$\alpha\beta\gamma \quad \alpha\gamma\beta$
$\beta\gamma\alpha \quad \beta\alpha\gamma$
$\gamma\alpha\beta \quad \gamma\beta\alpha$

5/23/71 (78) a) Eigenfcns of $\mathcal{H}$ will be product states like $\phi_\alpha(1)\phi_\beta(2)\phi_\gamma(3)$. To form symmetrized states, we take all $3! = 6$ possible permutations of the indices $\alpha\beta\gamma$ (or particles 123), and add them as

$$\psi(1,2,3) = \frac{1}{\sqrt{6}}\Big[\phi_\alpha(1)\phi_\beta(2)\phi_\gamma(3) \pm \phi_\alpha(1)\phi_\gamma(2)\phi_\beta(3) + \phi_\beta(1)\phi_\gamma(2)\phi_\alpha(3) \pm \phi_\beta(1)\phi_\alpha(2)\phi_\gamma(3) + \phi_\gamma(1)\phi_\alpha(2)\phi_\beta(3) \pm \phi_\gamma(1)\phi_\beta(2)\phi_\alpha(3)\Big]$$

Use upper (+) signs for boson case; lower (−) signs for fermion case. The norm factor is obvious.

b) For fermions, both $\psi(1,2)$ and $\psi(1,2,3)$ above can be written as

$$\psi(1,2,\ldots,N) = A \det[\phi_\lambda(k)], \quad A = 1/\sqrt{N!} \quad \text{(obvious?)}$$

Generalization to the case of N (identical) fermions is obvious (sic). To check out ψ note the det can be expanded as a sum of all possible permutations of the product states

$$\det[\phi_\lambda(k)] = \sum_\mu (-1)^\mu P_\mu\, \phi_\alpha(1)\phi_\beta(2)\cdots\phi_\nu(N)$$

N.B. indices $\alpha, \beta, \ldots, \nu$ are N in #

Here P_μ is an operator which interchanges pairs of particles μ times in succession. We find then, with $\mathcal{H} = \sum_{k=1}^N H(k)$...

$$\mathcal{H}\psi = A\sum_\mu (-1)^\mu P_\mu \left\{\left[\sum_{k=1}^N H(k)\right]\phi_\alpha(1)\phi_\beta(2)\cdots\phi_\nu(N)\right\}$$

In the product here, the k^{th} particle appears just once, say in the state κ, so that $H(k)\phi_\kappa(k) = E_\kappa\phi_\kappa(k)$. Then we have

$$\mathcal{H}\psi = A \sum_{\mu} (-1)^{\mu} P_{\mu} \left\{ [E_\alpha + E_\beta + \dots + E_\nu]\, \phi_\alpha(1)\phi_\beta(2)\cdots\phi_\nu(N) \right\}$$

$$= [E_\alpha + E_\beta + \dots + E_\nu]\, A \sum_{\mu} (-1)^{\mu} P_{\mu}\, \phi_\alpha(1)\phi_\beta(2)\cdots\phi_\nu(N)$$

or

$$\mathcal{H}\psi = [E_\alpha + E_\beta + \dots + E_\nu]\,\psi$$

and we see ψ is an eigenfcn of the total system energy, as desired. Again, the norm cnst $A = 1/\sqrt{N!}$ is "obvious". If we write ψ in square array as

$$\psi = \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \phi_\alpha(1) & \phi_\alpha(2) & \phi_\alpha(3) & \cdots \\ \phi_\beta(1) & \phi_\beta(2) & \phi_\beta(3) & \cdots \\ \phi_\gamma(1) & \phi_\gamma(2) & \phi_\gamma(3) & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix}$$

then it is easy to see that if any two fermions are in the same state (i.e. $\beta \equiv \alpha$) then two rows of the det are identical, which $\Rightarrow$ $\psi \equiv 0$, in accordance with the Exclusion Principle. Finally, if any pair of particles are interchanged, say $1 \leftrightarrow 2$, this interchanges two columns of the det, which makes it change sign (by rules of dets). Thus exchange symmetry is satisfied, i.e. ...

$$\psi(1,\dots,\ell,\dots,k,\dots,N) = (-)\,\psi(1,\dots,k,\dots,\ell,\dots,N)$$

The appropriate ψ for N bosons would be

$$\psi(1,2,\dots,N) = \frac{1}{\sqrt{N!}} \sum_{\mu} P_{\mu}\, \phi_\alpha(1)\phi_\beta(2)\cdots\phi_\nu(N)$$

which differs from the fermion case by deletion of the antisymmetrizing factor $(-1)^{\mu}$.

