

# Homework #3

## Due by 11/12/2025 before class

1. Adiabatic theorem and geometric phase. Consider a spin-1/2 particle in a magnetic field  $\vec{B}$ . The Hamiltonian is given by

$$H = -\mu\vec{\sigma} \cdot \vec{B}, \quad (1)$$

where  $\mu$  is the magnetic moment of the particle and  $\vec{\sigma}$  represents the three Pauli matrices. Suppose the magnetic field has a fixed magnitude  $B$  and a time-dependent orientation in space described by the polar angle  $\theta$  and the azimuthal angle  $\varphi$ .

(a) [5 pt] Express the  $x$ ,  $y$  and  $z$  components of the magnetic field in terms of  $\theta$  and  $\varphi$ . Further give an expression for the Hamiltonian in the matrix form.

(b) [5 pt] Solve the instantaneous eigenstates of this Hamiltonian at the polar angle  $\theta$  and the azimuthal angle  $\varphi$ .

(c) [10 pt] Suppose we keep  $\theta$  constant, and increase  $\varphi$  from 0 to  $2\pi$  adiabatically. In the class, we know the coefficient on an instantaneous eigenstate  $|n\rangle$  evolves as

$$\dot{a}_n(t) = -\langle n(t)|\dot{n}(t)\rangle a_n(t). \quad (2)$$

Now express the coefficient  $a_n$  in terms of  $\varphi$  for both instantaneous eigenstates, and derive an expression for the accumulated phase between these two states when  $\varphi$  increases from 0 to  $2\pi$ . Note that when  $\varphi = 2\pi$ , we return to the original basis at  $\varphi = 0$ . Therefore we simply get an additional phase on the original basis. It shall only depend on the trajectory of the adiabatic evolution, and is thus called a geometric phase.

2. (a) [10 pt] When two operators  $A$  and  $B$  satisfy  $[A, [A, B]] = 0$  and  $[B, [A, B]] = 0$ , we have a special case to the Zassenhaus formula:  $e^{A+B} = e^A e^B e^{-\frac{1}{2}[A, B]}$ . To prove this formula, we can construct a function  $f(\lambda) \equiv e^{\lambda A + B} \equiv \sum_n \frac{(\lambda A + B)^n}{n!}$ . Prove that

$$\frac{df}{d\lambda} = Af(\lambda) - \frac{1}{2}[A, B]f(\lambda). \quad (3)$$

Further integrate it from  $\lambda = 0$  to  $\lambda = 1$  to get the desired formula.

(b) [5 pt] As an application, consider the displacement operator for a simple harmonic oscillator  $D(\alpha) \equiv e^{\alpha a^\dagger - \alpha^* a}$ , where  $\alpha \in \mathbb{C}$  is the direction of the displacement on the complex plane. Suppose we apply 4 displacement operations sequentially as the unitary time evolution of the system:  $D(u)$ ,  $D(iv)$ ,  $D(-u)$  and  $D(-iv)$ , where  $u, v \in \mathbb{R}$ . Prove that the overall

unitary  $U = D(-iv)D(-u)D(iv)D(u) = e^{i\phi}I$  is a global phase, and that the phase  $\phi$  is related to the area enclosed by this trajectory on the complex plane.

(c) [5 pt] A coherent state is an eigenstate of the annihilation operator:  $a|\alpha\rangle = \alpha|\alpha\rangle$  ( $\alpha \in \mathbb{C}$ ). We can obtain a coherent state by applying a displacement to the ground state (vacuum) of the simple harmonic oscillator:  $|\alpha\rangle = D(\alpha)|0\rangle$ . Give an expression for the coherent state  $|\alpha\rangle$  in the particle number basis ( $\{|n\rangle\}$ , also known as the Fock basis).

