HW #10

1) BD P. 1 $\qquad V = \frac{\lambda}{2} m\omega^2 x^2 = \frac{\lambda \hbar\omega}{2}\left(\frac{a+a^{\dagger}}{\sqrt{2}}\right)^2$

$$\Delta E_n^{(2)} = \sum_{m\neq n} \frac{|\langle m|V_0|n\rangle|^2}{E_n - E_m}$$

$m = n-2$ $\qquad$ $m = n+2$

only terms that contribute are aa & $a^{\dagger}a^{\dagger}$

$$= \frac{\lambda^2(\hbar\omega)^2}{16}\left[\frac{(n+1)(n+2)}{-2\hbar\omega} + \frac{n(n-1)}{2\hbar\omega}\right]$$

~~$= \frac{\lambda^2\hbar^2\omega^2}{8\hbar\omega}(2n^2-2n+2) = \frac{\lambda^2\hbar\omega}{4}(n^2-n+1)$~~

$$= \frac{\lambda^2\hbar\omega}{32}\left[n^2 - n - n^2 - 3n - 2\right]$$

$$= \frac{\lambda^2\hbar\omega}{32}(-4)(n+1/2) = \frac{-\lambda^2\hbar\omega}{8}(n+1/2)$$

$$\sqrt{1+\lambda} = 1 + \lambda - \lambda^2/8 \quad ✓$$

- **#2-5**

In[36]:= `toPolar[x_] := x /. a_ → Abs[a] Exp[ⅈ Arg[a]]`

In[37]:= `$Assumptions = {Im[b] == 0};`

unperturbed hamiltonian, in atom position basis

In[38]:= $$h0 = \begin{pmatrix} 0 & -a & 0 & 0 & 0 & -a \\ -a & 0 & -a & 0 & 0 & 0 \\ 0 & -a & 0 & -a & 0 & 0 \\ 0 & 0 & -a & 0 & -a & 0 \\ 0 & 0 & 0 & -a & 0 & -a \\ -a & 0 & 0 & 0 & -a & 0 \end{pmatrix}$$

Out[38]= `{{0, -a, 0, 0, 0, -a}, {-a, 0, -a, 0, 0, 0}, {0, -a, 0, -a, 0, 0}, {0, 0, -a, 0, -a, 0}, {0, 0, 0, -a, 0, -a}, {-a, 0, 0, 0, -a, 0}}`

In[39]:= `Eigenvalues[h0]`

Out[39]= `{-2 a, -a, -a, a, a, 2 a}`

has degenerate eigenvalues, so need to find orthogonal eigenstates using the rotation operator

In[40]:= $$r = \begin{matrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{matrix}$$

Out[40]= `{{0, 1, 0, 0, 0, 0}, {0, 0, 1, 0, 0, 0}, {0, 0, 0, 1, 0, 0}, {0, 0, 0, 0, 1, 0}, {0, 0, 0, 0, 0, 1}, {1, 0, 0, 0, 0, 0}}`

check that h0 communtes with r

In[41]:= `h0.r - r.h0 // Simplify`

Out[41]= `{{0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}}`

In[42]:= `{rs, kets} = Eigensystem[r] // toPolar`

Out[42]= $\left\{\left\{-1, 1, e^{\frac{2 i \pi}{3}}, e^{-\frac{2 i \pi}{3}}, e^{\frac{i \pi}{3}}, e^{-\frac{i \pi}{3}}\right\}, \left\{\{-1, 1, -1, 1, -1, 1\}, \{1, 1, 1, 1, 1, 1\}, \left\{e^{\frac{2 i \pi}{3}}, e^{-\frac{2 i \pi}{3}}, 1, e^{\frac{2 i \pi}{3}}, e^{-\frac{2 i \pi}{3}}, 1\right\}, \left\{e^{-\frac{2 i \pi}{3}}, e^{\frac{2 i \pi}{3}}, 1, e^{-\frac{2 i \pi}{3}}, e^{\frac{2 i \pi}{3}}, 1\right\}, \left\{e^{\frac{i \pi}{3}}, e^{\frac{2 i \pi}{3}}, -1, e^{-\frac{2 i \pi}{3}}, e^{-\frac{i \pi}{3}}, 1\right\}, \left\{e^{-\frac{i \pi}{3}}, e^{-\frac{2 i \pi}{3}}, -1, e^{\frac{2 i \pi}{3}}, e^{\frac{i \pi}{3}}, 1\right\}\right\}\right\}$

