Solution 10

1. Time-dependent Hamilton operators

(i) In the Schrödinger picture, let $\psi(s)$ denote an arbitrary state at time s. Then the state evolved to time t is given by $\psi(t) \coloneqq U(t,s)\psi(s)$, since $U(t,s)\psi(s)$ is the unique solution of (1) with initial condition $\psi(s)$ at $t = s$. For the Heisenberg picture, let $A(s)$ be a (possibly time-dependent) operator in the Schrödinger picture. We have

$$\begin{aligned}\langle\psi(t), A(s)\psi(t)\rangle =&\langle U(t,s)\psi(s), A(s)U(t,s)\psi(s)\rangle\\ =&\langle\psi(s), U(t,s)^* A(s)U(t,s)\psi(s)\rangle\,,\end{aligned}$$

hence the operator in the Heisenberg picture is $A(t) = U(t,s)^* A(s)U(t,s)$.

(ii) We make the following preliminary observations:

$$\begin{aligned}0 = \mathrm{i}\partial_s\psi(t) = \mathrm{i}\partial_s(U(t,s)\psi(s)) =&(\mathrm{i}\partial_s U(t,s))\psi(s) + U(t,s)\mathrm{i}\partial_s\psi(s)\\ =&(\mathrm{i}\partial_s U(t,s))\psi(s) + U(t,s)H(s)\psi(s)\,;\end{aligned}$$

and thus $\mathrm{i}\partial_s U(t,s) = -U(t,s)H(s)$. Moreover, the dual of equation (2) is

$$-\mathrm{i}\partial_t U(t,s)^* = U(t,s)^* H(t)\,.$$

Hence $U(s,t)$ and $U(t,s)^*$ satisfy the same differential equation, and also the initial condition at time $t = s$, $U(s,s) = U(s,s)^* = \mathbb{1}$. Thus $U(t,s)^* \equiv U(s,t)$.

For the first part, consider now two elements of the Hilbert space at time s, $\psi(s)$ and $\phi(s)$. We have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(s), U(t,s)^*U(t,s)\phi(s)\rangle =&\frac{\mathrm{d}}{\mathrm{d}t}\langle U(t,s)\psi(s), U(t,s)\phi(s)\rangle\\ =&\langle -\mathrm{i}H(t)U(t,s)\psi(s), U(t,s)\phi(s)\rangle\\ &+ \langle U(t,s)\psi(s), -\mathrm{i}H(t)U(t,s)\phi(s)\rangle\\ =&\mathrm{i}\langle U(t,s)\psi(s), H(t)U(t,s)\phi(s)\rangle\\ &+ (-\mathrm{i})\langle U(t,s)\psi(s), H(t)U(t,s)\phi(s)\rangle = 0\,.\end{aligned}$$

Furthermore, $\langle\psi(s), U(t,s)^*U(t,s)\phi(s)\rangle = \langle\psi(s), U(s,t)U(s,t)^*\phi(s)\rangle$ by our preliminary observations. Hence the operators $U(t,s)^*U(t,s)$, $U(t,s)U(t,s)^*$ and $\mathbb{1}$ all satisfy the same differential equation with common initial value at $t = s$ and therefore coincide, which implies the unitarity of $U(t,s)$.

For the second part, we get

$$\begin{aligned}\mathrm{i}\partial_s U(t,s)U(s,r) =&(\mathrm{i}\partial_s U(t,s))U(s,r) + U(t,s)\mathrm{i}\partial_s U(s,r)\\ =& - U(t,s)H(s)U(s,r) + U(t,s)H(s)U(s,r) = 0\,,\end{aligned}$$

and the same argument as above yields the desired equality.

(iii) In the j-th component, Newton's equation of motion is $m\ddot{x}_j = F_j$, with F_j the j-th component of the Lorentz force,

$$F = e(E + \frac{1}{c}\dot{x} \times B) = -e\nabla\varphi - \frac{e}{c}\partial_t A + \frac{e}{c}\dot{x} \times (\nabla \times A)\,.$$

Hamilton's equations of motion on the other hand imply

$$\frac{\mathrm{d}p_j}{\mathrm{d}t} = -\frac{\mathrm{d}H}{\mathrm{d}x_j} = -\frac{1}{m}\sum_{i=1}^{3}(p_i - \frac{e}{c}A_i)(-\frac{e}{c})\partial_j A_i - e\partial_j\varphi\,, \tag{4}$$

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = \frac{\mathrm{d}H}{\mathrm{d}p_j} = \frac{1}{m}(p_j - \frac{e}{c}A_j)\,. \tag{5}$$

Thus $p_i = m\dot{x}_i + (e/c)A_i$ by (5), and plugging this into (4) yields

$$m\ddot{x}_j + \frac{e}{c}\partial_t A_j + \frac{e}{c}\sum_{k=1}^{3}\dot{x}_k\partial_k A_j = \frac{e}{c}\sum_{i=1}^{3} m\dot{x}_i\partial_j A_i - e\partial_j\varphi\,,$$

where the last term on the left-hand side appears due to the time-dependence of the x_j's. The statement follows now by comparison.

