P8.4 Consider an electron moving in an electrostatic potential $A^0(\mathbf{x})$, the steady-state equation being

$$E\psi = (c\boldsymbol{\alpha}\,.\,\hat{\mathbf{p}} + \beta mc^2 + V)\psi, \qquad V = -eA^0(\mathbf{x})$$

Perform a reduction to 'large components' (analogous to that in section 8.6) by the following steps.

(a) Writing $E = mc^2 + E'$, $\psi = \begin{pmatrix}\Psi\\ \Phi\end{pmatrix}$, show that

$$(E' - V)\Psi = c\boldsymbol{\sigma}\,.\,\hat{\mathbf{p}}\Phi$$

$$(2mc^2 + E' - V)\Phi = c\boldsymbol{\sigma}\,.\,\hat{\mathbf{p}}\Psi$$

(b) By expressing Φ in terms of Ψ, and keeping terms of first order in $(E - V)/2mc^2$ only, show that Ψ satisfies the equation

$$(E' - V)\Psi = \frac{1}{2m}\boldsymbol{\sigma}.\,\hat{\mathbf{p}}\left\{1 - \frac{(E' - V)}{2mc^2}\right\}\boldsymbol{\sigma}\,.\,\hat{\mathbf{p}}\Psi$$

(c) Prove that $\boldsymbol{\sigma}.\boldsymbol{\nabla}\, V(\mathbf{x})\boldsymbol{\sigma}.\boldsymbol{\nabla} = \boldsymbol{\nabla}V(\mathbf{x})\,.\boldsymbol{\nabla} + \mathrm{i}\boldsymbol{\sigma}\,.\,(\boldsymbol{\nabla}V(\mathbf{x}) \times \boldsymbol{\nabla}) + V(\mathbf{x})\boldsymbol{\nabla}^2$ and use this result to reduce the equation derived in (b) to

$$(E' - V)\Psi = \left\{\left(1 - \frac{E' - V}{2mc^2}\right)\frac{\hat{\mathbf{p}}^2}{2m} - \frac{\mathrm{i}\hbar}{4m^2c^2}\boldsymbol{\nabla}V\,.\,\hat{\mathbf{p}} + \frac{\hbar}{4m^2c^2}\boldsymbol{\sigma}\,.\,(\boldsymbol{\nabla}V \times \hat{\mathbf{p}})\right\}\Psi$$

Thus $E'\Psi = \hat{\mathbf{p}}^2/2m + V$ + terms of order $\mathbf{v}^2/c^2$. Deduce that to order $\mathbf{v}^2/c^2$ we can write

$$E'\Psi = \left\{\frac{\hat{\mathbf{p}}^2}{2m} - \frac{\hat{\mathbf{p}}^4}{8m^2c^2} + V - \frac{\mathrm{i}\hbar}{4m^2c^2}\boldsymbol{\nabla}V\,.\,\hat{\mathbf{p}} + \frac{\hbar}{4m^2c^2}\boldsymbol{\sigma}\,.\,(\boldsymbol{\nabla}V \times \hat{\mathbf{p}})\right\}\Psi$$

(d) Show that, if $V = V(r)$, $(r = |\mathbf{x}|)$ the last term in the above equation is the spin–orbit interaction

$$\frac{1}{r}\frac{\mathrm{d}V}{\mathrm{d}r}\frac{\mathbf{S}\,.\,\hat{\mathbf{L}}}{2m^2c^2}\Psi$$

where $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$.

(e) This is not quite the whole story, however. The quantity multiplying Ψ on the right-hand side of the third equation of part (c) ought, presumably, to be the Hamiltonian, to this order in v/c (namely, to order v^2/c^2). But it contains non-Hermitian terms (which?). This means that the 'total probability' $\int \Psi^\dagger\Psi\, \mathrm{d}^3\mathbf{x}$ would not be conserved. The reason (and the remedy) for this is well explained by Baym (1969). The true probability density is $\psi^\dagger\psi$, where $\psi = \begin{pmatrix}\Psi\\ \Phi\end{pmatrix}$; to order v^2/c^2 this is $\Psi^\dagger(1 + \hat{\mathbf{p}}^2/4m^2c^2)\Psi$, not $\Psi^\dagger\Psi$ itself. We therefore expect that, if we define the wave function Ψ' by $\Psi' = (1 + \hat{\mathbf{p}}^2/4m^2c^2)^{1/2}\Psi = (1 + \hat{\mathbf{p}}^2/8m^2c^2)\Psi$ to this order, then Ψ' would satisfy an equation of the form of part (c) but with a Hermitian Hamiltonian. Check that this is so, by showing that $\hat{\mathbf{p}}^2V\Psi' - V\hat{\mathbf{p}}^2\Psi' = -\hbar^2(\boldsymbol{\nabla}^2V)\Psi - 2\mathrm{i}\hbar\boldsymbol{\nabla}V.\hat{\mathbf{p}}\Psi'$ and using this result to deduce that

$$E'\Psi' = \left\{\frac{\hat{\mathbf{p}}^2}{2m} - \frac{\hat{\mathbf{p}}^4}{8m^2c^2} + \frac{\hbar^2}{8m^2c^2}\boldsymbol{\nabla}^2V + \frac{\hbar}{4m^2c^2}\boldsymbol{\sigma}\,.\,(\boldsymbol{\nabla}V \times \hat{\mathbf{p}})\right\}\Psi'$$