In[43]:= `bras = Inverse[kets`$^{\mathsf{T}}$`] // Simplify // toPolar`

Out[43]=
$$\left\{\left\{-\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}, \frac{1}{6}, -\frac{1}{6}, \frac{1}{6}\right\}, \left\{\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}\right\}, \left\{\frac{1}{6}\, e^{-\frac{2 i \pi}{3}}, \frac{1}{6}\, e^{\frac{2 i \pi}{3}}, \frac{1}{6}, \frac{1}{6}\, e^{-\frac{2 i \pi}{3}}, \frac{1}{6}\, e^{\frac{2 i \pi}{3}}, \frac{1}{6}\right\}, \left\{\frac{1}{6}\, e^{\frac{2 i \pi}{3}}, \frac{1}{6}\, e^{-\frac{2 i \pi}{3}}, \frac{1}{6}, \frac{1}{6}\, e^{\frac{2 i \pi}{3}}, \frac{1}{6}\, e^{-\frac{2 i \pi}{3}}, \frac{1}{6}\right\}, \left\{\frac{1}{6}\, e^{-\frac{i \pi}{3}}, \frac{1}{6}\, e^{-\frac{2 i \pi}{3}}, -\frac{1}{6}, \frac{1}{6}\, e^{\frac{2 i \pi}{3}}, \frac{1}{6}\, e^{\frac{i \pi}{3}}, \frac{1}{6}\right\}, \left\{\frac{1}{6}\, e^{\frac{i \pi}{3}}, \frac{1}{6}\, e^{\frac{2 i \pi}{3}}, -\frac{1}{6}, \frac{1}{6}\, e^{-\frac{2 i \pi}{3}}, \frac{1}{6}\, e^{-\frac{i \pi}{3}}, \frac{1}{6}\right\}\right\}$$

now we have an orthogonal basis to work with for perturbation theory

In[44]:= `es = Diagonal[bras.h.kets`$^{\mathsf{T}}$` // Simplify] // Chop`

Out[44]= `{2 a, -2 a, a, a, -a, -a}`

note that the (3rd and 4th), and (5th and 6th) pairs are degenerate

perturbation in atom basis

In[45]:=
$$\mathbf{h1} = -\mathbf{b} \begin{array}{cccccc} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}$$

Out[45]= `{{0, -b, 0, 0, 0, 0}, {-b, 0, -b, 0, 0, 0}, {0, -b, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}}`

need to rewrite it in the basis of h0

In[46]:= `h1p = bras.h1.kets`$^{\mathsf{T}}$` // Simplify // MatrixForm`

Out[46]//MatrixForm=
$$\left(\begin{array}{ccccc} \frac{2 b}{3} & 0 & -\frac{1}{6}\left(1+(-1)^{1/3}\right)^2 b & \frac{1}{4}\, i \left(i+\sqrt{3}\right) b & \frac{1}{12}\, i\, (i + \sqrt{} \\ 0 & -\frac{2 b}{3} & -\frac{1}{6}\left(-1+(-1)^{1/3}\right)^2 b & \frac{1}{12}\left(1-i\sqrt{3}\right) b & \frac{1}{4}\, (1 - i\sqrt{} \\ \frac{1}{4}\, i\left(i+\sqrt{3}\right) b & \frac{1}{12}\left(1-i\sqrt{3}\right) b & \frac{b}{3} & -\frac{1}{3}\left(1+(-1)^{2/3}\right) b & 0 \\ -\frac{1}{6}\left(1+(-1)^{1/3}\right)^2 b & -\frac{1}{6}\left(-1+(-1)^{1/3}\right)^2 b & \frac{1}{3}\left(-1+(-1)^{1/3}\right) b & \frac{b}{3} & 0 \\ -\frac{1}{6}(-1)^{1/3} b & \frac{1}{6}\left(1+(-1)^{1/3}\right)^2 b & 0 & 0 & -\frac{b}{3} \\ \frac{1}{12}\, i\left(i+\sqrt{3}\right) b & \frac{1}{4}\left(1-i\sqrt{3}\right) b & 0 & 0 & \frac{1}{3}\, (1 + (-1) \end{array}\right.$$

now, because the 3rd and 4th, and (5th and 6th) pairs are degenerate, we have to treat them specially

take the 3rd&4th submatrix:

In[47]:=
$$\mathbf{a} + \mathbf{Eigenvalues}\left[\begin{array}{cc} \frac{b}{3} & -\frac{1}{3}\left(1+(-1)^{2/3}\right) b \\ \frac{1}{3}\left(-1+(-1)^{1/3}\right) b & \frac{b}{3} \end{array}\right]$$

Out[47]=
$$\left\{a, a+\frac{2 b}{3}\right\}$$

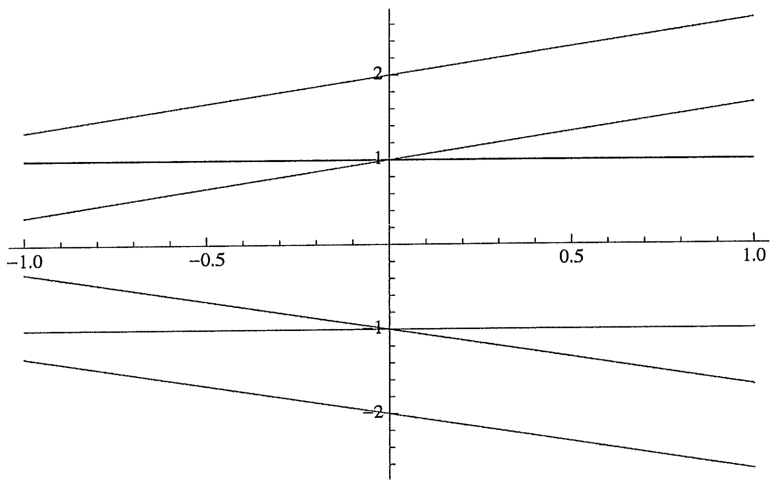
now the 5 th and 6 th

In[48]:=
$$-a + \text{Eigenvalues}\begin{bmatrix} -\frac{b}{3} & -\frac{1}{3}\left(-1+(-1)^{1/3}\right) b \\ \frac{1}{3}\left(1+(-1)^{2/3}\right) b & -\frac{b}{3} \end{bmatrix}$$

Out[48]=
$$\left\{-a,\ -a-\frac{2\,b}{3}\right\}$$

so the first order energy shifts, plotted, are

In[49]:=
$$\text{Plot}\left[\text{Flatten}\left[\left\{2\,a+2\,b/3,\ -2\,a-2\,b/3,\ \left\{a,\ a+\frac{2\,b}{3}\right\},\ \left\{-a,\ -a-\frac{2\,b}{3}\right\}\right\}\right] /.\ a\to 1,\ \{b,\ -1,\ 1\}\right]$$

Out[49]=


find the exact results

In[50]:= Eigenvalues[h0 + h1 /. a → 1]

Out[50]=
$$\left\{-1,\ 1,\ -\frac{\sqrt{5+4\,b+2\,b^2-\sqrt{9+8\,b+20\,b^2+16\,b^3+4\,b^4}}}{\sqrt{2}},\right.$$

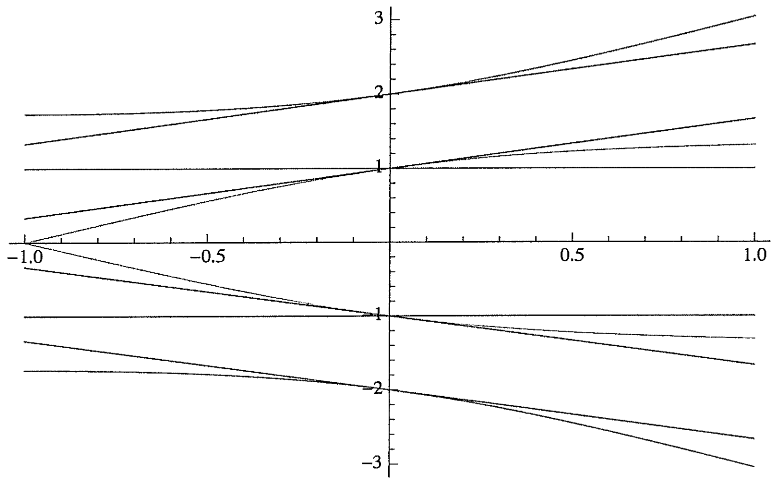
$$\frac{\sqrt{5+4\,b+2\,b^2-\sqrt{9+8\,b+20\,b^2+16\,b^3+4\,b^4}}}{\sqrt{2}},$$