5/23/71 (77) a) $\psi_k = \psi_k^{(0)} + \sum_n' a_{nk}^{(1)} \psi_n^{(0)}$, $a_{nk}^{(1)} = \dfrac{V_{nk}}{E_k^{(0)} - E_n^{(0)}}$ to $O(V)$

~~Prob. # (30)~~
~~ϕ 507~~
(Mar. '92)

The desired energy is : $E_k = \langle \psi_k | \mathcal{H} | \psi_k \rangle / \langle \psi_k | \psi_k \rangle$

$$\text{num.} = \left\langle \psi_k^{(0)} + \sum_m' a_{mk}^{(1)} \psi_m^{(0)} \right| H_0 + V \left| \psi_k^{(0)} + \sum_n' a_{nk}^{(1)} \psi_n^{(0)} \right\rangle$$

$$= E_k^{(0)} + V_{kk} + \sum_n' a_{nk}^{(1)} \langle \psi_k^{(0)} | H_0 + V | \psi_n^{(0)} \rangle + \sum_m' a_{mk}^{(1)*} \langle \psi_m^{(0)} | H_0 + V | \psi_k^{(0)} \rangle$$

$$+ \sum_{m,n}' a_{mk}^{(1)*} a_{nk}^{(1)} \langle \psi_m^{(0)} | H_0 + V | \psi_n^{(0)} \rangle$$

to $\Theta(V^2)$

$$\simeq \left(E_k^{(0)} + V_{kk} \right) + \sum_n' a_{nk}^{(1)} V_{kn} + \sum_m a_{mk}^{(1)*} V_{mk} + \sum_{m,n}' a_{mk}^{(1)*} a_{nk}^{(1)} E_n^{(0)} \delta_{mn}$$

$$= \left(E_k^{(0)} + V_{kk} \right) + 2 \sum_n' \frac{|V_{nk}|^2}{E_k^{(0)} - E_n^{(0)}} + \sum_n' \frac{E_n^{(0)}}{E_k^{(0)} - E_n^{(0)}} \frac{|V_{nk}|^2}{E_k^{(0)} - E_n^{(0)}}$$

$$= E_k^{(0)} + V_{kk} + \sum_n' \left(2 + \frac{E_n^{(0)}}{E_k^{(0)} - E_n^{(0)}} \right) \frac{|V_{nk}|^2}{E_k^{(0)} - E_n^{(0)}}$$

$$\text{den.} = \left\langle \psi_k^{(0)} + \sum_m' a_{mk}^{(1)} \psi_m^{(0)} \right| \left. \psi_k^{(0)} + \sum_n' a_{nk}^{(1)} \psi_n^{(0)} \right\rangle = 1 + \sum_n' |a_{nk}^{(1)}|^2$$

$$\therefore \; E_k = \text{num}/\text{den.} \underset{\text{to } \Theta(V^2)}{\simeq} E_k^{(0)} \left(1 - \sum_n' |a_{nk}^{(1)}|^2 \right) + V_{kk} + \sum_n' \left(2 + \frac{E_n^{(0)}}{E_k^{(0)} - E_n^{(0)}} \right) \frac{|V_{nk}|^2}{E_k^{(0)} - E_n^{(0)}}$$

or $E_k \simeq E_k^{(0)} + V_{kk} + \sum_n' \dfrac{|V_{nk}|^2}{E_k^{(0)} - E_n^{(0)}}$ } this is the desired energy to $\Theta(V^2)$ QED

b) We consult THE FUNDAMENTAL EQTN of lecture (71), 5/10/71, p287. For $\nu = 1$, $k \neq m$, it gives

