Final Test: 2021.

Multiple-test:

1. The wavelength 488 nm belongs to Visible.
2. The momentum operator in quantum mechanics has real eigenvalues, is self-adjoint
3. Solid materials have a bulk modulus different from zero
4. Metals are characterized by The presence of free electrons, A good electrical conductivity
5. The effectivity mass of an electron in a crystal lattice. May be negative or positive.
6. The rotational-vibrational absorption spectrum of gas of diatomic molecules may be observed in the infrared spectral region, (show a P-branch)
7. The atomic state $^1S_7$ is impossible $l=0,\ s=0\ \ j=7$
8. All crystalls are ______

Treer wrong.

a) From $[\hat{A},\hat{B}]=0$ and $[\hat{B},\hat{C}]=0$ it follows that $[\hat{A},\hat{C}]=0$ Wrong

b) The operator of discrete translations $\hat{T}_n$ defined by $\hat{T}_n\psi(\vec r)=\psi(\vec r+\vec r_n)$ (r_n - lattice vector) with the eigenvalues $t_n=e^{ik r_n}$ is self-adjoint ______

c) All self-adjoint operators commute with each other Wrong

d) Amorphous solids lack any short-range order in their atomic configuration wrong

e) If a crystal lattice has inversion symmetry, the corresponding solid must be a metal wrong

3. In a 1-D harmonic oscillator, obtain the oscillator strength for the quantum transitions. from the eigenstate with quantum number $n=99$ to $n=100$?

$f_{in}=\frac{2m}{\hbar}W_{in}|X_{ni}|^2.$

~~$n=99$ $n=100$~~ $n=99$ $l=100$

~~$n=100$ $l=99$~~

解: $(X_{100,99})^2=(X_{n,n-1})^2\Big|_{n=100}=\frac{n\hbar}{2mW_0}=\frac{100\hbar}{2mW_0}$

$W_{100,99}=W_0$ $\quad(W_{m,n}=W_0 \Leftrightarrow m=n-1)$

$\therefore f_{in}=\frac{2m}{\hbar}W_{in}|X_{ni}|^2=f_{100,99}=\frac{2m}{\hbar}W_{100,99}\cdot|X_{99,100}|^2=100$

4. From Planck's formula, find an expression for the energy density of radiation in equilibrium conditions per wavelength interval i.e: $u(\lambda,T)=\frac{1}{V}\frac{dE}{d\lambda}$.

解: $u(w,T)=\frac{dE}{Vdw}=\frac{\hbar w^3}{c^3\pi^2}\cdot\frac{1}{e^{\frac{\hbar w}{k_0T}}-1}$ $\qquad W=\frac{2\pi c}{\lambda}$

$u(\lambda,T)=\frac{1}{V}\frac{dE}{d\lambda}=\frac{1}{V}\frac{dE}{dw}\cdot\frac{dw}{d\lambda}=-\frac{8\hbar}{\lambda^3}\cdot\frac{1}{e^{\frac{\hbar 2\pi c}{\lambda k_0T}}-1}\cdot\left(-\frac{2\pi c}{\lambda^2}\right)$

$=\frac{16\hbar\pi c}{\lambda^5}\cdot\frac{1}{e^{\frac{2\hbar\pi c}{\lambda k_0T}}-1}$

$w=\frac{2\pi c}{\lambda}$ $\quad dw=-\frac{2\pi c}{\lambda^2}d\lambda$ $\Rightarrow u(w,T)dw=-u(\lambda,T)d\lambda$ $\qquad u(\lambda,T)=\frac{8\pi hc}{\lambda^5}\cdot\frac{1}{e^{\frac{hc}{\lambda k_0T}}-1}$

$\because u(\lambda,T)=\frac{1}{V}\frac{dE}{d\lambda}$ $\quad\therefore \frac{E}{V}=\int_{-\infty}^{\infty}u(\lambda,T)d\lambda=8\pi hc\int_{-\infty}^{\infty}\frac{\left(\frac{1}{\lambda}\right)^5}{e^{\frac{hc}{k_0T}\frac{1}{\lambda}}-1}d\lambda$

$x=\frac{hc}{k_0T}\frac{1}{\lambda}\Rightarrow d\lambda=-\frac{hc}{k_0T}\frac{1}{\lambda^2}dx$

$\therefore$ ~~$\frac{E}{V}$~~ $\therefore \frac{dE}{d\lambda}=\frac{8\pi hcV}{\lambda^5}\frac{1}{e^{\frac{hc}{\lambda k_0T}}-1}$

5. Imagine that you have measured the IR absorption spectrum of a gas of $(CF_3)_3CH$ molecules, You observe the fundamental transition wavenumber of the ~~strength~~ stretching vibration of the CH-group as $\nu_{1,0}=2992\,cm^{-1}$, You also register the transition wavenumber corresponding to the first overtone as $\nu_{2,0}=5882\,cm^{-1}$, From these data, assuming a Morse potential and neglecting any rotations, estimate the transition wavenumber corresponding to the second overtone $\nu_{3,0}$!

