Q3. $H_0 = \frac{p^2}{2m}$, $V(x+a) = V(x)$.

$E_0(k) = \frac{\hbar^2 k^2}{2m}$. $H = H_0 + V(x)$.

$V(x+a) = V(x)$

(i) Matrix element.

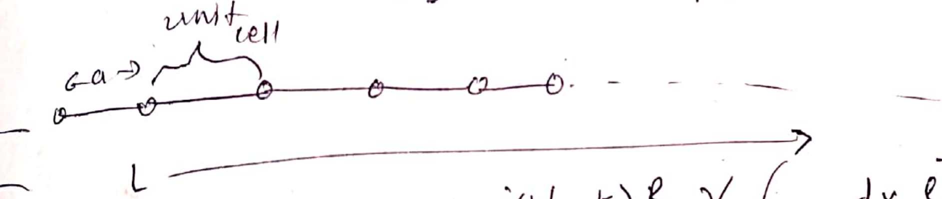
$$\langle k'|V|k\rangle = \frac{1}{L^3}\int dx \cdot e^{i(k-k')x} V(x) = V_{k'-k}$$

$$= \underline{V_{k'-k}}.$$

Now let $R = na$, be lattice position, $n \in \mathbb{Z}$.

and $\underline{V(x+R) = V(x)}$.

$$\langle k'|V|k\rangle = \cancel{\frac{1}{L}\sum_R} = \frac{1}{L}\sum_R \int_{\text{unit cell}} dx\, e^{-i(k'-k)(x+R)} V(x+R).$$



$$= \frac{1}{L}\left(\sum_R e^{-i(k'-k)R}\right)\left(\int_{\text{unit cell}} dx\, e^{-i(k'-k)x} V(x+R)\right)$$

$$= \frac{1}{L}\left(\sum_R e^{-i(k'-k)R}\right)\left(\int_{\text{unit cell}} dx\, e^{-i(k'-k)x} V(x)\right)$$

$\boxed{V(x) = V(x+R)}$

~~Now take density~~ we have to find out $\sum_R e^{-i(k'-k)R}$.

take $\rho(x) = \sum \delta(x-na)$.

$F(\rho(x)) = \frac{2\pi}{a}\sum_m \delta\left(k - \frac{2\pi m}{a}\right) = \sum_n \int dx\, e^{ikx}\delta(x-na)$

fourier transfer $= \sum_n e^{ikna}$.

$\Rightarrow \sum e^{i(k)na} = \sum e^{ikR} \propto \sum \delta\left(k - \frac{2\pi m}{a}\right)$.

$\Rightarrow k = \frac{2\pi m}{a}$ for this to be non-zero.

(Poisson summation formula)

$\Rightarrow \quad k' - k = \frac{2\pi m}{a}. \qquad m \in \mathbb{Z}.$

$\Rightarrow \quad V_{k'-k}$ is only non-zero for

$k' - k = \frac{2\pi m}{a}.$

$$V_{\frac{2\pi m}{a}} = \frac{1}{L}\int dx\, e^{i\frac{2\pi m x}{a}} V(x) \qquad \text{let } G = \frac{2\pi m}{a}.$$

(ii). Treating $V(x)$ as a perturbation.

$$\varepsilon^{(1)}(k) = \langle k | V | k \rangle = V_0 = \frac{1}{L}\int_{-\infty}^{\infty} dx\, V(x).$$

a constant energy shift

(we can redefine $V(x)$ as $V(x) + V_0$ to get rid of it).

$$\varepsilon^{(2)}(k) = \sum_{\substack{k' = k+G \\ G \neq 0}} \frac{|\langle k' | V | k \rangle|^2}{\varepsilon_0(k) - \varepsilon_0(k')}$$

$$\boxed{G = \frac{2\pi m}{a}.}$$

$$\varepsilon_0(k) = \frac{\hbar^2 k^2}{2m}.$$

Degeneracy exists when $\varepsilon_0(k) = \varepsilon_0(k')$ and $k' = k + G$.

for $\varepsilon_0(k) = \frac{\hbar^2 k^2}{2m}$, this only happens at

$k' = -k = \frac{n\pi}{a}. \quad n \in \mathbb{Z}.$

Brillouin zone boundary

$$\boxed{-k = k + G \Rightarrow k = \frac{G}{2} = \frac{m\pi}{a}}$$

(iii). To do degenerate perturbation theory.

we pick a two level system with.