$$\left(E_k^{(0)} - E_m^{(0)} \right) a_{mk}^{(2)} = \sum_n V_{mn} a_{nk}^{(1)} - \sum_{\mu=0}^{0} E_k^{(1-\mu)} a_{mk}^{(\mu+1)} = \sum_n' \frac{V_{mn} V_{nk}}{E_k^{(0)} - E_n^{(0)}} - \overset{V_{kk}}{E_k^{(1)}} a_{mk}^{(1)}$$

or $$a_{mk}^{(2)} = \sum_n{}' \frac{V_{mn}V_{nk}}{(E_k^{(0)}-E_n^{(0)})(E_k^{(0)}-E_m^{(0)})} - \frac{V_{kk}V_{mk}}{(E_k^{(0)}-E_m^{(0)})(E_k^{(0)}-E_m^{(0)})}$$ $m \neq k$; interchange m & n for notation;

i.e. $$a_{nk}^{(2)} = \sum_m{}' \frac{V_{nm}V_{mk}}{(E_k^{(0)}-E_m^{(0)})(E_k^{(0)}-E_n^{(0)})} - \frac{V_{kk}V_{nk}}{(E_k^{(0)}-E_n^{(0)})^2}$$

Thus, to 2ND order, the wavefcn is ...

$$\psi_k \simeq \psi_k^{(0)} + \sum_n{}' \left[a_{nk}^{(1)} + a_{nk}^{(2)}\right]\psi_n^{(0)}$$

$$= \left[\frac{V_{nk}}{E_k^{(0)}-E_n^{(0)}}\left(1 - \frac{V_{kk}}{E_k^{(0)}-E_n^{(0)}}\right) + \sum_m{}' \frac{V_{nm}V_{mk}}{(E_k^{(0)}-E_n^{(0)})(E_k^{(0)}-E_m^{(0)})}\right]$$

This agrees with Schiff, eq. (31.14), p. 247. QED.

Now for $v=2$, $k=m$, THE FUNDAMENTAL EQTN gives

$$E_k^{(3)} = \sum_n V_{kn}a_{nk}^{(2)} - \sum_{\mu=0}^{1} E_k^{(2-\mu)} \cancel{a_{kk}^{(\mu+1)}} = \sum_n{}' V_{kn}a_{nk}^{(2)}$$

Can choose all $a_{kk}^{(v)} \equiv 0$ by norm.

Plugging in the above result for $a_{nk}^{(2)}$, we get

$$E_k^{(3)} = \sum_n{}' \left\{ \sum_m{}' \frac{V_{kn}V_{nm}V_{mk}}{(E_k^{(0)}-E_m^{(0)})(E_k^{(0)}-E_n^{(0)})} - \frac{V_{kn}V_{nk}V_{kk}}{(E_k^{(0)}-E_n^{(0)})^2} \right\}$$ QED

5/23/71 **30** Schiff works out this problem on p. 248. We need matrix elements of x^2. From the results of problem 25, we note -- for example

$$V_{nn} = \tfrac{1}{2}q\langle n|x^2|n\rangle = \tfrac{1}{2}q\left(n+\tfrac{1}{2}\right)\frac{\hbar}{m\omega}$$

The perturbed energy to $O(q^2)$ is given by

$$E_n \simeq E_n^{(0)} + V_{nn} + \sum_k{}' |V_{kn}|^2/(E_n^{(0)} - E_k^{(0)}) \leftarrow k \neq n \text{ in sum}$$

Where: $E_n^{(0)} = (n+\frac{1}{2})\hbar\omega$, $\omega = \sqrt{k/m}$, and V_{nn} is as above.

