Molecular quantum dynamics: Solutions 11

Canonical momentum:

$$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}} = m\mathbf{v} + e\mathbf{A} \tag{1}$$

Hamiltonian:

$$\begin{aligned}
H(\mathbf{x}, \mathbf{p}) &= \mathbf{p} \cdot \mathbf{v} - L && (2)\\
&= (m\mathbf{v} + e\mathbf{A}) \cdot \mathbf{v} - \frac{1}{2}mv^2 + e\varphi - e\mathbf{v} \cdot \mathbf{A} && (3)\\
&= \frac{1}{2}mv^2 + e\varphi && (4)\\
&= \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\varphi && (5)
\end{aligned}$$

Hamilton's equations:

$$\begin{aligned}
\dot{\mathbf{x}} &= \frac{\partial H}{\partial \mathbf{p}} = \frac{1}{m}(\mathbf{p} - e\mathbf{A}) && (6)\\
\dot{\mathbf{p}} &= -\frac{\partial H}{\partial \mathbf{x}} && (7)\\
&= \frac{1}{m}\left[(\mathbf{p} - e\mathbf{A})\, e \cdot \nabla\right]\mathbf{A} + \frac{1}{m}e\,(\mathbf{p} - e\mathbf{A}) \times (\nabla \times \mathbf{A}) - e\nabla\varphi && (8)\\
&= e\left[(\mathbf{v} \cdot \nabla)\,\mathbf{A} + \mathbf{v} \times \mathbf{B}\right] - e\nabla\varphi && (9)
\end{aligned}$$

Also:

$$\dot{\mathbf{p}} = m\ddot{\mathbf{x}} + e\dot{\mathbf{A}} = m\ddot{\mathbf{x}} + e\left[\frac{\partial \mathbf{A}}{\partial t} + (\dot{\mathbf{x}} \cdot \nabla)\mathbf{A}\right] \tag{10}$$

Altogether:

$$m\ddot{\mathbf{x}} = e[-\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t} + \mathbf{v} \times \mathbf{B}] = e\,(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \tag{11}$$