$|k\rangle$ & $|k+G\rangle$.

$\langle k | H | k \rangle = \varepsilon_0(k), \quad \langle k' | H | k' \rangle = \varepsilon_0(k+G) = \varepsilon_0(k).$

$\langle k | H | k' \rangle = (\langle k' | H | k \rangle)^* = V_G^*$

$|\psi\rangle = \alpha |k\rangle + \beta |k+G\rangle.$

$$\begin{pmatrix} \varepsilon_0(k) & V_G^* \\ V_G & \varepsilon_0(k+G) \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E\begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$$

$$(\varepsilon_0(k) - E)^2 = |V_G|^2$$

$$\Rightarrow \quad E_\pm = \varepsilon_0(k) \pm |V_G|$$

So at zone boundary "G", the energy splits with a gap of $E_+ - E_- = 2|V_G|$.

(iv). Say $k = \frac{n\pi}{a} + \delta$. & $k' = -\frac{n\pi}{a} + \delta$.

$$\mathcal{E}_0\left(\frac{n\pi}{a} + \delta\right) = \frac{\hbar^2}{2m}\left(\left(\frac{n\pi}{a}\right)^2 + \delta^2 + \frac{2n\pi\delta}{a}\right).$$

$$\mathcal{E}_0\left(-\frac{n\pi}{a} + \delta\right) = \frac{\hbar^2}{2m}\left(\left(\frac{n\pi}{a}\right)^2 + \delta^2 - \frac{2n\pi\delta}{a}\right).$$

Now the degenerate perturbation theory eq is.

$$\cancel{(\mathcal{E}_0(k) - E)} \; (\mathcal{E}_0(k+\delta) - E)(\mathcal{E}_0(k'+\delta) - E) - |V_G|^2 = 0.$$

$$\Rightarrow \left(\frac{\hbar^2}{2m}\left(\left(\frac{n\pi}{a}\right)^2 + \delta^2\right) + \frac{\hbar^2}{2m}\frac{2n\pi\delta}{a} - E\right)\left(\frac{\hbar^2}{2m}\left(\left(\frac{n\pi}{a}\right)^2 + \delta^2\right) - E - \frac{\hbar^2}{2m}\frac{2n\pi\delta}{a}\right) - |V_G|^2 = 0.$$

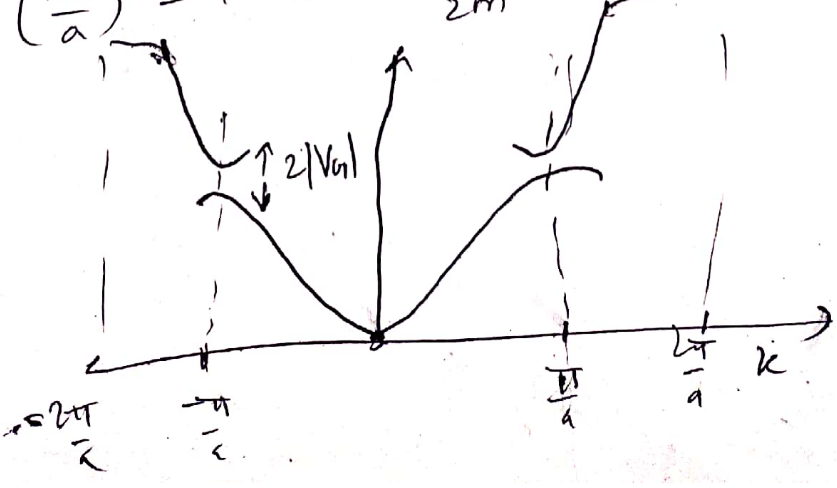
$$\Rightarrow \left(\frac{\hbar^2}{2m}\left(\left(\frac{n\pi}{a}\right)^2 + \delta^2\right) - E\right)^2 = \left(\frac{\hbar^2}{2m}\frac{2n\pi\delta}{a}\right)^2 + |V_G|^2.$$

$$E_\pm = \frac{\hbar^2}{2m}\left(\left(\frac{n\pi}{a}\right)^2 + \delta^2\right) \pm \sqrt{|V_G|^2 + \left(\frac{\hbar^2}{2m}\frac{2n\pi\delta}{a}\right)^2}$$

expand in small "δ".