So we also need the matrix elt

$V_{kn} = \frac{1}{2} q \langle k|x^2|n\rangle$ Again, use results of prob. 25 ... 18

$$\langle k|x^2|n\rangle = \frac{1}{\alpha}\sqrt{\frac{n+1}{2}}\langle k|x|n+1\rangle + \frac{1}{\alpha}\sqrt{\frac{n}{2}}\langle k|x|n-1\rangle, \quad \alpha = \sqrt{\frac{m\omega}{\hbar}}$$

$$= \begin{cases} (n+\frac{1}{2})\frac{\hbar}{m\omega}, & \text{for } k=n \text{ (as above)} \\ \frac{1}{\alpha^2}\sqrt{\frac{(n+1)(n+2)}{4}}, & \text{for } k=n+2 \\ \frac{1}{\alpha^2}\sqrt{\frac{(n-1)n}{4}}, & \text{for } k=n-2 \end{cases} \Bigg\} \text{ and } 0 \text{ otherwise}$$

So the second order term collapses to

$$\sum_k{}' \frac{|V_{kn}|^2}{(E_n^{(0)} - E_k^{(0)})} = \left(\frac{1}{2}q\right)^2 \left\{ -\frac{(n+1)(n+2)}{4\alpha^4\, 2\hbar\omega} + \frac{n(n-1)}{4\alpha^4\, 2\hbar\omega} \right\}$$

$$= -\frac{1}{8} q^2 (n+\tfrac{1}{2}) \frac{\hbar}{m^2\omega^3}$$

The perturbation calculation thus gives, to $\mathcal{O}(q^2)$

$$E_n \simeq (n+\tfrac{1}{2})\hbar\omega\left[1 + \tfrac{1}{2}(q/k) - \tfrac{1}{8}(q/k)^2\right], \quad k = m\omega^2$$

The exact result would be

$$E_n = (n+\tfrac{1}{2})\hbar\omega', \quad \omega' = \sqrt{(k+q)/m} = \left(1+\frac{q}{k}\right)^{\frac{1}{2}}\omega$$

Expanding the $\sqrt{\ }$, we find $(1+\frac{q}{k})^{\frac{1}{2}} \simeq 1 + \frac{1}{2}(q/k) - \frac{1}{8}(q/k)^2 + \dots$. Clearly, E_n by the perturbation calculation agrees exactly, term by term, with the exact result, to $O(q^2)$

5/23/71 (8) Prob. # (34) ϕ507 (Mar.'92)

This problem is discussed in Saxon "Elementary QM" (Holden-Day, 1968) pp. 195-196. We start from...

$$|E_k^{(2)}| \leqslant \sum_n{}' |V_{nk}|^2 / |E_k^{(0)} - E_n^{(0)}| \leqslant \frac{1}{|\Delta E_k^{(0)}|_{AV}} \sum_n{}' \langle k|V|n\rangle\langle n|V|k\rangle$$

If, as Saxon uses it, $|\Delta E_k^{(0)}|_{AV}$ is the energy gap between state k and its nearest neighbor only, then obviously the inequality is strengthened by the 2ND step here (since then $|\Delta E_k^{(0)}|_{AV}$ is smaller than all but one of the denominators which occurs in the sum). If, however, $|\Delta E_k^{(0)}|_{AV}$ is a vague sort of average, all we can do is wave our arms while saying that it would reasonably be smaller than "most" of the energy denominators which enter the sum -- in which case the inequality would again be strengthened. If that is OK, then we can use the last expression to write

$$|E_k^{(2)}| \leqslant (1/|\Delta E_k^{(0)}|_{AV}) \left[\sum_n \langle k|V|n\rangle\langle n|V|k\rangle - \langle k|V|k\rangle^2 \right]$$

Here we have added & subtracted the diagonal term. Using compleatness, $\sum_n |n\rangle\langle n| = 1$, we have

$$|E_k^{(2)}| \leqslant (1/|\Delta E_k^{(0)}|_{AV}) \underbrace{\left[\langle k|V^2|k\rangle - \langle k|V|k\rangle^2 \right]}_{\langle V^2\rangle_k - \langle V\rangle_k^2 \,=\, (\Delta V)_k^2 \text{, by defn}}$$

So,

$$|E_k^{(2)}| \leqslant (\Delta V)_k^2 / |\Delta E_k^{(0)}|_{AV} \qquad \text{QED}$$

See Saxon, pp. 197-198.