3. (a) [10 pt] From the above formula, we have  $e^A e^B = e^B e^A e^{[A,B]}$ , or  $e^A e^B e^{-A} = e^B e^{[A,B]}$  when  $[A, [A, B]] = 0$  and  $[B, [A, B]] = 0$ . Substitute  $B \leftarrow \log B$ , we have  $e^A B e^{-A} = B + [A, B]$  when  $[A, [A, B]] = 0$  and  $[B, [A, B]] = 0$ . In general when  $[A, B]$  does not commute with  $A$  or  $B$ , we have

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2}[A, [A, B]] + \cdots = \sum_n \frac{1}{n!} \underbrace{[A, \cdots [A, [A, B]] \cdots]}_{n \text{ times}}. \quad (4)$$

To prove this formula, we can construct  $g(\lambda) \equiv e^{\lambda A} B e^{-\lambda A}$ . Show that this formula is given by the Taylor series of  $g(\lambda)$  around  $\lambda = 0$ .

(b) [5 pt] Again, consider the displacement operator  $D(\alpha) \equiv e^{\alpha a^\dagger - \alpha^* a}$ . Compute the unitary transformation of the annihilation and creation operators under  $D(\alpha)$ :  $D^\dagger(\alpha) a D(\alpha)$  and  $D^\dagger(\alpha) a^\dagger D(\alpha)$ . Further show that the position  $x$  and the momentum  $p$  operators will be shifted by constants proportional to  $\text{Re}[\alpha]$  and  $\text{Im}[\alpha]$ , respectively, under such a unitary transformation. These are the reasons why  $D(\alpha)$  is called a displacement operator.

4. Numerically simulate the single-qubit dynamics by discretizing into single-qubit gates. Specifically, consider the Hamiltonian

$$H = B_x \sigma_x + B_y \sigma_y + B_z \sigma_z \quad (5)$$

with  $B_x = B_y = B_z = 2\pi$ . Start from  $|0\rangle$  and evolve the system for time  $T = 2$ . Decompose the unitary evolution into a sequence of rotations around  $x$ ,  $y$  and  $z$  axes.

(a) [5 pt] This problem can be solved analytically as a rotation around the  $[1, 1, 1]$  axis. Compute how the population in the state  $|0\rangle$  evolves with time.

(b) [10 pt] Consider the first-order discretization and Trotter decomposition. Plot the population in the state  $|0\rangle$  versus time  $t$  (at the discretized time points) for different number of steps  $M = 100, 200, 500, 1000$ . Observe how the curves converge to the exact solution as  $M$  increases.

(c) [5 pt] Repeat the calculation for the second-order discretization and Trotter decomposition. Compare your results with the first-order method.

5. Given a 6-bit odd integer  $N$ . Factor it into two 3-bit integers  $N = p \times q$  by solving a combinatorial optimization problem.

(a) [5 pt] For a general 6-bit odd integer  $N$ , following the procedure in the class to express the factoring problem as to find the ground state of an Ising model Hamiltonian

$$H = - \sum_i h_i s_i - \sum_{i < j} J_{ij} s_i s_j + C. \quad (6)$$

Express the matrices  $h$  and  $J$ , and the constant  $C$ , in terms of the bits in the binary representation of the integer  $N = n_5 n_4 n_3 n_2 n_1$ .

(b) [5 pt] Below we take  $N = 35$ . Classically, solve this optimization problem by the brutal-force method to enumerate all the possible spin states. Verify that the ground state has an energy of zero, and that it corresponds to the correct factoring  $35 = 5 \times 7$  or  $35 = 7 \times 5$ .

(c) [10 pt] Write a Qiskit code to solve this optimization problem by quantum annealing with first order Trotter decomposition. Run a classical simulation for an evolution time  $T = 10$  and a step number  $M = 100$ . You can use an initial transverse field  $B = 1$ , and vary your Hamiltonian linearly with time. Repeat the simulation for 1000 trials. For each of the measured spin configuration, compute the corresponding energy, and plot a histogram of the energy for 1000 trials.

(d) [5 pt] Run your quantum annealing code for  $N = 27$ . What is the result you get? Note that for  $N = 27$ , no factoring into two 3-bit integers exists.