$$E_\pm = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 \pm |V_G| + \frac{\hbar^2\delta^2}{2m}\left(1 \pm \frac{\hbar^2}{m}\left(\frac{n\pi}{a}\right)^2\frac{1}{|V_G|}\right)$$

$\Rightarrow$



(V). $V(x) = 2V_1 \cos\left(\frac{2\pi x}{a}\right)$.

$$V_G = \frac{1}{a}\int dx\, e^{iGx}\, V(x)$$

$$V(x) = V_1 e^{i\frac{2\pi x}{a}} + V_1 e^{-i\frac{2\pi x}{a}}.$$

$$V_G = \frac{V_1}{a}\int dx\left(e^{i(G+\frac{2\pi}{a})x} + e^{+i(G-\frac{2\pi}{a})x}\right).$$

This is non-zero only for.

$G = \frac{2\pi}{a}$ or $-\frac{2\pi}{a}$.

$$V_{\frac{2\pi}{a}} = V_{-\frac{2\pi}{a}} = V_1$$

$k = -k' = \frac{\pi}{a}$ ~~or~~

$$E_\pm = \varepsilon_0\left(\pm\frac{\pi}{a}\right) \pm |V_G|$$
$$= \frac{\hbar^2}{2m}\frac{\pi^2}{a^2} \pm V_1.$$

for. $E_+ = \frac{\hbar^2\pi^2}{2ma^2} + V_1$.

$$\begin{pmatrix} \hbar^2\pi^2/2ma^2 & V_1 \\ V_1 & \hbar^2\pi^2/2ma^2 \end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = \frac{\hbar^2\pi^2}{2ma^2} + V_1 \begin{pmatrix}\alpha \\ \beta\end{pmatrix}.$$

Solving this gives $\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = \begin{pmatrix}1/\sqrt{2} \\ 1/\sqrt{2}\end{pmatrix}$ .. normalised.

and for $E_- = \frac{\hbar^2\pi^2}{2ma^2} - V_1$

$$\begin{pmatrix} \hbar^2\pi^2/2ma^2 & V_1 \\ V_1 & \hbar^2\pi^2/2ma^2 \end{pmatrix}\begin{pmatrix}\alpha' \\ \beta'\end{pmatrix} = \frac{\hbar^2\pi^2}{2ma^2} + V_1 \begin{pmatrix}\alpha' \\ \beta'\end{pmatrix}$$

$$\Rightarrow \begin{pmatrix}\alpha' \\ \beta'\end{pmatrix} = \begin{pmatrix}1/\sqrt{2} \\ -1/\sqrt{2}\end{pmatrix}$$

$\Rightarrow$ eigenstates to first order are

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|k\rangle \pm |k'\rangle\right)$$

as $|k\rangle \to e^{ikx} = e^{i\pi x/a}$, $|k'\rangle \to e^{-i\pi x/a}$

$$\psi_+ \approx e^{i\pi x/a} + e^{-i\pi x/a} \approx \cos\left(\frac{\pi x}{a}\right)$$

$$\psi_- \approx e^{i\pi x/a} - e^{-i\pi x/a} \approx \sin\left(\frac{\pi x}{a}\right)$$

Q2

(i) $\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \hbar\omega\left(\frac{1}{2} + a^\dagger a\right)$.

$H_1 = g_1\hat{x} = g_1\sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a} + \hat{a}^\dagger)$.

$|\phi_n^0\rangle = |n\rangle$, $E_n^0 = \hbar\omega(n+\frac{1}{2})$.

$E_n^1 = \langle n|H_1|n\rangle = g_1\sqrt{\frac{\hbar}{2m\omega}}\,\langle n|a + a^\dagger|n\rangle = 0$.

$E_n^2 = \sum_{n' \neq n} \frac{|\langle n'|H_1|n\rangle|^2}{E_n - E_{n'}}$

$\left(\langle n'|H_1|n\rangle = g_1\sqrt{\frac{\hbar}{2m\omega}}\,\langle n'|a + a^\dagger|n\rangle \right.$

$= g_1\sqrt{\frac{\hbar}{2m\omega}}\,\left.\left(\sqrt{n+1}\,\langle n'|n+1\rangle + \sqrt{n}\,\langle n'|n-1\rangle\right)\right)$

This is non-zero for $n' = n+1, n-1$.

