Problem set 8

Problem 1.

(1.a) $\Delta V = \lambda(x^4+y^4+z^4)$

Using spherical polar coordinates $\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases}$

$$\Delta V = \lambda(x^4+y^4+z^4) = \lambda r^4(\sin^4\theta\cos^4\varphi + \sin^4\theta\sin^4\varphi + \cos^4\theta)$$
$$= \lambda r^4[\sin^4\theta(1-2\cos^2\varphi\sin^2\varphi) + \cos^4\theta]$$

Unlike $\Delta V = f(x^2+y^2+z^2) = f(r^2)$, ΔV can not be rewritten independent of θ, φ, which means rotational symmetry ($SO(3)$) is broken.

But it still has finite symmetry of $x\to -x$, $y\to -y$, $z\to -z$ and any permutation of x, y, z, which is a cubic symmetry (O_h)

(2.a)

Spherical harmonics ($l=2$)

$$Y_2^{\pm2}(\theta,\varphi) = \frac{1}{4}\cdot\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{\pm 2i\varphi}$$
$$Y_2^{\pm1}(\theta,\varphi) = \frac{1}{2}\cdot\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\, e^{\pm i\varphi}$$
$$Y_2^{0}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1)$$

Rewrite $\Delta V = \lambda V_R(r) V_Y(\theta,\varphi)$, $|nlm\rangle = R_{nl}(r) Y_l^m(\theta,\varphi)$

$$\langle nlm_1|\Delta V|nlm_2\rangle = \lambda\langle R_{nl}|\Delta V_R|R_{nl}\rangle\langle Y_l^{m_1}|\Delta V_Y|Y_l^{m_2}\rangle$$

Note that $\lambda\langle R_{nl}|\Delta V_R|R_{nl}\rangle$ is constant for all d-orbitals, we only need to calculate

$$\langle Y_l^{m_1}|\Delta V_Y|Y_l^{m_2}\rangle = \int_0^\pi \sin\theta\, d\theta\int_0^{2\pi} d\varphi\,(\sin^4\theta(1-2\sin^2\varphi\cos^2\varphi)+\cos^4\theta)\, Y_l^{m_1 *}(\theta,\varphi)\, Y_l^{m_2}(\theta,\varphi)$$

Consider integral $\int_0^{2\pi} d\varphi\cdot e^{i(m_2-m_1)\varphi} = 2\pi\,\delta_{m_1,m_2}$

Consider integral $\int_0^{2\pi} d\varphi\,(1-2\sin^2\varphi\cos^2\varphi)e^{i(m_2-m_1)\varphi}$, using $\sin^2\varphi\cos^2\varphi = -\frac{1}{16}(e^{4i\varphi}+e^{-4i\varphi}-2)$

$$= 2\pi\,\delta_{m_1,m_2} + 2\times\frac{1}{16}\int_0^{2\pi}(e^{4i\varphi}+e^{-4i\varphi}-2)e^{i(m_2-m_1)\varphi}$$
$$= \frac{3}{2}\pi\,\delta_{m_1,m_2} + \frac{1}{4}\pi(\delta_{m_2+4,m_1}+\delta_{m_2,m_1+4})$$

Which means by integrating φ, $\langle Y_l^{m_1}|\Delta V_Y|Y_l^{m_2}\rangle$ has off-diagonal elements only when $m=\pm2$.

① $m=\pm 2$ $\qquad -\cos\theta \to x$

$$\int_0^\pi d\theta \sin\theta\,(\sin^2\theta)^2 \sin^4\theta = 2\int_0^1 dx\,(1-x^2)^4 = \frac{256}{315}$$

$$\int_0^\pi d\theta \sin\theta(\sin^2\theta)^2\cos^4\theta = 2\int_0^1 dx\,(1-x^2)^2 x^4 = \frac{16}{315}$$

$$\langle Y_2^{\pm2}|\Delta V_Y|Y_2^{\pm2}\rangle = \frac{15}{16}\frac{1}{2\pi}\left(\frac{256}{315}\times 2\pi + \frac{16}{315}\times\frac{3}{2}\pi\right) = \frac{13}{21}$$

$$\langle Y_2^{\pm2}|\Delta V_Y|Y_2^{\mp2}\rangle = \frac{15}{16}\frac{1}{2\pi}\frac{256}{315}\cdot\frac{\pi}{4} = \frac{2}{21}$$

② $m=\pm1$, similarly.

$$\langle Y_2^{\pm1}|\Delta V_Y|Y_2^{\pm1}\rangle = \frac{11}{21}$$

③ $m=0$

$$\langle Y_2^{0}|\Delta V_Y|Y_2^{0}\rangle = \frac{5}{7} = \frac{15}{21}$$

$$M_{m_1 m_2} = \begin{array}{c} \begin{array}{ccccc} 0 & +1 & -1 & +2 & -2 \end{array} \\ \begin{pmatrix} 5/7 & & & & \\ & 11/21 & & & \\ & & 11/21 & & \\ & & & 13/21 & 2/21 \\ & & & 2/21 & 13/21 \end{pmatrix} \end{array} = \frac{1}{21}\left(11 + 2\begin{pmatrix} 2 & & & & \\ & 0 & & & \\ & & 0 & & \\ & & & 1 & 1 \\ & & & 1 & 1 \end{pmatrix}\right)$$

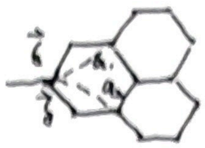
$\to$ eigenvalues 0, 2,
eigenstates $\frac{1}{\sqrt{2}}(Y_2^{+2} \mp Y_2^{-2})$.