5/23/71 (3) The 1st order correction to the energy will be the matrix elt

$$V_{nn} = (k/2b^2)\langle n|x^4|n\rangle$$

To calculate the $\langle x^4\rangle_n$, we use the ladder operators a & $a^\dagger$

$$x = \sqrt{\hbar/2m\omega}\,(a+a^\dagger)$$

In taking x^4, the only terms in the a's which will contribute to the diagonal elements will be those with two powers of both a & $a^\dagger$ (a term like $a^3a^\dagger$ operating on $|n\rangle$ gives $|n-2\rangle$, etc.). Retaining only these terms, we have

$$x^4 = \left(\frac{\hbar}{2m\omega}\right)^2\left[a^2a^{\dagger 2} + aa^\dagger aa^\dagger + aa^{\dagger 2}a + a^\dagger a^2 a^\dagger + a^\dagger a a^\dagger a + a^{\dagger 2}a^2\right]$$

Now we can use the fundamental relations

$$a|n\rangle = \sqrt{n}\,|n-1\rangle \quad , \quad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

to generate results like...

$$a^2a^{\dagger 2}|n\rangle = (n+1)(n+2)|n\rangle \quad , \quad a^{\dagger 2}a^2|n\rangle = (n-1)n\,|n\rangle$$

$$aa^\dagger aa^\dagger|n\rangle = (n+1)^2|n\rangle \quad , \quad a^\dagger aa^\dagger a\,|n\rangle = n^2|n\rangle$$

$$aa^{\dagger 2}a\,|n\rangle = n(n+1)|n\rangle \;; \quad a^\dagger a^2 a^\dagger|n\rangle = n(n+1)|n\rangle$$

Then we have...

$$\langle n|x^4|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^2\left[(n+1)(n+2)+(n-1)n + (n+1)^2+n^2+2n(n+1)\right]$$

$$= 6(\hbar/2m\omega)^2\left[n^2+(n+\tfrac{1}{2})\right]$$

The corrected energy (to $\mathcal{O}(1/b^2)$) will be (8)

$$E_n \simeq \underbrace{E_n^{(0)}}_{=(n+\frac{1}{2})\hbar\omega} + V_{nn} = (n+\tfrac{1}{2})\left[\hbar\omega + \frac{3k}{b^2}\left(\frac{\hbar}{2m\omega}\right)^2\right] + n^2\,\frac{3k}{b^2}\left(\frac{\hbar}{2m\omega}\right)^2$$

If we define : $\delta\omega = \frac{3k}{b^2}\left(\frac{\hbar}{2m\omega}\right)^2\Big/\hbar = \underline{\underline{3\hbar/4mb^2}}$ (with $k=m\omega^2$)

then,, $E_n \simeq (n+\frac{1}{2})\,\hbar\,(\omega+\delta\omega) + n^2\hbar\,\delta\omega$ **QED**

6/7/71 (13) This is Drumheller's problem -- from his QM 507 substitute lectures of 5/17/71 & 5/19/71. See folder "Odd Notes on QM".

For S=1, the spin matrices are (Schiff, p. 203)...

$$S_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},\quad S_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix},\quad S_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

In the Ham^n : $H = AS_z^2 + B(S_x^2 - S_y^2)$, we shall absorb the $\hbar^2$ into the constants A & B, i.e. we can define new cnsts $a = A\hbar^2$ & $b = B\hbar^2$. So drop the $\hbar$ here, and calculate...

$$S_x^2 = \frac{1}{2}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix},\quad S_y^2 = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix},\quad S_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The eigenvectors of S_z are one-comp spinors...

$$\psi_1^{(0)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},\quad \psi_2^{(0)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},\quad \psi_3^{(0)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$\hookrightarrow S_z = +1$ ($m_s = +1$) $\hookrightarrow S_z = 0$ ($m_s = 0$) $\hookrightarrow S_z = -1$ ($m_s = -1$)