$\Rightarrow E_n^2 = g_1^2\frac{\hbar}{2m\omega}\left[-\frac{n+1}{\hbar\omega} + \frac{n}{\hbar\omega}\right] = \underline{-\frac{g_1^2}{2m\omega^2}}$

Shifting

~~New~~ Eigenstate correction

$|\phi_n^1\rangle = \sum_{n' \neq n} \frac{\langle n'|H_1|n\rangle}{E_n - E_{n'}}|n'\rangle$.

$= g_1\sqrt{\frac{\hbar}{2m\omega}}\cdot\frac{1}{\hbar\omega}\left(-\cancel{\;}\sqrt{n+1}\,|n+1\rangle + \sqrt{n}\,|n-1\rangle\right)$.

$= g_1\sqrt{\frac{\hbar}{2m\omega}}\cdot\frac{1}{\hbar\omega}(-a^\dagger + a)|n\rangle$

$|\phi_n^1\rangle = \frac{ig_1}{m\hbar\omega^2}(\hat{p}|n\rangle)$

This is like ~~__~~ applying translation operator on wave function

$\phi_n\left(x + \frac{g_1}{m\omega^2}\right) = \phi_n(x) + \frac{g_1}{m\omega^2}\frac{\partial\phi_n}{\partial x} + \cdots$

$= \langle x|n\rangle + \frac{ig_1}{m\omega^2\hbar}\langle x|\hat{p}|n\rangle$.

(ii). $H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$, $H_1 = \frac{1}{2} g_2 x^2$

$$H = \frac{p^2}{2m} + \frac{1}{2} m\left(\omega^2 + \frac{g_2}{m}\right) x^2.$$

$$\omega' = \sqrt{\omega^2 + \frac{g_2}{m}}$$

$$E_n' = \hbar\omega'(n+\tfrac{1}{2}) , \quad \omega' = \omega\sqrt{1+\frac{g_2}{m\omega^2}}$$

$$E_n' = (n+\tfrac{1}{2})\hbar\omega\left(1 + \frac{g_2}{2m\omega^2} - \frac{g_2^2}{8m^2\omega^4} + \cdots\right).$$

$H_0|n\rangle = E_n|n\rangle \Rightarrow E_n = \hbar\omega(n+\tfrac{1}{2})$

$$E_n' = E_n + \langle n|H_1|n\rangle + \sum_{n'\neq n} \frac{|\langle n'|H|n\rangle|^2}{E_n - E_{n'}} + \cdots$$

$$\langle n|H_1|n\rangle = \frac{g_2}{2}\langle n|x^2|n\rangle$$

$$= \frac{g_2}{2}\left(\frac{\hbar}{2m\omega}\right) \langle n|(a+a^\dagger)(a+a^\dagger)|n\rangle$$

$$= \frac{g_2}{2}\left(\frac{\hbar}{2m\omega}\right) \langle n| a^2 + a^{\dagger 2} + aa^\dagger + a^\dagger a|n\rangle$$

$$= \frac{\hbar g_2}{4m\omega}(n+1+n) = \frac{\hbar g_2}{4m\omega}(2n+1)$$

$$= \hbar\omega(n+\tfrac{1}{2})\left(\frac{g_2}{2m\omega^2}\right)$$

which is the same as above

$$\langle n'|H_1|n\rangle = \frac{g_2}{2}\langle n'|x^2|n\rangle$$

$$= \frac{g_2}{2}\frac{\hbar}{2m\omega}\left(\sqrt{(n+1)(n+2)}\,\delta_{n',n+2} + \sqrt{n(n-1)}\,\delta_{n',n-2} + (2n+1)\,\delta_{n',n}\right)$$

$$\sum_{n'\neq n} \frac{|\langle n'|H_1|n\rangle|^2}{\hbar\omega(n'-n)} = \frac{\hbar g_2^2}{16 m^2\omega^3}\cdot\left(-\frac{1}{2}(n+1)(n+2) + \frac{n(n-1)}{2}\right)$$

