Molecular quantum dynamics: Solutions 2

Problem 1: Normalization of the momentum wavefunction

From the lecture, we have

$$a(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(q) e^{-ikq} dq. \tag{1}$$

Using Eq. (1), we obtain

$$\begin{aligned}
\int_{-\infty}^{\infty} |a(k)|^2 dk &= \int_{-\infty}^{\infty} dk \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dq' \psi(q') e^{-ikq'} \right]^* \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dq'' \psi(q'') e^{-ikq''} && (2)\\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} dq' \int_{-\infty}^{\infty} dq'' \int_{-\infty}^{\infty} dk \; \psi(q')^* \psi(q'') e^{ikq'} e^{-ikq''} && (3)\\
&= \int_{-\infty}^{\infty} dq' \int_{-\infty}^{\infty} dq'' \psi(q')^* \psi(q'') \delta(q' - q'') \quad (\text{using } \mathit{Hint}) && (4)\\
&= \int_{-\infty}^{\infty} dq' \psi(q')^* \psi(q') \quad (\text{using the property of the delta function}) && (5)\\
&= \int_{-\infty}^{\infty} dq' |\psi(q')|^2 && (6)\\
&= 1 \quad (\text{because the wavefunction in the position representation is normalized}). && (7)
\end{aligned}$$