Basic Physical Chemistry I

Jun Okabayashi
2020.6.2

Q1
Prove the following relation,

$$\vec{S^2}\chi_s{}^{\mathrm{III}} = 2\hbar^2\chi_s^{\mathrm{III}}.$$

Q2
Prove the following relation,

$$\vec{S^2} = S(S+1)\hbar^2.$$

Q3
Discuss the case that the ferromagnetic states are stable.

Q4
Explain the difference between molecular orbital and valence bond approaches.

Q5
Explain the advantage of configuration interaction approach.

Q6
Prove the relation in $F(x)$.

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|$$

Q7
Prove the Fourier transformation in k-representation of Coulomb potential $U(r) = \frac{1}{4\pi\epsilon}\frac{1}{r}$;

$$\int \frac{e^{-i\vec{k}\cdot\vec{r}}}{|\vec{r}|}d\vec{r} = \frac{4\pi}{k^2}$$

Q8
Explain Koopman ' s theorem.

Q9
Discuss Hartree-Fock-Roothaan approximation.

Q10
Summarize about super-exchange interaction.

Q11
Summarize about double-exchange interaction.