Real form. $Y_2^{\pm2} \propto \left(\frac{x\pm iy}{r}\right)^2$, $Y_2^{\pm1} \propto \frac{z(x\pm iy)}{r^2}$, $Y_2^0 \propto \frac{2z^2-x^2-y^2}{r^2}$

$5/7 \to 2z^2-x^2-y^2,\ x^2-y^2$ $\qquad$ (E_g of O_h)

$11/21 \to xz,\ yz,\ xy$ $\qquad$ (T_{2g} of O_h)

Problem 2. Dirac cone



(2.a) $\vec{a}_1 = \frac{a}{2}(3, \sqrt{3})$, $\vec{a}_2 = (3, -\sqrt{3})$

$\vec{b}_1 = \frac{2\pi}{3a}(1, \sqrt{3})$, $\vec{b}_2 = \frac{2\pi}{3a}(1, -\sqrt{3})$

$$\hat{H} = -t \sum_{\langle R, R' \rangle} C_A^\dagger(\vec{R}) C_B(\vec{R'}) + h.c. = -t \sum_\delta \sum_R C_A^\dagger(R) C_B(R+\delta) + h.c.$$

Using k-representation $C_A(R) = \frac{1}{\sqrt{N}} \sum_k e^{ikR} C_A^\dagger(R)$, $C_B(R) = \frac{1}{\sqrt{N}} \sum_k e^{ikR} C_B^\dagger(R)$

$$\hat{H} = -t \sum_\delta \sum_R \sum_{kk'} \underbrace{\frac{1}{N} e^{i(k'-k)R}}_{\delta(k-k')} \cdot e^{ik'\delta} C_A^\dagger(k) C_B(k') + h.c.$$

$$= -t \sum_k \sum_\delta e^{+ik\delta} C_A^\dagger(k) C_B(k) + h.c. = \sum_k (C_A^\dagger(k), C_B^\dagger(k)) \begin{pmatrix} 0 & f(k) \\ f^*(k) & 0 \end{pmatrix} \begin{pmatrix} C_A(k) \\ C_B(k) \end{pmatrix}$$

~~f(k)~~ $\delta_1 = (-a, 0)$, $\delta_2 = (\frac{1}{2}a, \frac{\sqrt{3}}{2}a)$, $\delta_3 = (\frac{1}{2}a, -\frac{\sqrt{3}}{2}a)$

$$f(k) = -t \sum_\delta e^{ik\delta} = -t\left(e^{-ik_x a} + 2e^{ik_x a/2} \cos\left(\frac{\sqrt{3}}{2} k_y a\right)\right)$$

with on-site energy ε_A, ε_B

$$\varepsilon_A \sum_R n_A(R) = \frac{1}{N} \sum_R \sum_{kk'} e^{i(k-k')R} C_A^\dagger(k) C_A(k) = \sum_k \varepsilon_A n(k)$$

$$\hat{H} = \sum_k (\quad , \quad) \begin{pmatrix} V & f(k) \\ f^*(k) & -V \end{pmatrix} \begin{pmatrix} \quad \end{pmatrix}$$

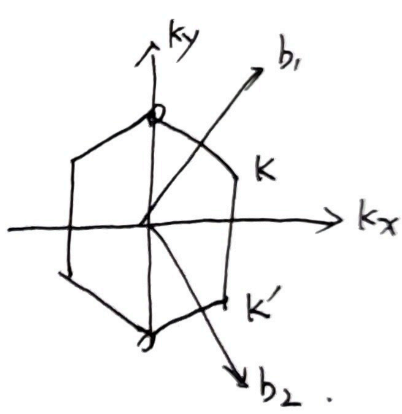
Dirac cone at $f(k) = 0$ yields

$$\begin{cases} \cos(k_x a) + 2\cos(k_x a/2) \cos(k_y a\sqrt{3}/2) = 0 \\ -\sin(k_x a) + 2\sin(k_x a/2) \cos(k_y a\sqrt{3}/2) = 0 \end{cases}$$

Solution

① $\sin(k_x a) = 0$, $\cos(\frac{\sqrt{3}}{2} k_y a) = -\frac{1}{2}$

② $\cos\frac{k_x a}{2} = \cos(\frac{\sqrt{3}}{2} k_y a) = \pm\frac{1}{2}$



at $k=K$

$$\frac{\partial f}{\partial k_x} = iat\left(e^{-ik_x a} - e^{ik_x a/2}\cos\frac{\sqrt{3}}{2}k_y a\right) = -\frac{3}{2}iat\, e^{\pi i/3}$$

$$\frac{\partial f}{\partial k_y} = \sqrt{3}\,at\left(e^{ik_x a/2}\sin\left(\frac{\sqrt{3}}{2}k_y a\right)\right) = \frac{3}{2}at\cdot e^{\pi i/3}$$

$$\sqrt{E^2} = \frac{3}{2}at\sqrt{\left[e^{\pi i/3}(-iq_x+q_y)\right]\left[e^{-\pi i/3}(+iq_x+q_y)\right]} = v_F\sqrt{q_x^2+q_y^2} = v_F(\sigma_x q_x + \sigma_y q_y)$$

With $\varepsilon_A = V$, $\varepsilon_B = -V$

$$\sqrt{E^2} = v_F\sqrt{q_x^2+q_y^2+(V/v_F)^2} = v_F\left(\sigma_x q_x + \sigma_y q_y + \frac{V}{v_F}\cdot\sigma_z\right)$$