$$= -\frac{1}{8}\frac{g_2^2\hbar}{m^2\omega^3}$$

which also same as above

$$|\phi_n'\rangle = \sum_{n'\neq n} \frac{\langle n'|H_1|n\rangle}{E_n - E_{n'}}|n'\rangle$$

$$= \frac{g_2\hbar}{4m\omega}\frac{\sqrt{(n+1)(n+2)}}{\hbar\omega(2)}|n+2\rangle - \frac{g_2\hbar}{4m\omega}\frac{\sqrt{n(n-1)}}{\hbar\omega(2)}|n-2\rangle.$$

$$|\phi_n'\rangle = \frac{g_2}{8m\omega^2}(a^\dagger)^2|n\rangle - \frac{g_2}{8m\omega^2}a^2|n\rangle.$$

First order eigenstate correction

(iii) $H_1 = \frac{g_3}{2} x^3$

$\langle n | x^3 | n \rangle = 0$. --- odd.

$$\langle n' | x^3 | n \rangle = \left(\frac{\hbar}{2m\omega} \right)^{3/2} \Big[\sqrt{(n+1)(n+2)(n+3)}\, \delta_{n',n+3} + \sqrt{n(n-1)(n-2)}\, \delta_{n',n-3} + (n+1)^{3/2}\, \delta_{n',n+1} + n^{3/2}\, \delta_{n',n-1} \Big]$$

$$\Rightarrow \frac{g_3^2}{4} \sum_{n' \neq n} \frac{|\langle n' | x^3 | n \rangle|^2}{\hbar\omega (n'-n)}$$

$$= \left(\frac{\hbar}{2m\omega} \right)^{3/2} \frac{1}{\hbar\omega} \left(-\frac{1}{3} (n+1)(n+2)(n+3) + \frac{n(n-1)(n-2)}{3} \;\cancel{+3}\; - 9(n+1)^3 + 9n^3 \right)$$

$$E_n^2 = \frac{-\hbar^2}{8m^3\omega^4} \left(\frac{7}{2} + 30\left(n+\frac{1}{2}\right)^2 \right)$$

Second order energy correction.

$$\phi_n^1 \approx \frac{g_3}{2} \left(\frac{\hbar}{2m\omega} \right)^{3/2} \Big(\sqrt{(n+1)(n+2)(n+3)}\, |n+3\rangle + \sqrt{n(n-1)(n-2)}\, |n-3\rangle + (n+1)^{3/2} |n+1\rangle + n^{3/2} |n-1\rangle \Big).$$

Eigenstate correction

Adwait Naravane 19MS151.

Q1

$H_0 = \alpha \mathbb{1}_{2\times 2} + \omega \sigma_z$.

take basis as $|\uparrow\rangle \to \begin{pmatrix}1\\0\end{pmatrix}$, $|\downarrow\rangle \to \begin{pmatrix}0\\1\end{pmatrix}$.

$$H_0 \to \alpha\begin{pmatrix}1&0\\0&1\end{pmatrix} + \omega\begin{pmatrix}1&0\\0&-1\end{pmatrix} = \begin{pmatrix}\alpha+\omega & 0\\ 0 & \alpha-\omega\end{pmatrix}$$

$\begin{pmatrix}1\\0\end{pmatrix}$ & $\begin{pmatrix}0\\1\end{pmatrix}$ are eigenstates with energies, $E(\uparrow) = \alpha+\omega$, $E(\downarrow) = \alpha-\omega$.

$$H_1 = \varepsilon\Gamma\hat{\sigma}_x$$

$$E_1^{(1)} = \langle\uparrow|H_1|\uparrow\rangle = \varepsilon\Gamma\begin{pmatrix}1&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 0$$

$$E_2^{(1)} = \langle\downarrow|H_1|\downarrow\rangle = 0$$

First order energy corrections

second order energy.