(iv) Let $\tilde{H}(t)$ be given by replacing A, φ by $\tilde{A}, \tilde{\varphi}$ in $H(t)$. We are looking for $\tilde{\psi}(t)$ such that

$$\begin{aligned} \mathrm{i}\partial_t\tilde{\psi}(t) =& \tilde{H}(t)\tilde{\psi}(t) \\ =& \frac{1}{2m}\sum_{i=1}^{3}(-\mathrm{i}\partial_i - \frac{e}{c}A_i - \frac{e}{c}\partial_i\chi)^2\tilde{\psi}(t) + e\varphi\tilde{\psi}(t) - \frac{e}{c}(\partial_t\chi)\tilde{\psi}(t)\,. \end{aligned} \tag{6}$$

We have $\tilde{H}(t) = H(t) + H'(t)$ with

$$H'(t) = \frac{1}{2m}\sum_{i=1}^{3}((\frac{e}{c})^2(\partial_i\chi)^2 + 2\mathrm{i}\frac{e}{c}(\partial_i\chi)\partial_i + \mathrm{i}\frac{e}{c}\partial_i^2\chi + 2(\frac{e}{c})^2 A_i\partial_i\chi) - \frac{e}{c}\partial_t\chi\,;$$

hence comparing (1) and (6) leads to the conclusion that $\tilde{\psi}$ has to have the form $\tilde{\psi} = f\psi$ for some function $f = f(t,x)$. The l.h.s. of (6) therefore is

$$f\mathrm{i}\partial_t\psi(t) + \mathrm{i}(\partial_t f)\psi(t)\,, \tag{7}$$

whereas the r.h.s. is

$$fH(t)\psi + \sum_{i=1}^{3}(2\mathrm{i}\frac{e}{c}A_i(\partial_i f)\psi - (\partial_i^2 f)\psi - 2(\partial_i f)\partial_i\psi) + H'(t)f\psi\,. \tag{8}$$

The fist terms of (7) and (8) coincide. Furthermore, comparing the coefficients of $\partial_i\psi$ in the left over parts, we get

$$\partial_i f = \mathrm{i}\frac{e}{c}(\partial_i\chi)f\,,$$

and hence $f = \mathrm{e}^{\mathrm{i}\frac{e}{c}\chi}$ (up to a multiplicative constant which is chosen to be 1 in order for the wave function to be normalized). This is verified by plugging in f into the remaining terms of (7) and (8).

2. Self-adjointness of Schrödinger operators with Coulomb potential

(i) We have

$$\begin{aligned}\sum_{i=1}^n \langle \psi\,, A_i^* A_i \psi \rangle &= \sum_{i=1}^n \langle \psi\,, \left(\mathrm{i}\partial_i - \mathrm{i}\alpha \frac{x^i}{|x|^2} \right) \left(\mathrm{i}\partial_i + \mathrm{i}\alpha \frac{x^i}{|x|^2} \right) \psi \rangle \\ &= \sum_{i=1}^n \langle \psi\,, -\partial_i^2 \psi \rangle + \alpha^2 \langle \psi\,, \frac{(x^i)^2}{|x|^4} \psi \rangle - \alpha \langle \psi\,, \partial_i (\frac{x^i}{|x|^2}) \psi \rangle \\ &= \langle \psi\,, -\Delta \psi \rangle + \alpha^2 \langle \psi\,, \frac{1}{|x|^2} \psi \rangle - \sum_{i=1}^n \alpha \langle \psi\,, \left(\frac{1}{|x|^2} - \frac{2(x^i)^2}{|x|^4} \right) \psi \rangle \\ &= \langle \psi\,, -\Delta \psi \rangle + (\alpha^2 - \alpha(n-2)) \langle \psi\,, \frac{1}{|x|^2} \psi \rangle\,.\end{aligned}$$

Note that this expression is positive (as indicated on the exercise sheet), since $\langle \psi\,, A_i^* A_i \psi \rangle = \langle A_i \psi\,, A_i \psi \rangle = \|A_i \psi\|^2$. It attains a minimum for $\alpha = (n-2)/2$, where $\alpha^2 - \alpha(n-2) = -(n-2)^2/4$.

(ii) Set $\hbar = 1$. We have

$$\begin{aligned}\|w(x)\psi\|^2 =& d^2 \langle |x|^{-1}\psi, |x|^{-1}\psi \rangle \\ =& d^2 \langle \psi, |x|^{-2} \psi \rangle \\ \leqslant& 4d^2 \langle \psi, -\Delta \psi \rangle \\ =& 4d^2 \langle \hat{\psi}, |p|^2 \hat{\psi} \rangle\,,\end{aligned}$$

where the inequality follows from the Hardy inequality and we used Fourier transform for the last step. By Young's inequality we have $|p|^2 \leqslant c|p|^4 + 1/c$ for some (arbitrary) positive constant c. Thus

$$\begin{aligned}\|w(x)\psi\|^2 \leqslant& 4d^2 c \langle \hat{\psi}, |p|^4 \hat{\psi} \rangle + \frac{4d^2}{c} \langle \hat{\psi}, \hat{\psi} \rangle \\ \leqslant& 4d^2 c \| |p|^2 \hat{\psi} \|^2 + \frac{4d^2}{c} \|\hat{\psi}\|^2 \\ =& 4d^2 c \| -\Delta \psi \|^2 + \frac{4d^2}{c} \|\psi\|^2\,.\end{aligned}$$

In order to satisfy the conditions for the Kato-Rellich theorem, we must have

$$\|w(x)\psi\| \leqslant a\| -\Delta \psi\| + b\|\psi\|\,,$$

for some $a, b > 0$, $a < 1$, i.e.

$$\|w(x)\psi\|^2 \leqslant a^2 \| -\Delta \psi \|^2 + b^2 \|\psi\|^2 + 2ab \| -\Delta \psi \| \|\psi\|\,.$$

By the above computation, we actually have

$$\|w(x)\psi\|^2 \leqslant a^2 \| -\Delta \psi \|^2 + b^2 \|\psi\|^2$$

for $a = 2|d|\sqrt{c}$ and $b = 2|d|/\sqrt{c}$. Moreover, we can choose the constant $c > 0$ such that $\sqrt{c} < 1/2|d|$, whence $a < 1$ and the conditions of the theorem are satisfied.