Advanced Quantum Theory

Homework 5

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4.2 Wavefunction

Consider a bosonic, spinless system with three single-particle states. Write down the normalised wavefunction of the multiple-particle state $|\,3,0,1\,\rangle$ in occupation-number representation.

For bosons, we have that:

$$\psi_{i_1,\ldots,i_N}(\vec{r}_i,\ldots\vec{r}_N) = C\sum_{\pi}\psi_{i_{\pi(1)}}(\vec{r}_1)\ldots\psi_{i_{\pi(N)}}(\vec{r}_N),\ C = \frac{1}{\sqrt{N!\,\Pi_i n_i!}} \tag{4.2.1}$$

For $N=4$:

$$C = \frac{1}{\sqrt{4!\,3!\,0!\,1!}} = \frac{1}{12}$$

There are $4! = 24$ permutations of the indices $i_1,\ldots,i_4$. Hence:

$$\begin{aligned}
\psi_{3,0,1}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4) &= \frac{1}{12}\sum_{\pi}\psi_{i_{\pi(1)}}(\vec{r}_1)\psi_{i_{\pi(2)}}(\vec{r}_2)\psi_{i_{\pi(3)}}(\vec{r}_3)\psi_{i_{\pi(4)}}(\vec{r}_4) \\
&= \frac{1}{12}\Big(\psi_1(\vec{r}_1)\psi_1(\vec{r}_2)\psi_1(\vec{r}_3)\psi_3(\vec{r}_4) \ + \ \psi_1(\vec{r}_1)\psi_1(\vec{r}_2)\psi_1(\vec{r}_4)\psi_3(\vec{r}_3) + \\
&\qquad \psi_1(\vec{r}_1)\psi_1(\vec{r}_3)\psi_1(\vec{r}_2)\psi_3(\vec{r}_4) \ + \ \psi_1(\vec{r}_1)\psi_1(\vec{r}_3)\psi_1(\vec{r}_4)\psi_3(\vec{r}_2) + \\
&\qquad \psi_1(\vec{r}_1)\psi_1(\vec{r}_4)\psi_1(\vec{r}_2)\psi_3(\vec{r}_3) \ + \ \psi_1(\vec{r}_1)\psi_1(\vec{r}_4)\psi_1(\vec{r}_3)\psi_3(\vec{r}_2) + \\
&\qquad \psi_1(\vec{r}_2)\psi_1(\vec{r}_1)\psi_1(\vec{r}_3)\psi_3(\vec{r}_4) \ + \ \psi_1(\vec{r}_2)\psi_1(\vec{r}_1)\psi_1(\vec{r}_4)\psi_3(\vec{r}_3) + \\
&\qquad \psi_1(\vec{r}_2)\psi_1(\vec{r}_3)\psi_1(\vec{r}_1)\psi_3(\vec{r}_4) \ + \ \psi_1(\vec{r}_2)\psi_1(\vec{r}_3)\psi_1(\vec{r}_4)\psi_3(\vec{r}_1) + \\
&\qquad \psi_1(\vec{r}_2)\psi_1(\vec{r}_4)\psi_1(\vec{r}_1)\psi_3(\vec{r}_3) \ + \ \psi_1(\vec{r}_2)\psi_1(\vec{r}_4)\psi_1(\vec{r}_3)\psi_3(\vec{r}_1) + \\
&\qquad \psi_1(\vec{r}_3)\psi_1(\vec{r}_1)\psi_1(\vec{r}_2)\psi_3(\vec{r}_4) \ + \ \psi_1(\vec{r}_3)\psi_1(\vec{r}_1)\psi_1(\vec{r}_4)\psi_3(\vec{r}_2) + \\
&\qquad \psi_1(\vec{r}_3)\psi_1(\vec{r}_2)\psi_1(\vec{r}_1)\psi_3(\vec{r}_4) \ + \ \psi_1(\vec{r}_3)\psi_1(\vec{r}_2)\psi_1(\vec{r}_4)\psi_3(\vec{r}_1) + \\
&\qquad \psi_1(\vec{r}_3)\psi_1(\vec{r}_4)\psi_1(\vec{r}_1)\psi_3(\vec{r}_2) \ + \ \psi_1(\vec{r}_3)\psi_1(\vec{r}_4)\psi_1(\vec{r}_2)\psi_3(\vec{r}_1) + \\
&\qquad \psi_1(\vec{r}_4)\psi_1(\vec{r}_1)\psi_1(\vec{r}_2)\psi_3(\vec{r}_3) \ + \ \psi_1(\vec{r}_4)\psi_1(\vec{r}_1)\psi_1(\vec{r}_3)\psi_3(\vec{r}_2) + \\
&\qquad \psi_1(\vec{r}_4)\psi_1(\vec{r}_2)\psi_1(\vec{r}_1)\psi_3(\vec{r}_3) \ + \ \psi_1(\vec{r}_4)\psi_1(\vec{r}_2)\psi_1(\vec{r}_3)\psi_3(\vec{r}_1) + \\
&\qquad \psi_1(\vec{r}_4)\psi_1(\vec{r}_3)\psi_1(\vec{r}_1)\psi_3(\vec{r}_2) \ + \ \psi_1(\vec{r}_4)\psi_1(\vec{r}_3)\psi_1(\vec{r}_2)\psi_3(\vec{r}_1)\Big)
\end{aligned}$$

4.5 Bose-Hubbard model

Consider a system with an arbitrary number of indistinguishable bosonic particles. It has two sites and the Hamiltonian:

$$\hat{H} = -\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1 + \frac{1}{2}\sum_i \hat{n}_i(\hat{n}_i - 1), \;\; \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i \tag{4.5.1}$$

(a) Show that applying $\hat{H}$ to a state does not change its particle number.