$$E_1^{(2)} = \frac{\langle\uparrow|H_1|\downarrow\rangle}{E(\uparrow)-E(\downarrow)} = \varepsilon^2\Gamma^2 \frac{\left[\begin{pmatrix}1&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}\right]^2}{\alpha+\omega-\alpha+\omega}$$

$$= \frac{\varepsilon^2\Gamma^2}{2\omega},$$

$$E_2^{(2)} = -\frac{\langle\downarrow|H_1|\uparrow\rangle}{E(\uparrow)-E(\downarrow)} = -\frac{\varepsilon^2\Gamma^2\left(\begin{pmatrix}0&1\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}\right)^2}{\alpha+\omega-\alpha+\omega}.$$

$$= -\frac{\varepsilon^2\Gamma^2}{2\omega}.$$

$$\Rightarrow E_1 \approx \alpha+\omega+\frac{\varepsilon^2\Gamma^2}{2\omega}, \quad E_2 \approx \alpha-\omega-\frac{\varepsilon^2\Gamma^2}{2\omega}.$$

First order eigenstate corrections

$$|1^{(1)}\rangle = -\frac{|\downarrow\rangle\langle\uparrow|H_1|\downarrow\rangle}{E(\downarrow)-E(\uparrow)} = -\frac{\varepsilon\Gamma}{\alpha-\omega-\alpha-\omega}|\downarrow\rangle = \frac{\varepsilon\Gamma}{2\omega}|\downarrow\rangle.$$

$$|2^{(1)}\rangle = -\frac{|\uparrow\rangle\langle\downarrow|H_1|\uparrow\rangle}{E(\uparrow)-E(\downarrow)} = -\frac{\varepsilon\Gamma}{2\omega}|\uparrow\rangle.$$

$$\Rightarrow |1\rangle \approx |\uparrow\rangle + \frac{\varepsilon\Gamma}{2\omega}|\downarrow\rangle, \quad |2\rangle \approx |\downarrow\rangle - \frac{\varepsilon\Gamma}{2\omega}|\uparrow\rangle$$

Non-perturbatively :—

$$H_0 + h_1 = \begin{pmatrix} \alpha+\omega & \varepsilon\Gamma \\ \varepsilon\Gamma & \alpha-\omega \end{pmatrix}$$

Solving the eigenvalue equation,

$(\alpha+\omega-\lambda)(\alpha-\omega-\lambda) - \varepsilon^2\Gamma^2 = 0.$

$(\alpha-\lambda)^2 = \omega^2 + \varepsilon^2\Gamma^2 \Rightarrow \quad \lambda = \alpha \pm \sqrt{\omega^2 + \varepsilon^2\Gamma^2}.$

$\Rightarrow E = \alpha \pm \omega \sqrt{1 + \frac{\varepsilon^2\Gamma^2}{\omega^2}}$. -- energy eigenvalues.

Expand in power series -

$E = \alpha \pm \omega \left(1 + \frac{\varepsilon^2\Gamma^2}{2\omega^2} - \frac{\varepsilon^4\Gamma^4}{8\omega^4} + \cdots\right)$

$E \approx \alpha \pm \omega\left(1 + \frac{\varepsilon^2\Gamma^2}{2\omega^2}\right).$

$E_+ = \alpha + \omega + \frac{\varepsilon^2\Gamma^2}{2\omega}$, $E_- = \alpha - \omega - \frac{\varepsilon^2\Gamma^2}{2\omega}.$

eigenstate → take $\begin{pmatrix} a \\ b \end{pmatrix}$.

$a(\alpha+\omega) + b\varepsilon\Gamma = \lambda a, \quad a\varepsilon\Gamma + b(\alpha-\omega) = \lambda b.$

for E_+, $a(\omega+\beta) + b(\beta-\omega) = \sqrt{\beta^2+\omega^2}\,(a+b)$

$a(\omega-\beta) + b(\omega+\beta) = \sqrt{\beta^2+\omega^2}\,(a-b).$

(let $\varepsilon\Gamma = \beta$) $\quad \frac{a\beta}{\omega + \sqrt{\beta^2+\omega^2}} = b.$

$|1\rangle \propto \begin{pmatrix} \frac{\omega + \sqrt{\beta^2+\omega^2}}{\beta} \\ 1 \end{pmatrix}$ ... normalisation will give a constant.

Similarly we can get second eigenstate.

$|2\rangle \propto \begin{pmatrix} \frac{\omega - \sqrt{\beta^2+\omega^2}}{\beta} \\ 1 \end{pmatrix}$.

(iv).