear superpositions of the states $|\uparrow, \uparrow\rangle$, $|\downarrow, \downarrow\rangle$, $|\uparrow, \downarrow\rangle$, $|\downarrow, \uparrow\rangle$, $|\uparrow\downarrow, 0\rangle$ and $|0, \uparrow\downarrow\rangle$. Label the eigenstates with the eigenvalues of S_{Tot}^z and \hat{P} . (4 marks)

(iii) Compute the action of the Hamiltonian (1) on these 6 eigenstates, and write the resultant as a 6×6 matrix. Show that this matrix separates into three 2×2 block matrices, of which two blocks are already diagonal and the third can be written completely in terms of the Pauli matrices and the 2×2 identity matrix. (3 marks)

(iv) Diagonalise the third block, i.e., compute the eigenvalues and eigenstates of this block. Draw a simple diagram for the entire eigenspectrum from the 6 eigenvalues you have obtained, denoting the eigenstates alongside the energy levels. (3 marks)

(v) **The Mott insulating limit** : In the strong-coupling limit of $U \gg t$, show that the eigenspectrum can be (roughly) visualised as two bands of states (the lower and upper Hubbard bands) separated by an energy gap $\Delta = U$. Argue that, in this limit, the eigenstates of the upper Hubbard band are (almost completely) composed of linear superpositions of the “holon-doublon” states ($|\uparrow\downarrow, 0\rangle$ and $|0, \uparrow\downarrow\rangle$). Similarly, show that, in the same limit, the lower Hubbard band are (almost completely) composed of linear superpositions of the “Néel” states ($|\uparrow, \downarrow\rangle$ and $|\downarrow, \uparrow\rangle$), together with the polarised states ($|\uparrow, \uparrow\rangle$ and $|\downarrow, \downarrow\rangle$). This shows how U mixes states in the upper and lower Hubbard bands. Further, show that the lower Hubbard band has the structure of a *unique* ground state and a *triplet* of lowest excited states. (4 marks)

(vi) **The antiferromagnetic Heisenberg model** : Demonstrate that the eigenspectrum of the lower Hubbard band in the strong-coupling limit ($U \gg t$) is identical to that of the two-site Heisenberg Hamiltonian with antiferromagnetic spin exchange ($J \equiv \frac{t^2}{U} > 0$) (3 marks)

$$H_{Heisenberg} = J \vec{S}_1 \cdot \vec{S}_2 - \frac{J}{4}. \quad (2)$$

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2. Kohn's theorem, magnetic translations and the quantum Hall effect. (10 marks)

The Hamiltonian for the centre of mass of a system of 2-dimensional electrons in a transverse magnetic field can be written as

$$H_{\text{COM}} = \frac{1}{2mN_e} [\Pi_x^2 + \Pi_y^2] , \quad (3)$$

where $\Pi_x = -i\hbar \frac{\partial}{\partial x}$, $\Pi_y = -i\hbar \frac{\partial}{\partial y} + eBN_e x$, N_e is the no. of electrons and we've used the Landau gauge for the e-m vector potential $\vec{A} = (0, eBx, 0)$.

(i) Provide simple arguments demonstrating that H_{COM} commutes with the Hamiltonian for the internal relative motion of the system (H_{rel})

$$H_{\text{rel}} = \frac{1}{2mN_e} \sum_{i < j} [(\vec{\Pi}_i - \vec{\Pi}_j)^2 + V(\vec{r}_i - \vec{r}_j)] , \quad (4)$$

i.e., $[H_{\text{COM}}, H_{\text{rel}}] = 0$ (Kohn's theorem, Phys. Rev. **123**, 1242 (1961)). (1 mark)

(ii) Compute the commutator $[\Pi_x, \Pi_y]$ for Π_x and Π_y defined below eqn.(3). (1 mark)

(iii) Define the pseudomomenta $K_x = \Pi_x + eBN_e y$, $K_y = \Pi_y - eBN_e x$. Now, compute the commutators $[\Pi_x, K_x]$, $[\Pi_x, K_y]$, $[\Pi_y, K_x]$, $[\Pi_y, K_y]$ and $[K_x, K_y]$. (4 marks)

(iv) From the results of (ii), compute the commutators $[K_x, H_{\text{COM}}]$ and $[K_y, H_{\text{COM}}]$. What do your answers indicate? (1 mark)

(v) Define the magnetic translation operators $T_1 = e^{\frac{iL_1}{N_B\hbar} K_x}$, $T_2 = e^{\frac{iL_2}{N_B\hbar} K_y}$ where L_1 and L_2 are the sidelengths of the two-dimensional system in the x- and y-directions and N_B is the magnetic flux through the system $N_B = \frac{e}{h} BL_1 L_2$. Now compute the quantity $T_1^{-1} T_2^{-1} T_1 T_2$, which corresponds to translating adiabatically the centre of mass through a closed loop. (2 marks)

Hint: In the above, you may use the relation $e^{-A} e^{-B} e^A e^B = e^{-[A, B]}$ (which uses the Baker-Campbell-Hausdorff relation $e^A e^B = e^{A+B+\frac{1}{2}[A, B]}$) and the relations $[A, [A, B]] = 0 = [B, [A, B]]$.

(vi) Using the answer you obtained in (v), compute the quantity

$$\gamma = -\frac{1}{2\pi} \text{Im} [\ln(T_1^{-1} T_2^{-1} T_1 T_2)] . \quad (5)$$

Quantisation of Hall conductivity : The quantity γ corresponds to a geometric phase of the centre of mass gained while traversing the closed loop, and is related to the quantised Hall conductivity of the 2-dimensional electronic system in a transverse B-field, $\sigma_{\text{Hall}} = \gamma \frac{e^2}{h}$ (see, e.g., Tao and Haldane, Phys. Rev. B. **33**, 3844 (1986)). What is the value of σ_{Hall} obtained from your calculation? (1 mark)

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