TISE = time independent Schrödinger equation. SS = stationary state. 1D = one dimension.

$$\hat{H}\,|\Psi(t)\rangle = i\hbar\frac{d}{dt}\,|\Psi(t)\rangle \qquad \text{Schrödinger equation} \qquad (1)$$

$$H(\hat{x},\hat{p},t)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \qquad \text{Schrödinger eq., } x\text{-repr, spinless particle in 1D} \qquad (2)$$

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle \qquad \text{TISE: } \frac{\partial\hat{H}}{\partial t}=0,\ \text{SS, } |\Psi(t)\rangle \equiv \exp(-iEt/\hbar)\,|\psi\rangle \qquad (3)$$

$$\hat{\mathcal{T}}(\Delta x) = \exp\left(-i\frac{\Delta x\,\hat{p}}{\hbar}\right) \qquad \text{translation operator in 1D} \qquad (4)$$

$$\hat{\mathcal{R}}(\Delta\theta) = \exp\left(-i\frac{\Delta\theta\,\hat{L}_\theta}{\hbar}\right) \qquad \text{rotation operator} \qquad (5)$$

$$[\hat{x},\hat{p}] = i\hbar \qquad \text{also for other canonical conjugate pairs} \qquad (6)$$

$$[\hat{\theta},\hat{L}_\theta] = i\hbar \qquad \therefore\ \ \hat{L}_\theta \doteq -i\hbar\frac{\partial}{\partial\theta} \qquad (7)$$

$$[\hat{L}_j,\hat{L}_k] = i\hbar\epsilon_{jkl}\hat{L}_l \qquad \text{similarly, if all } L\to S \text{ or if all } L\to J \qquad (8)$$

$$[\hat{L}_j,\hat{p}_k] = i\hbar\epsilon_{jkl}\hat{p}_l \qquad j,k,l = \text{any of } 1,2,3 \text{ (or } x,y,z) \qquad (9)$$

$$[\hat{L}_j,\hat{x}_k] = i\hbar\epsilon_{jkl}\hat{x}_l \qquad \epsilon_{jkl} = \text{Levi-Civita symbol} \qquad (10)$$

$$[\hat{L}_j,\hat{L}^2] = 0 \qquad \text{similarly, if all } L\to S \text{ or if all } L\to J \qquad (11)$$

$$[\hat{L}_j,\hat{p}^2] = 0 = [\hat{L}_j,\hat{r}^2] \qquad \hat{p}^2 \equiv \hat{p}_x^2+\hat{p}_y^2+\hat{p}_z^2,\quad \hat{r}^2 \equiv \hat{x}^2+\hat{y}^2+\hat{z}^2 \qquad (12)$$

$$[\hat{L}_j,\hat{S}_k] = 0 \qquad \hat{L} \text{ and } \hat{S} \text{ live in orthogonal Hilbert spaces} \qquad (13)$$

$$\hat{H} = -\hat{\vec{\mu}}\cdot\hat{\vec{B}} \qquad \text{for magnetic moment } \vec{\mu} \text{ in a } \vec{B} \text{ field} \qquad (14)$$

$$\hat{\vec{\mu}} = -\frac{\mu_B}{\hbar}(2\hat{\vec{S}}+\hat{\vec{L}}) \qquad \text{for electron } (g_{spin}\approx 2),\ \mu_B = \frac{e\hbar}{2m_e} = \text{Bohr magneton} \qquad (15)$$

$$[\hat{A},f(\hat{B})] = 0 \ \text{ if } \ [\hat{A},\hat{B}] = 0 \qquad \text{for any analytic function } f \qquad (16)$$

$$f(\hat{B})\,|B\rangle = f(B)\,|B\rangle \ \text{ if } \ \hat{B}\,|B\rangle = B\,|B\rangle \qquad \text{for any analytic function } f \qquad (17)$$

$$\langle\hat{T}\rangle = \frac{n}{2}\langle\hat{V}\rangle \qquad \text{Virial theorem for } \hat{V}\propto\hat{x}^n,\hat{r}^n,\ \text{SS} \qquad (18)$$

$$\int_{-\infty}^{\infty} dx\, e^{i(k-k')x} = 2\pi\delta(k-k') \qquad \delta(k) = \text{Dirac delta function} \qquad (19)$$

$$\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad \sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \qquad \text{Pauli matrices, spin 1/2, } \hat{S}_j \doteq \frac{\hbar}{2}\sigma_j \qquad (20)$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}+\hat{a}^\dagger\right) \qquad \text{1D simple harmonic oscillator} \qquad (21)$$

$$\hat{p} = \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a}-\hat{a}^\dagger\right) \qquad \text{one-dimensional (1D) SHO} \qquad (22)$$

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle,\quad \hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad \text{1D SHO, “ladder” operators} \qquad (23)$$

Please organize your solutions as neatly as you can.
**Please start by writing down your name on your solution sheet.**
Show **sufficient minimal derivation** for all your answers.

To the zeroth order approximation, the perfect score of this exam is 350 points.

**Good luck!**

**Problem 1** (50 points) Consider a spin 1/2 particle. Represent the $\hat{S}_z$ operator as a 2×2 matrix, using the eigenvectors of $\hat{S}_y$ as the basis vectors. [The Pauli matrices are given in the first page.]