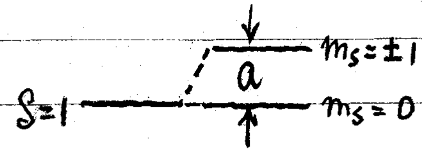
a) Now write : $H = H_0 + V \begin{cases} H_0 = a S_z^2 \\ V = b(S_x^2 - S_y^2) \end{cases} a \gg b$

The unperturbed eigenenergies are

$$E_1^{(0)} = \psi_1^{(0)\dagger} H_0 \psi_1^{(0)} = a\,(1\,0\,0)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = +a,$$

$$E_2^{(0)} = 0, \quad E_3^{(0)} = +a \text{ also.}$$

So, after H_0, the levels are still two fold degenerate, as indicated in the dgm.



b) Forming the perturbation matrix ...

$$V = b(S_x^2 - S_y^2) = b\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

We note V is not diagonal, and $V_{kk} = \psi_k^{(0)\dagger} V \psi_k^{(0)} \equiv 0$ for $k = 1,2,3$. But $V_{13} = \psi_1^{(0)\dagger} V \psi_3^{(0)} = +b$, and $V_{31} = +b$, so V will couple states 1 & 3 (i.e. $m_s = +1$ & -1) and will lift the degeneracy.

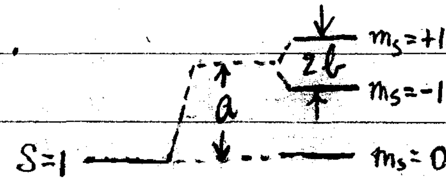
To get the energy corrections $E_k^{(1)}$ due to V, we must diagonalize the V matrix (lecture of 5/17/71). Thus we take

$$\det(\underset{m}{V} - \lambda \underset{m}{I}) = \begin{vmatrix} -\lambda & 0 & b \\ 0 & -\lambda & 0 \\ b & 0 & -\lambda \end{vmatrix} = \lambda(b^2 - \lambda^2) = 0$$

$\Rightarrow \lambda = 0$ (for state $\psi_2^{(0)}$), $\lambda = \pm b$ (for states $\psi_1^{(0)}$ & $\psi_3^{(0)}$).

So the energies of the states are now...

$$E_1 = a + b, \quad E_2 = 0, \quad E_3 = a - b$$



The new eigenfcns are found from (p. 295 of notes)...

$$\underset{\sim}{V}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \lambda \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}, \quad \text{with } \psi_M = \sum_k c_k^M \psi_k^{(0)}$$

where there are 3 sets of c_k^M, $M = 1,2,3$ for the 3 λ values

Choosing $\lambda = 0$, we have

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \equiv 0 \Rightarrow c_1 = c_3 = 0, \; c_2 = 1 \text{ (for norm.)}$$

Choosing $\lambda = \pm b$, we have

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \pm \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \Rightarrow c_1 = \pm c_3, \; c_2 \equiv 0$$

Here, choose $c_1 = \frac{1}{\sqrt{2}}$ & $c_3 = \pm \frac{1}{\sqrt{2}}$ for normalization. Then

$$E_1 = a + b \Rightarrow \psi_1 = \frac{1}{\sqrt{2}}\left(\psi_1^{(0)} + \psi_3^{(0)}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

$$E_2 = 0 \Rightarrow \psi_2 = \psi_2^{(0)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$E_3 = a - b \Rightarrow \psi_3 = \frac{1}{\sqrt{2}}\left(\psi_1^{(0)} - \psi_3^{(0)}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

These are the desired eigenfcns. We note that the above solution to this problem is <u>exact</u>, as -- w.r.t. the new eigenfcns ψ_M, the matrix of H is diagonal...

$$H = \begin{pmatrix} a & 0 & b \\ 0 & 0 & 0 \\ b & 0 & a \end{pmatrix} \Rightarrow \left.\begin{aligned} \psi_1^\dagger H \psi_1 &= a + b = E_1 \\ \psi_2^\dagger H \psi_2 &= 0 = E_2 \\ \psi_3^\dagger H \psi_3 &= a - b = E_3 \end{aligned}\right\} \langle M|H|N\rangle = E_M \delta_{MN}$$