$$-\sqrt{\frac{5}{2}+2\,b+b^2+\frac{1}{2}\sqrt{9+8\,b+20\,b^2+16\,b^3+4\,b^4}},$$

$$\left.\sqrt{\frac{5}{2}+2\,b+b^2+\frac{1}{2}\sqrt{9+8\,b+20\,b^2+16\,b^3+4\,b^4}}\right\}$$

In[51]:= `Show[Plot[%, {b, -1, 1}], %%]`

Out[51]=



so the results work pretty well out to about b=0.1 a. The answers would be substantially improved if we included the second order shifts as well.

- **#6**

In[52]:= $\{\text{evals}, \text{kets}\} = \text{Eigensystem}\left[\begin{matrix} a & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -a/2 \end{matrix}\right]$

Out[52]= $\left\{\left\{0, -\frac{a}{2}, a\right\}, \{\{0, 1, 0\}, \{0, 0, 1\}, \{1, 0, 0\}\}\right\}$

In[53]:= $\text{bras} = \text{Inverse}[\text{kets}^T]$

Out[53]= `{{0, 1, 0}, {0, 0, 1}, {1, 0, 0}}`

In[54]:= $V = \begin{matrix} 0 & b & 0 \\ b & 0 & b \\ 0 & b & 0 \end{matrix};\ \text{bras}.V.\text{kets}^T \text{ // MatrixForm}$

Out[54]//MatrixForm=

$$\begin{pmatrix} 0 & b & b \\ b & 0 & 0 \\ b & 0 & 0 \end{pmatrix}$$

In[55]:= $\text{evals}[[1]] + \frac{(\text{bras}[[2]].V.\text{kets}[[1]])^2}{\text{evals}[[1]] - \text{evals}[[2]]} + \frac{(\text{bras}[[3]].V.\text{kets}[[1]])^2}{\text{evals}[[1]] - \text{evals}[[3]]} \text{ // Simplify}$

Out[55]= $\frac{b^2}{a}$

In[56]:= $\text{evals}[[2]] + \frac{(\text{bras}[[3]].V.\text{kets}[[2]])^2}{\text{evals}[[2]] - \text{evals}[[3]]} + \frac{(\text{bras}[[1]].V.\text{kets}[[2]])^2}{\text{evals}[[2]] - \text{evals}[[1]]} \text{ // Simplify}$

Out[56]= $-\frac{a}{2} - \frac{2 b^2}{a}$

In[57]:= $\text{evals}[[3]] + \frac{(\text{bras}[[1]].\text{V}.\text{kets}[[3]])^2}{\text{evals}[[3]] - \text{evals}[[1]]} + \frac{(\text{bras}[[2]].\text{V}.\text{kets}[[3]])^2}{\text{evals}[[3]] - \text{evals}[[2]]}$ // Simplify

Out[57]= $a + \frac{b^2}{a}$

another way: define an effective second-order operator. First define an outer product

In[58]:= `OP[ket_, bra_] := KroneckerProduct[{ket}`$^{\mathsf{T}}$`, {bra}]`

now do the general sum over intermediate states

In[59]:= $\text{G2} = \text{Sum}\left[\text{V}.\frac{\text{OP}[\text{kets}[[m]], \text{bras}[[m]]]}{e - \text{evals}[[m]]}.\text{V}, \{m, 3\}\right]$

Out[59]= $\left\{\left\{\frac{b^2}{e}, 0, \frac{b^2}{e}\right\}, \left\{0, \frac{b^2}{-a+e} + \frac{b^2}{\frac{a}{2}+e}, 0\right\}, \left\{\frac{b^2}{e}, 0, \frac{b^2}{e}\right\}\right\}$

In[60]:= `evals + Table[bras[[i]].G2.kets[[i]] /. e → evals[[i]], {i, 3}] // Simplify`

Out[60]= $\left\{\frac{b^2}{a}, -\frac{a}{2} - \frac{2 b^2}{a}, a + \frac{b^2}{a}\right\}$