解: $\nu_{nm}=G(v=n)-G(v=m)=\nu_0(n-m)-\nu_0x_e[(n+\frac{1}{2})^2-(m+\frac{1}{2})^2]$

$=\nu_0(1-x_e)(n-m)-\nu_ex_e[n^2-m^2]$

$m=0\rightarrow \nu_{n,0}=\nu_e[(1-x_e)n-x_en^2]$

assume $a=\frac{\nu_{n_2,0}}{\nu_{n_1,0}}=\frac{[(1-x_e)n_2-x_en_2^2]}{[(1-x_e)n_1-x_en_1^2]}$ $\Rightarrow x_e=\frac{a(-n_2)}{a(n_1+n_1^2)-(n_2+n_2^2)}$

when $n_1=1,\ n_2=2$ $\quad a=\frac{\nu_{2,0}}{\nu_{1,0}}=\frac{5882}{2992}\approx1.966$

$\rightarrow x_e\approx0.0164$

from $\nu_{n_1,0}=\nu_e[(1-x_e)n_1-x_en_1^2]\rightarrow \nu_e\approx3093.5\,cm^{-1}$

$x_e=\frac{\nu_e}{4D_e}\rightarrow D_e\approx47156.5\,cm^{-1}$

$\therefore$ ~~$E_{diss}=hcD_e(1-x_e)^2\approx5.66eV$~~

$\therefore \nu_{3,0}=\nu_e(1-x_e)\times2-\nu_ex_e\times3$

$=8670\,cm^{-1}$

$\nu_{1,0}=\nu_e(1-x_e)-\nu_ex_e=2992$

$\nu_{2,0}=2\nu_e(1-x_e)-4\nu_ex_e=5882$

$\therefore$ We know $\begin{cases}\nu_e(1-x_e)=3043\\ \nu_ex_e=51\end{cases}$

$\therefore \nu_{3,0}=3\nu_e(1-x_e)-9\nu_ex_e=3\times3043-9\times51$

$=8670\,cm^{-1}$

6. Consider the hydrogen $2p_z$ state $(=|210\rangle)$ with $n=2,\ l=1,\ m=0$, Calculate the variance of r defined as $Var(r)\equiv\langle r^2\rangle-\langle r\rangle^2$ in this state.!

$\int_0^{\infty}r^ne^{-pr}dr=\frac{n!}{p^{n+1}}$

make use of $|210\rangle=\frac{1}{4\sqrt{2\pi}\,a_0^{\frac{3}{2}}}\frac{r}{a_0}e^{-\frac{r}{2a_0}}\cos\theta$

解: $\langle r^2\rangle=\int_{-\infty}^{\infty}\psi^*r^2\psi dV=\frac{1}{32\pi a_0^5}\int_{-\infty}^{\infty}r^4e^{-\frac{r}{a_0}}\cos^2\theta\, dV$

$=\frac{1}{32\pi a_0^5}\underbrace{\int_0^{\infty}r^5e^{-\frac{r}{a_0}}dr}_{120a_0^6}\underbrace{\int_0^{2\pi}d\phi}_{2\pi}\underbrace{\int_0^{\pi}\cos^2\theta\sin\theta d\theta}_{\frac{2}{3}}$

$=5a_0$

$\langle r\rangle=\int_{-\infty}^{\infty}\psi^*r\psi dV=\frac{1}{32\pi a_0^5}\underbrace{\int_0^{\infty}r^4e^{-\frac{r}{a_0}}dr}_{24a_0^5}\underbrace{\int_0^{2\pi}d\phi}_{2\pi}\underbrace{\int_0^{\pi}\cos^2\theta\sin\theta\, d\theta}_{\frac{2}{3}}$

$=1$

$\therefore Var(r)\equiv\langle r^2\rangle-\langle r\rangle^2=5a_0-1$