4.2

a, b see lecture 28

$$\psi(x,y,z) = \psi_x(x)\,\psi_y(y)\,\psi_z(z) = \left(\sqrt{\frac{2}{a}}\right)^3 \sin\frac{n_x\pi x}{a}\,\sin\frac{n_y\pi y}{a}\,\sin\frac{n_z\pi z}{a}$$

(c)

	n_x, n_y, n_z	
E_7:	2 2 3	17
E_8:	4 1 1	18
E_9:	3 3 1	19
E_{10}:	4 2 1	21
E_{11}:	3 3 2	22
E_{12}:	4 2 2	24
E_{13}:	4 3 1	26
E_{14}:	$\left.\begin{matrix} 5\ 1\ 1 \\ 3\ 3\ 3 \end{matrix}\right\}$	27 "accidental" degeneracy!

4.1

$$\Theta(\theta) = A \ln\left(\tan\frac{\theta}{2}\right)$$

$l = m = 0$

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d}{d\theta}\Theta\right) = 0$$

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{A\sec^2\frac{\theta}{2}}{2\tan\frac{\theta}{2}}\right)$$

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{A\cancel{\cos\frac{\theta}{2}}}{2\cos^{\cancel{2}}\frac{\theta}{2}\,\sin\theta/2}\right)$$

$$\sin\theta \frac{d}{d\theta}\left(\cancel{\sin\theta}\frac{A}{\cancel{\sin\theta}}\right) = 0$$

$$\left.\begin{array}{l}\Theta(\theta=0) \Rightarrow -\infty \\ \Theta(\theta=\pi) \Rightarrow +\infty\end{array}\right\}$$ So it is unacceptable

4.5

$$Y_\ell^\ell(\theta,\phi) = (-1)^\ell \left[\frac{2\ell+1}{4\pi(2\ell)!}\right]^{1/2} e^{i\ell\phi} P_\ell^\ell$$

$$P_\ell = \frac{1}{2^\ell \ell!} \frac{\partial^{|\ell|}}{\partial x} (x^2-1)^\ell$$

$$P_\ell^\ell = (1-x^2)^{\ell/2} \frac{\partial^{|\ell|}}{\partial x} P_\ell = \frac{1}{2^\ell \ell!} (1-x^2)^{\ell/2} \underbrace{\frac{\partial^{|2\ell|}}{\partial x} (x^2-1)^\ell}$$

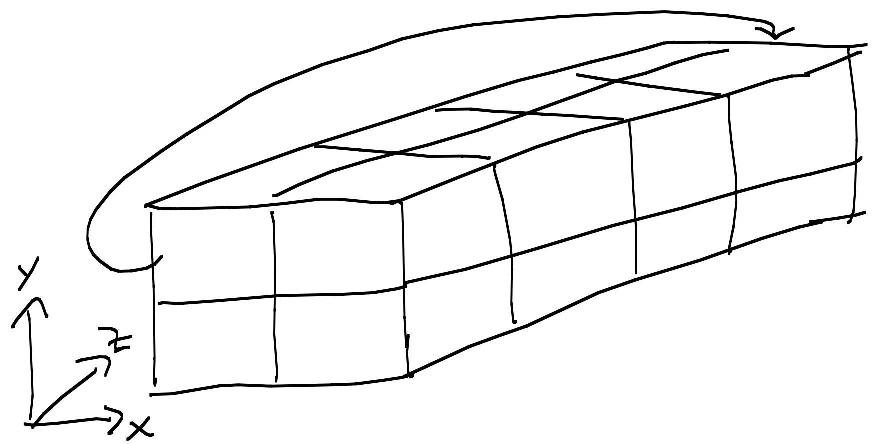
$$\frac{\partial^{|2\ell|}}{\partial x} x^{2\ell} + \cancel{\frac{\partial^{|2\ell|}}{\partial x} x^{<2\ell}} \to 0 = (2\ell)!$$