6/9/71 (8) We have worked out this problem "S-Matrix for Time Indpt Interaction" on 2/3/71 in our Odd Notes on QM folder. It follows quite closely the derivation in Davydov, pp. 331-333.

a) Referring to QM 506 lecture # (38), 1/29/71, p. 172 of notes, we note that with $\beta \neq \alpha$, $S^{(0)}_{\beta\alpha} = \delta_{\beta\alpha} \equiv 0$, so the S-matrix series is

$$S_{\beta\alpha} = S^{(1)}_{\beta\alpha} + S^{(2)}_{\beta\alpha} + \dots \qquad \beta \neq \alpha$$

where (with interaction $\Omega = V/\hbar$)...

$$S^{(1)}_{\beta\alpha} = -i \int dx \int dt \; \phi^*_\beta(x,t)\,\Omega(x,t)\,\phi_\alpha(x,t)$$

$$S^{(2)}_{\beta\alpha} = -i \int dx_2 \int dt_2 \int dx_1 \int dt_1 \; \phi^*_\beta(x_2,t_2)\left[\Omega(x_2,t_2)\,G_0\,\Omega(x_1,t_1)\right]\phi_\alpha(x_1,t_1)$$

$\vdots$

Here $G_0 = G_0(x_2,t_2; x_1,t_1)$ is the free particle propagator. Now if we take $\Omega(x,t) = V(x)/\hbar$ indpt of time, and the ϕ's with a separable time dependence, namely...

$$\phi_\alpha(x,t) = \varphi_\alpha(x)\, e^{-\frac{i}{\hbar}E_\alpha t}, \text{ etc.}$$

then the 1st term in the S-expansion is

$$S^{(1)}_{\beta\alpha} = -\frac{i}{\hbar}\int dx\, \varphi^*_\beta(x)\,V(x)\,\varphi_\alpha(x) \int_{-\infty}^{+\infty} dt\, e^{\frac{i}{\hbar}(E_\beta - E_\alpha)t}$$

$$= -\frac{i}{\hbar}\langle\beta|V|\alpha\rangle \times 2\pi\hbar\,\delta(E_\beta - E_\alpha)$$

$$= -2\pi i\,\delta(E_\beta - E_\alpha)\,\langle\beta|V|\alpha\rangle$$

The $S^{(2)}_{\beta\alpha}$ term is considerably more complicated. We have...

$$S^{(2)}_{\beta\alpha} = -\frac{i}{\hbar^2}\int dx_2 \int_{-\infty}^{+\infty} dt_2 \int dx_1 \int_{-\infty}^{+\infty} dt_1\, \varphi_\beta^*(x_2)\, e^{+\frac{i}{\hbar}E_\beta t_2} \times$$

$$\times \left[V(x_2)\, G_0(x_2,t_2;x_1,t_1)\, V(x_1)\right] \varphi_\alpha(x_1)\, e^{-\frac{i}{\hbar}E_\alpha t_1}$$

But the free particle propagator can be represented by (p.159 of notes)

$$G_0(x_2,t_2;x_1,t_1) = -i\sum_n \varphi_n^*(x_1)\,\varphi_n(x_2)\,e^{-\frac{i}{\hbar}E_n(t_2-t_1)}, \quad \text{for } t_2 > t_1$$

Because $G_0 = 0$ for $t_1 > t_2$, the t_1 integration truncates to $\int_{-\infty}^{t_2}$. Plugging this G_0 in, we find we can write...

$$S^{(2)}_{\beta\alpha} = -\frac{i}{\hbar^2}\sum_n \langle\beta|V|n\rangle\langle n|V|\alpha\rangle \int_{-\infty}^{+\infty} dt_2\, e^{+\frac{i}{\hbar}(E_\beta-E_n)t_2} \times \frac{1}{i}\int_{-\infty}^{+t_2} dt_1\, e^{\frac{i}{\hbar}(E_n-E_\alpha)t_1}$$

