Molecular quantum dynamics: Exercise series 10

Read: Tannor 11.6.5, 11.7.1.

Problem 1: Fourier method for a molecule in magnetic field

Imagine that you would like to use one of the computational methods described in class for a molecule in magnetic field $\mathbf{B}$ (for simplicity, assume $\mathbf{B}$ constant in time), described by the Hamiltonian

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2m} \left(\mathbf{p} - \mathbf{A}(\mathbf{q})\right)^2,$$

where $\mathbf{A}$ is the vector potential satisfying $\mathbf{B} = \nabla \times \mathbf{A}$. For simplicity, consider only the first-order split-operator and Fourier methods.

a) Explain why you cannot directly apply the split operator method to this problem.

b) You can quite easily apply the Fourier method. Describe (as in class) the steps of the algorithm specific to this Hamiltonian. Particularly, mention the differences from the case $H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q})$ studied in class.

Hint: Remember that both $\mathbf{p}$ and $\mathbf{A}(\mathbf{q})$ are operators which do not commute, and that $\mathbf{A}(\mathbf{q})$, being a function of $\mathbf{q}$, commutes with any other function of $\mathbf{q}$.