Exercises

一、 Filling the blanks

1. If the operator $\hat{R}$ is a self-conjugate operator, it should satisfy the relationship

    _____, and the eigenvalues of self-conjugate operators are

    _____.

2. The wavefunction should satisfy the three requirements: _____, _____ and

    _____.

3. $|\Psi (x_1, y_1, z_1, x_2, y_2, z_2)|^2$ represents_____.

4. For the following functions, (A) $\cos kx$ (B) e^{-bx} (C) e^{-ikx} (D) e^{-kx^2}, _____are the

    eigenfunctions of $\dfrac{d}{dx}$, and _____are the eigenfunctions of $\dfrac{d^2}{dx^2}$.

5. The angular distribution of d_{z^2} orbital is $d_{z^2} = \dfrac{1}{4}\sqrt{\dfrac{5}{\pi}}(3\cos^2\theta - 1)$, then the angle(s) for the

    angular nodal plane is(are)_____, and the angle(s) for the extremum

    is(are)_____.

6. For the electronic configuration p^2, all the corresponding spectrum terms are

    _____, among which the ground-state spectrum term is _____.

二、 Short answer questions

1. Please write the electronic configurations of the ground-state O_2, O_2^+, O_2^-, O_2^{2-}, and tell if

each of them is paramagnetic or diamagnetic, calculate their bond orders, and list the order of

the O-O bond strength.

三、 Calculations

1. The wavefunction of 1s orbital of H is $\psi_{1s} = \left(\dfrac{1}{\pi a_0^3}\right)^{\frac{1}{2}} \exp\left(-\dfrac{r}{a_0}\right)$, please calculate the position

    (r) corresponding to the maximum of the radial distribution function.