Exercises

一、 Filling the blanks

1. If the operator $\hat{R}$ is a self-conjugate operator, it should satisfy the relationship $\int g^*(\hat{R}f)d\tau = \int f(\hat{R}g)^*d\tau$, and the eigenvalues of self-conjugate operators are real numbers.

2. The wavefunction should satisfy the three requirements: single valued, continuous and square integrable.

3. $|\Psi(x_1, y_1, z_1, x_2, y_2, z_2)|^2$ represents the probability density of finding No.1 and No.2 particles at the two positions.

4. For the following functions, (A) cos *kx* (B) e^{-bx} (C) e^{-ikx} (D) e^{-kx^2}, B.C are the eigenfunctions of $\frac{d}{dx}$, and A.B.C are the eigenfunctions of $\frac{d^2}{dx^2}$.

5. The angular distribution of d_{z^2} orbital is $d_{z^2} = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1)$, then the angle(s) for the angular nodal plane is(are) $\theta = \arccos(\pm\frac{1}{\sqrt{3}})$ and the angle(s) for the extremum is(are) $0^\circ, 90^\circ, 180^\circ$ ← $\sin 2\theta = 0 \Rightarrow 2\theta = 0^\circ, 180^\circ, 360^\circ$

6. For the electronic configuration p^2, all the corresponding spectrum terms are $^1D, ^3P, ^1S$, among which the ground-state spectrum term is ^3P.

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.

paramagnetic ↑ ↑ ↑ → diamagnetic

$O_2: 1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 1\pi_u^4 1\pi_g^2$

$O_2^+: \ldots 1\pi_g^1$, $O_2^-: \ldots 1\pi_g^3$, $O_2^{2-} \ldots 1\pi_g^4$

$P(O_2) = 2$, $P(O_2^+) = 2.5$, $P(O_2^-) = 1.5$, $P(O_2^{2-}) = 1$, $O_2^+ > O_2 > O_2^- > O_2^{2-}$

三、Calculations

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

$D(r) = 4\pi r^2 \Psi_{1s}^2 = (4/a_0^3) r^2 \exp(-\frac{2r}{a_0})$

$D'(r) = (4/a_0^3)(2r - 2r^2/a_0)\exp(-2r/a_0) = 0$

$\rightarrow r = a_0$