$$Y_\ell^\ell(\theta,\phi) = (-1)^\ell \left[\frac{2\ell+1}{4\pi(2\ell)!}\right]^{1/2} e^{i\ell\phi} \frac{1}{2^\ell \ell!} (1-\cos^2\theta)^{\ell/2} (2\ell)!$$

$$= \frac{(2\ell)!}{2^\ell \ell!} (-1)^\ell \left[\frac{2\ell+1}{4\pi(2\ell)!}\right]^{1/2} (\sin\theta\, e^{i\phi})^\ell$$

$$= \frac{1}{\ell!} \left[\frac{(2\ell+1)!}{4\pi}\right]^{1/2} \left(-\frac{1}{2}\sin\theta\, e^{i\phi}\right)^\ell$$

#2

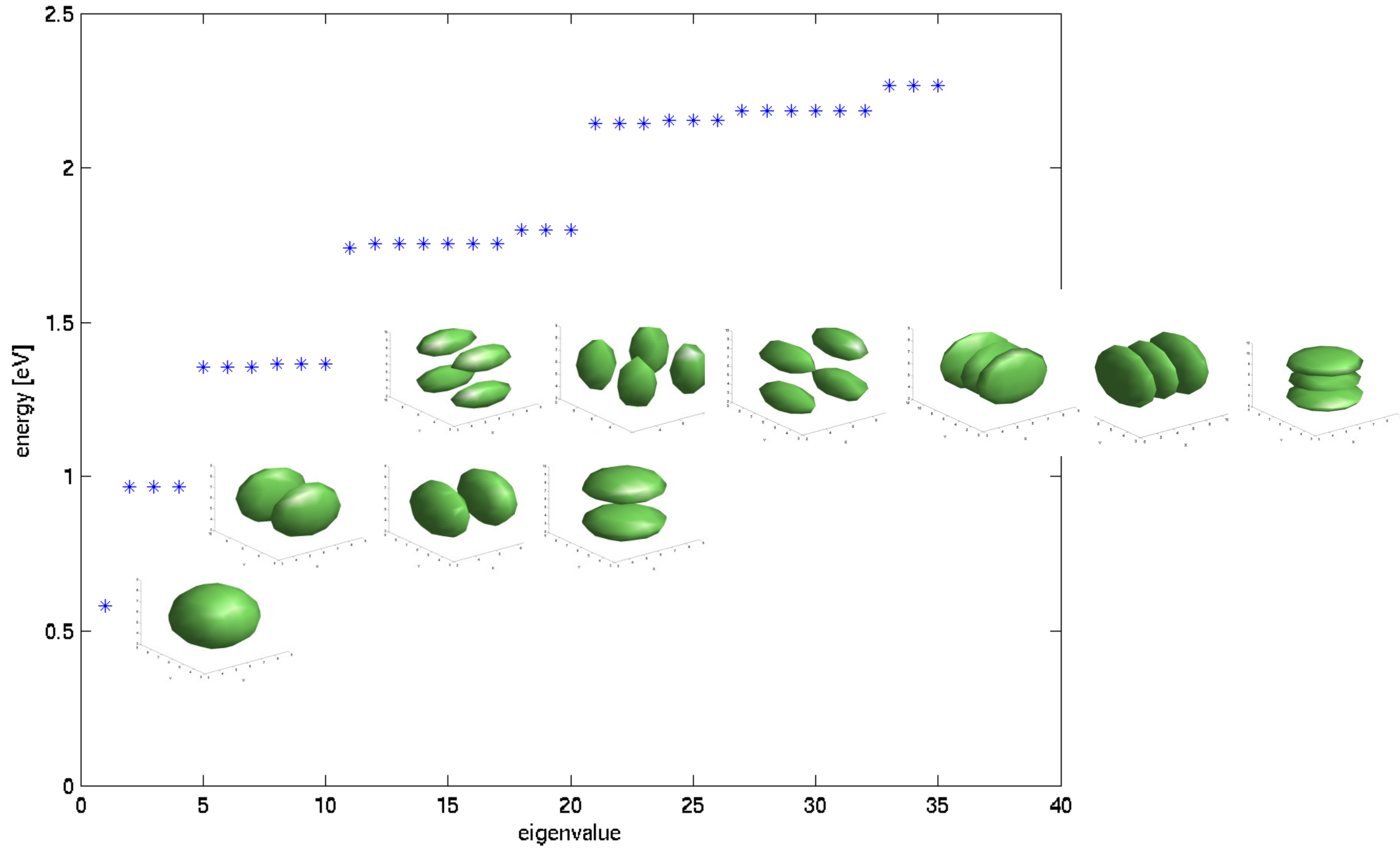


$$H = \left[\begin{array}{c|c|c|c} H_{xy} & t_z \hat{I}_4 & \hat{O} & t_z \hat{I}_4 \\ \hline t_z \hat{I}_4 & H_{xy} & t_z \hat{I}_4 & \hat{O} \\ \hline \hat{O} & t_z \hat{I}_4 & H_{xy} & t_z \hat{I}_4 \\ \hline t_z \hat{I}_4 & \hat{O} & t_z \hat{I}_4 & H_{xy} \end{array}\right]$$

$$H_{xy} = \left[\begin{array}{c|c} H_x & t_y \hat{I}_2 \\ \hline t_y \hat{I}_2 & H_x \end{array}\right]$$

$$H_x = \begin{pmatrix} -2(t_x+t_y+t_z) & t_x \\ t_x & -2(t_x+t_y+t_z) \end{pmatrix}$$

```
clear; close all

c=2.998e10;%cm/s
hbar=6.582e-16; %in eV*sec
m=5.11e5/c^2; %in eV/c^2

