Exercise 7.4

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to find the energies,
We need to find the eigenvalues of

$$H = H^0 + H' = \begin{pmatrix} E_a^0 + \lambda V_{aa} & \lambda V_{ab} \\ \lambda V_{ba} & E_b^0 + \lambda V_{bb} \end{pmatrix} = \begin{pmatrix} A & \lambda V_{ab} \\ \lambda V_{ba} & B \end{pmatrix}$$

$C = \lambda^2 V_{ab} V_{ba} = \lambda^2 |V_{ab}|^2$

solve characteristic equation:

$$(E_a^0 + \lambda V_{aa} - \alpha)(E_b^0 + \lambda V_{bb} - \alpha) - \lambda^2 V_{ab} V_{ba} = 0$$

$$E_a^0 E_b^0 + E_a^0 \lambda V_{bb} - E_a^0 \alpha + \lambda V_{aa} E_b^0 + \lambda^2 V_{aa} V_{bb} - \alpha \lambda V_{aa} - \alpha E_b^0 - \alpha \lambda V_{bb} + \alpha^2 - \lambda^2 V_{ab} V_{ba} = 0$$

$$\alpha^2 - \alpha\left(E_a^0 + \lambda V_{aa} + \lambda V_{bb} + E_b^0\right) + E_a^0 E_b^0 + E_a^0 \lambda V_{bb} + \lambda V_{aa} E_b^0 + \lambda^2 V_{aa} V_{bb} - \lambda^2 V_{ab} V_{ba} = 0$$

find discriminant:

$$D = \left(-E_a^0 - \lambda V_{aa} - \lambda V_{bb} - E_b^0\right)^2 - 4\left(E_a^0 E_b^0 + E_a^0 \lambda V_{bb} + \lambda V_{aa} E_b^0 + \lambda^2 V_{aa} V_{bb} - \lambda^2 V_{ab} V_{ba}\right)$$

$$= 2E_a^0 E_b^0 + 2E_a^0 \lambda V_{aa} + 2E_a^0 \lambda V_{bb} + E_a^{0\,2} + \lambda^2 V_{aa}^2 + \lambda^2 V_{bb}^2 + E_b^{0\,2} + 2\lambda^2 V_{aa} V_{bb} + 2\lambda V_{bb} E_b^0 + 2\lambda V_{aa} E_b^0 - 4\left(E_a^0 E_b^0 + E_a^0 \lambda V_{bb} + \lambda V_{aa} E_b^0 + \lambda^2 V_{aa} V_{bb} - \lambda^2 V_{ab} V_{ba}\right)$$

ABC-formula (but D seems to be far too long...)

$$\alpha = \frac{E_a^0 + \lambda V_{aa} + \lambda V_{bb} + E_b^0 \pm \sqrt{-2E_a^0 E_b^0 + 2E_a^0 \lambda V_{aa} - 2E_a^0 \lambda V_{bb} + E_a^{0\,2} + \lambda^2 V_{aa}^2 + \lambda^2 V_{bb}^2 + E_b^{0\,2} - 2\lambda^2 V_{aa} V_{bb} + 2\lambda V_{bb} E_b^0 - 2\lambda V_{aa} E_b^0 + 4\lambda^2 V_{ab} V_{ba}}}{2}$$

Then, α would have to be the energy of the perturbed system (there are 2 possible values for α, with either the + or the − sign)

$$(A - \lambda)(B - \lambda) - C = 0$$

$$AB - \lambda B - \lambda A + \lambda^2 - C = 0$$

$$\lambda^2 - \lambda(A + B) + AB - C = 0$$

$$D = (A+B)^2 - 4(AB - C)$$

$$\lambda = \frac{A + B \pm \sqrt{(A+B)^2 - 4(AB - C)}}{2}$$

$$\lambda = \frac{E_a^0 + \lambda V_{aa} + E_b^0 + \lambda V_{bb} \pm \sqrt{(E_a^0 + \lambda V_{aa})^2 + 2(E_a^0 + \lambda V_{aa})(E_b^0 + \lambda V_{bb}) + (E_b^0 + \lambda V_{bb})^2 - 4(E_a^0 + \lambda V_{aa})(E_b^0 + \lambda V_{bb}) + 4\lambda^2 |V_{ab}|^2}}{2}$$

$$= \frac{E_a^0 + \lambda V_{aa} + E_b^0 + \lambda V_{bb} \pm \sqrt{(E_a^0)^2 + 2E_a^0 \lambda V_{aa} + \lambda^2 V_{aa}^2 - 2E_a^0 E_b^0 - 2E_a^0 \lambda V_{bb} - 2E_b^0 \lambda V_{aa} - 2\lambda^2 V_{aa} V_{bb} + (E_b^0)^2 + 2E_b^0 \lambda V_{bb} + \lambda^2 V_{bb}^2 - 4\lambda^2 |V_{ab}|^2}}{2}$$