Heuristically, each term in the Hamiltonian contains an equal number of creation and annihilation operators. Apply $\hat{H}$ to a state $|\, n_1, n_2 \,\rangle$ in occupation-number representation:

$$\begin{aligned}
\hat{H} &= \left(-\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1 + \frac{1}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \right) |\, n_1, n_2 \,\rangle \\
&= -\hat{a}_1^\dagger \hat{a}_2 |\, n_1, n_2 \,\rangle - \hat{a}_2^\dagger \hat{a}_1 |\, n_1, n_2 \,\rangle + \left(\frac{1}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \right) |\, n_1, n_2 \,\rangle
\end{aligned}$$

The three terms are:

$$\begin{aligned}
-\hat{a}_1^\dagger \hat{a}_2 |\, n_1, n_2 \,\rangle &= -\sqrt{n_2}\; \hat{a}_1^\dagger |\, n_1, n_2 - 1 \,\rangle \\
&= -\sqrt{n_1 + 1}\; \sqrt{n_2}\; |\, n_1 + 1, n_2 - 1 \,\rangle
\end{aligned}$$

$$\begin{aligned}
-\hat{a}_2^\dagger \hat{a}_1 |\, n_1, n_2 \,\rangle &= -\sqrt{n_1}\; \hat{a}_2^\dagger |\, n_1 - 1, n_2 \,\rangle \\
&= -\sqrt{n_1}\; \sqrt{n_2 + 1}\; |\, n_1 - 1, n_2 + 1 \,\rangle
\end{aligned}$$

$$\left(\frac{1}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \right) |\, n_1, n_2 \,\rangle = \frac{1}{2}\left(n_1(n_1 - 1) + n_2(n_2 - 1) \right) |\, n_1, n_2 \,\rangle$$

In each case, the particle number is unchanged.

(b) Write down the basis states of the system with two particles.

In occupation-number representation, the basis states are $|\, 2, 0 \,\rangle, |\, 1, 1 \,\rangle, |\, 0, 2 \,\rangle$.

(c) Represent the Hamiltonian in matrix form and determine its eigenvalues.

Apply $\hat{H}$ to the basis states:

$$\hat{H}|\, 2, 0 \,\rangle = -\sqrt{2}\; \hat{a}_2^\dagger |\, 1, 0 \,\rangle = -\sqrt{2}\; |\, 1, 1 \,\rangle$$

$$\hat{H}|\, 1, 1 \,\rangle = -\hat{a}_1^\dagger |\, 1, 0 \,\rangle - \hat{a}_2^\dagger |\, 0, 1 \,\rangle = -\sqrt{2}\; |\, 2, 0 \,\rangle - \sqrt{2}\; |\, 0, 2 \,\rangle$$

$$\hat{H}|\, 0, 2 \,\rangle = -\sqrt{2}\; \hat{a}_1^\dagger |\, 0, 1 \,\rangle = -\sqrt{2}\; |\, 1, 1 \,\rangle$$

In matrix form:

$$\begin{aligned}
H(i,j) &= \begin{bmatrix} \langle\, 2, 0 \,|\hat{H}|\, 2, 0 \,\rangle & \langle\, 2, 0 \,|\hat{H}|\, 1, 1 \,\rangle & \langle\, 2, 0 \,|\hat{H}|\, 0, 2 \,\rangle \\ \langle\, 1, 1 \,|\hat{H}|\, 2, 0 \,\rangle & \langle\, 1, 1 \,|\hat{H}|\, 1, 1 \,\rangle & \langle\, 1, 1 \,|\hat{H}|\, 0, 2 \,\rangle \\ \langle\, 0, 2 \,|\hat{H}|\, 2, 0 \,\rangle & \langle\, 0, 2 \,|\hat{H}|\, 1, 1 \,\rangle & \langle\, 0, 2 \,|\hat{H}|\, 0, 2 \,\rangle \end{bmatrix} \\
&= \begin{bmatrix} 0 & -\sqrt{2} & 0 \\ -\sqrt{2} & 0 & -\sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{bmatrix}
\end{aligned}$$

The eigenvalues of A are the roots of its characteristic polynomial, $\det(A - \lambda I) = 0$.

$$\det(A - \lambda I) = \begin{vmatrix} -\lambda & -\sqrt{2} & 0 \\ -\sqrt{2} & -\lambda & -\sqrt{2} \\ 0 & -\sqrt{2} & -\lambda \end{vmatrix} = -\lambda \begin{vmatrix} -\lambda & -\sqrt{2} \\ -\sqrt{2} & -\lambda \end{vmatrix} + \sqrt{2} \begin{vmatrix} -\sqrt{2} & -\sqrt{2} \\ 0 & -\lambda \end{vmatrix}$$

$$= -\lambda \left(\lambda^2 - 2\right) + 2\lambda = -\lambda \left(4 - \lambda^2\right) = 0$$

Hence, the eigenvalues are $\lambda = 0, \pm 2$.