dx=2e-8+eps; %2 Ang, in cm
dy=2e-8; %2 Ang, in cm
dz=2e-8-eps; %2 Ang, in cm

tx=-hbar^2/(2*m*dx^2);
ty=-hbar^2/(2*m*dy^2);
tz=-hbar^2/(2*m*dz^2);

Nx=11;Ny=11;Nz=11;

Hx=diag(-2*(tx+ty+tz)*ones(Nx,1))+diag(tx*ones(Nx-
1,1),1)+diag(tx*ones(Nx-1,1),-1);
Hy=ty*eye(Nx);
Hz=tz*eye(Nx*Ny);

Hxy=kron(eye(Ny),Hx)+kron(diag(ones(Ny-1,1),1),Hy)+kron(diag(ones(Ny-
1,1),-1),Hy);
H=kron(eye(Nz),Hxy)+kron(diag(ones(Nz-1,1),1),Hz)+kron(diag(ones(Nz-
1,1),-1),Hz);

%add potential
for ii=1:Nx
 for jj=1:Ny
  for kk=1:Nz
    V((kk-1)*(Nx*Ny)+(jj-1)*Nx+ii)=1e14*((ii-(Nx+1)/2)^2*dx^2+(jj-
(Ny+1)/2)^2*dy^2+(kk-(Nz+1)/2)^2*dz^2);
  end
 end
end
H=H+diag(V);

[v,d]=eig(H);

E=diag(d);

figure(99)
plot(E,'*'); axis([0 40 0 2.5])
xlabel('eigenvalue')
ylabel('energy [eV]')

%show iso-density surfaces of eigenstates
vsv=conj(v).*v; %|Psi|^2

densitythresh=0.004;
for ii=1:10
  figure(ii);
  isosurface(reshape(vsv(:,ii),Nx, Ny, Nz),densitythresh);
  xlabel('X'); ylabel('Y');
end
```



energy [eV]
eigenvalue
0
0.5
1
1.5
2
2.5
0
5
10
15
20
25
30
35
40