AQT Problem class 4

3 sites • • •

single-particle Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m}\begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}$

interaction between particles at same site

Hamiltonian in 2nd quantisation

$$\hat{H}_{mult} = \sum_{ij} H(i,j)\, a_i^+ a_j + \frac{1}{2} U^{int} \sum_i \underbrace{a_i^+ a_i (a_i^+ a_i - 1)}_{a_i^{+2} a_i}$$

(a) energy levels for single particle

$$0 = \det\begin{pmatrix} -2-\lambda & 1 & 0 \\ 1 & -2-\lambda & 1 \\ 0 & 1 & -2-\lambda \end{pmatrix} = (-2-\lambda)((-2-\lambda)^2-1) - (-2-\lambda)$$

$\lambda_j = -2,\ -2 \pm \sqrt{2}$

$E_j = -\frac{\hbar^2}{2m}\lambda_j$

(b) show that the same follows in 2nd quantisation

need matrix representation of $\hat{H}_{mult}$ in basis $|1,0,0\rangle, |0,1,0\rangle, |0,0,1\rangle$

$$\begin{pmatrix} \langle 1,0,0|\hat{H}_{mult}|1,0,0\rangle & \langle 1,0,0|\hat{H}_{mult}|0,1,0\rangle & \dots \\ \langle 0,1,0|\hat{H}_{mult}|1,0,0\rangle & & \\ \vdots & & \end{pmatrix}$$

$$\langle \dots \overset{m}{1} \dots | \hat{H}_{mult} | \dots \overset{n}{1} \dots \rangle$$

Due to $a_i^+ a_i (a^+ a_i - 1)|\dots n_i \dots\rangle = n_i(n_i-1)|\dots n_i \dots\rangle$
$= 0$ for $n_i = 0,1$

we can ignore interaction

$$\langle \dots \overset{m}{1} \dots | \sum_{ij} H(i,j) a_i^+ \underbrace{a_j | \dots \overset{n}{1} \dots \rangle}_{\delta_{jn}|0,0,0\rangle}$$

$\langle \ldots \overset{\downarrow m}{1} \ldots | a_i^+$

$= (a_i | \ldots \overset{\downarrow m}{1} \ldots \rangle)^+$

$= (\delta_{im} | 0, 0, 0 \rangle)^+$

$= \langle 0, 0, 0 | \delta_{im}$

Hence the matrix elements in 2nd quantisation are

$$\langle 0,0,0 | \sum_{i,j} H(i,j) \delta_{im} \delta_{jn} | 0,0,0 \rangle = H(m,n)$$

as expected

(c) <u>basis states for 2 particles</u>

in occupation number repr:

$|1,1,0\rangle \qquad |2,0,0\rangle$

$|1,0,1\rangle \qquad |0,2,0\rangle$

$|0,1,1\rangle \qquad |0,0,2\rangle$

(d) <u>energy levels for 2 particles</u>

$$\hat{H} |1,1,0\rangle = -\frac{\hbar^2}{2m} \big(-2a_1^+ a_1 - 2a_2^+ a_2 - \cancel{2a_3^+ a_3} + a_2^+ a_1 + a_3^+ a_2 + a_1^+ a_2 + \cancel{a_2^+ a_3} \big) |1,1,0\rangle$$

$$= -\frac{\hbar^2}{2m} \big(-4 |1,1,0\rangle + a_2^+ |0,1,0\rangle + a_3^+ |1,0,0\rangle + a_1^+ |1,0,0\rangle \big)$$

$$= -\frac{\hbar^2}{2m} \big(-4 |1,1,0\rangle + \sqrt{2} |0,2,0\rangle + |1,0,1\rangle + \sqrt{2} |2,0,0\rangle \big)$$

$$\hat{H} |2,0,0\rangle = -\frac{\hbar^2}{2m} \big(-2a_1^+ a_1 + a_2^+ a_1 \big) |2,0,0\rangle + \frac{u^{int}}{2} a_1^+ a_1 (a_1^+ a_1 - 1) |2,0,0\rangle$$

$$= -\frac{\hbar^2}{2m}\left(-4\,|2,0,0\rangle + a_2^\dagger \sqrt{2}\,|1,0,0\rangle\right)$$

$$+\, U^{int}\,|2,0,0\rangle$$

$$= -\frac{\hbar^2}{2m}\left(-4\,|2,0,0\rangle + \sqrt{2}\,|1,1,0\rangle\right) + U^{int}\,|2,0,0\rangle$$

We now know the following entries of the matrix representation (where $\alpha = -\frac{\hbar^2}{2m}$)

$$\begin{pmatrix} \langle 1,1,0|\hat{H}_{mult}|1,1,0\rangle & \langle 1,1,0|\hat{H}_{mult}|0,1,0\rangle & \cdots \\ \langle 0,1,0|\hat{H}_{mult}|1,1,0\rangle & & \\ \vdots & & \ddots \end{pmatrix}$$

$$= \begin{array}{c} \\ \langle 1,1,0| \\ \langle 1,0,1| \\ \langle 0,1,1| \\ \langle 2,0,0| \\ \langle 0,2,0| \\ \langle 0,0,2| \end{array} \begin{array}{c} \begin{array}{cccccc} |1,1,0\rangle & |1,0,1\rangle & |0,1,1\rangle & |2,0,0\rangle & |0,2,0\rangle & |0,0,2\rangle \end{array} \\ \left(\begin{array}{ccc|ccc} -4\alpha & & & \sqrt{2}\alpha & & \\ \alpha & & & 0 & & \\ 0 & & & 0 & & \\ \hline \sqrt{2}\alpha & & & -4\alpha + U^{int} & & \\ \sqrt{2}\alpha & & & 0 & & \\ 0 & & & 0 & & \end{array}\right) \end{array}$$