**Problem 2** (50 points) Is the following statement true? If true, prove it. If false, provide one counter example.

*If two operators $\hat{A}$ and $\hat{B}$ are compatible, then any eigenstate of $\hat{A}$ is automatically an eigenstate of $\hat{B}$.*

**Problem 3** (100 points) Consider a quantum mechanical version of a mass on a vertical spring problem. [Although you cannot see them individually, there are gazillion (or more quantitatively, ~ $10^{21}$) molecules on the ceiling of this room right now, doing this motion!] We take

$$\hat{H}_0 \doteq \frac{p_x^2}{2m} + \frac{1}{2}kx^2$$

to be the unperturbed Hamiltonian, and

$$\hat{H}_1 \doteq mgx \tag{24}$$

as the perturbation, where $g$ is the surface gravity, $m > 0$ is the mass of the particle in question, and $k > 0$ is the spring constant. Here, $x$ is the vertical coordinate, $p_x$ is its conjugate momentum, and we do not consider the motion of the particle in the other two directions. The natural frequency defined by $\hat{H}_0$ is

$$\omega = \sqrt{k/m}.$$

(a) Using the perturbation theory, find the energies of the ground state and the first excited state of the system, including the leading order corrections by perturbation.

(b) Identify the *dimensionless* perturbation parameter ($\delta$) up to a multiplicative numerical constant.

[Note: You do not need to know anything about the actual forms of wave functions (except perhaps their parity properties; the ground state has the even parity and the first excited state has the odd parity); all you need to know about a simple harmonic oscillator is given near the bottom of the first page of this exam. Note that the energy eigenvalue for $\hat{H}_0$ is given by $\left(n + \frac{1}{2}\right)\hbar\omega$.]

**Problem 4** (100 points) Consider a two dimensional simple harmonic oscillator defined by

$$\hat{H}_0 \doteq \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2}k(x^2 + y^2),$$

with $m, k > 0$. The system is immersed in a laser field, which adds a perturbation

$$\hat{H}_1 \doteq \epsilon x^3 y.$$

[Note: A *state* that we refer to below should be understood as one of those states of the form $|n_x, n_y\rangle$, or any linear combination of them, where $n_x$ and $n_y$ are quantum numbers of one dimensional simple harmonic oscillators for the $x$ and $y$ coordinates, respectively.]

(a) Find the first excited state of $\hat{H}_0$, its energy, and its degeneracy. Express the energy in terms of $\omega \equiv \sqrt{k/m}$.

(b) Find the leading order corrections to the energy of the first excited states, and the corresponding eigenstates.

(c) Consider translation ($\hat{\mathcal{T}}_x$, $\hat{\mathcal{T}}_y$), rotation ($\hat{\mathcal{R}}_z$), and parity ($\hat{\mathcal{P}}_x$ ($x \leftrightarrow -x$), $\hat{\mathcal{P}}_y$ ($y \leftrightarrow -y$), $\hat{\mathcal{P}}_{x\leftrightarrow y}$, $\hat{\mathcal{P}}_{x\leftrightarrow -y}$) operators. Which of these are symmetry operators for $\hat{H}_0$? Which of them are symmetry operators for $\hat{H}_1$? Is there any way to use the symmetry argument to explain the eigenstates that you found in the previous part?

**Problem 5** (100 points) [The novel electronic properties of graphene and nanotube originate from a unique crystalline arrangement of certain molecular orbitals, namely the "$\pi$-bonding or $\pi^*$-anti-bonding" orbitals, which is the topic of this problem. In the following, the $xy$ plane corresponds to the (local) crystalline plane of graphene or nanotube.]

Consider an $xy$ plane, where two hydrogen-like atoms are placed at a certain distance. We consider only the $2p_z$ ($n = 2, l = 1, m_l = 0$) orbital for each atom. Then, the full wave function for the *atomic* orbital is given by

$$\psi(\vec{r}) = N z \exp\left(-\frac{r}{2a}\right)$$

if the origin of the coordinate system is taken to be the center of the atom in question. Here, $a > 0$ is a length scale parameter and $N$ is a normalization constant. Keep in mind that there are two such atomic orbitals, having this same form but centered at the two different atoms, and the mixing of these two atomic orbitals by quantum tunneling is the central physics of this problem. You may refer to the states corresponding to these two $2p_z$ orbitals as $|L\rangle$ and $|R\rangle$.

(a) Draw a "side view" diagram that includes the sketch of the following elements: the $xy$ plane (which must be a horizontal line from the side view), the two $2p_z$ orbitals (angular symmetry *and* radial behavior), and the two Coulomb potentials for the two Hydrogen-like atoms (at a finite distance from the side view). [Defining the line connecting the centers of the two atoms as the $x$ axis, the "side view" here is defined as the view of the $zx$ plane, as you look in the direction of the $y$ axis.]

(b) If an electron occupies one of the two $2p_z$ orbitals, and if the distance between two atoms is large, but not too large compared to $a$, then there will be a small but finite amount of quantum tunneling of the electron between the two orbitals. Assuming such scenario, and assuming that the above two $2p_z$ orbitals are orthogonal ($\langle L | R \rangle \equiv 0$; to make mathematics simple without damaging physics), prove that the Hamiltonian matrix for this problem is given by

$$\hat{H} \doteq \begin{pmatrix} E & -t \\ -t & E \end{pmatrix},$$

using $|L\rangle$ and $|R\rangle$ as the basis states for the representation. Here, $E$ is a real number, and $t$ is a *positive* real number; you must derive these properties of $E$ and $t$.

(c) Find eigenvalues and eigenvectors for the above matrix. The eigenvectors correspond to the two, bonding (lower energy) and anti-bonding (higher energy), molecular orbitals, which are commonly referred to as $\pi$ and $\pi^*$ orbitals, respectively.

(d) Explain, using the symmetry consideration, why the eigenvectors that you found in the previous part have the forms that they have.

(e) How many electrons can each molecular orbital hold? (Do not forget the spin 1/2 quantum number of the electron.)