Let $E_n - E_\alpha \to E_n - E_\alpha - i\epsilon$, with $\epsilon \to 0_+$ understood. Then the last integral is

$$\frac{1}{i}\int_{-\infty}^{+t_2} dt_1\, e^{\frac{i}{\hbar}(E_n-E_\alpha-i\epsilon)t_1} = \frac{1/i}{\frac{i}{\hbar}(E_n-E_\alpha-i\epsilon)}\, e^{+\frac{\epsilon}{\hbar}t_1}\, e^{\frac{i}{\hbar}(E_n-E_\alpha)t_1}\Big|_{-\infty}^{t_2}$$

because of this factor, get 0 at $t_1 = -\infty$.

$$= \frac{\hbar}{E_\alpha - E_n + i\epsilon}\, e^{\frac{i}{\hbar}(E_n-E_\alpha-i\epsilon)t_2}$$

$$\therefore\ S^{(2)}_{\beta\alpha} = -\frac{i}{\hbar}\sum_n \frac{\langle\beta|V|n\rangle\langle n|V|\alpha\rangle}{E_\alpha - E_n + i\epsilon}\underbrace{\int_{-\infty}^{+\infty} dt_2\, e^{\frac{i}{\hbar}(E_\beta-E_\alpha-i\epsilon)t_2}}_{=2\pi\hbar\,\delta(E_\beta-E_\alpha),\ \text{for } \epsilon\to 0_+}$$

or

$$S^{(2)}_{\beta\alpha} = -2\pi i\,\delta(E_\beta-E_\alpha)\sum_n \frac{\langle\beta|V|n\rangle\langle n|V|\alpha\rangle}{E_\alpha - E_n + i\epsilon}$$

agrees with Davydov eq (85.6), p. 332

So, for $\beta \neq \alpha$, the S-matrix expansion is $S_{\beta\alpha} = S^{(1)}_{\beta\alpha} + S^{(2)}_{\beta\alpha} + \cdots$, or

$$S_{\beta\alpha} = -2\pi i\, \delta(E_\beta - E_\alpha)\left[\langle\beta|V|\alpha\rangle + \sum_n \frac{\langle\beta|V|n\rangle\langle n|V|\alpha\rangle}{E_\alpha - E_n + i\epsilon} + \cdots\right]$$

QED Presumably the sum over n includes the term $n = \alpha$ (why not?).

b) Defining T by : $S_{\beta\alpha} = -2\pi i\, \delta(E_\beta - E_\alpha)\langle\beta|T|\alpha\rangle$, we have

$|S_{\beta\alpha}|^2 = 4\pi^2 |\langle\beta|T|\alpha\rangle|^2\, \delta^2(E_\beta - E_\alpha)$, prob of transition $\alpha \to \beta$.

Now $\delta(E_\beta - E_\alpha) = \frac{1}{2\pi\hbar} \lim_{T\to\infty} \int_{-T}^{+T} e^{\frac{i}{\hbar}(E_\beta - E_\alpha)t}\, dt$, so we have

$$\delta^2(E_\beta - E_\alpha) = \frac{1}{2\pi\hbar} \lim_{T\to\infty} \delta(E_\beta - E_\alpha) \int_{-T}^{+T} e^{\frac{i}{\hbar}(E_\beta - E_\alpha)t}\, dt$$

Because of the δ-fcn in front of the integral, only energy values $E_\beta \simeq E_\alpha$ count, so we may write the integral as

$$\left.\int_{-T}^{+T} e^{\frac{i}{\hbar}(E_\beta - E_\alpha)t}\, dt\right|_{E_\beta \simeq E_\alpha} \simeq \int_{-T}^{+T} dt = 2T \text{, collision duration}$$

$$\therefore |S_{\beta\alpha}|^2 = 4\pi^2 |\langle\beta|T|\alpha\rangle|^2 \frac{1}{2\pi\hbar}\, \delta(E_\beta - E_\alpha)\, \underbrace{\lim_{T\to\infty} 2T}_{\text{define this as collision time}}$$

or/ $|S_{\beta\alpha}|^2 / 2T = W(\alpha \to \beta) = \frac{2\pi}{\hbar} |\langle\beta|T|\alpha\rangle|^2\, \delta(E_\beta - E_\alpha)$

This is the desired transition prob. per unit time.