

Exercises

一、Filling the blanks

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

$$\int \psi^*(\hat{R}\psi) d\tau = \int (\hat{R}\psi)^* \psi d\tau$$

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 No. 1 and No. 2 particles at the two positions

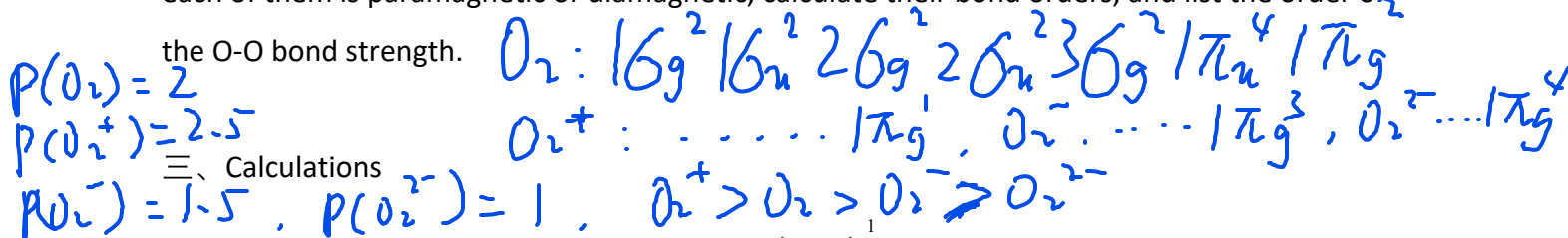
4. For the following functions, (A) $\cos kx$ (B) e^{-bx} (C) e^{-ikx} (D) e^{-kx^2} , B, C are the eigenfunctions of $\frac{d}{dx}$, and A, B, C are the eigenfunctions of $\frac{d^2}{dx^2}$.

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) $0^\circ, 90^\circ, 180^\circ$ $\leftarrow \sin 2\theta = 0 \Rightarrow 2\theta = 0^\circ, 180^\circ, 360^\circ$

6. For the electronic configuration p^2 , all the corresponding spectrum terms are $^1P, ^3P, ^1S$, 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.



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.

$$P(r) = 4\pi r^2 \psi_{1s}^2 = (4/a_0^3) r^2 \exp(-2r/a_0)$$

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

$$\rightarrow r = a_0$$