Applications of Quantum Mechanics - Examples III

(Starred questions are optional)

1. The Schrödinger equation for a particle in a background electromagnetic field is

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left( \nabla + \frac{ie}{\hbar} A \right)^2 \psi - e\phi \psi - \mu \mathbf{B} \cdot \mathbf{s} \psi. \]

Under a gauge transformation, the potentials \( A \) and \( \phi \) transform to \( \tilde{A} = A + \nabla f \) and \( \tilde{\phi} = \phi - \frac{\partial f}{\partial t} \).

Show that with a suitable transformation of \( \psi \), the Schrödinger equation transforms into itself, i.e. is gauge invariant. Show that the probability density \( |\psi|^2 \) and the expectation value of \(-i\hbar \nabla + eA\) are gauge invariant.

2. Consider a particle of charge \(-e\) and mass \(m\) moving in the \(x\)-\(y\) plane under the influence of a constant, uniform magnetic field \(\mathbf{B} = (0, 0, B)\). Write down the classical Hamiltonian \(H\) in the gauge \(A = B(-y/2, x/2, 0)\) and use Hamilton’s equations,

\[ \dot{x} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial x}, \]

to show that that classical orbits are circles. Show that the coordinates \((x_0, y_0, 0)\) of the center of any circular orbit are related to the position and momentum of the particle as,

\[ x_0 = \frac{x}{2} - \frac{Py}{eB}, \]
\[ y_0 = \frac{y}{2} + \frac{Px}{eB}. \]

Show that the quantum operators corresponding to the classical quantities \(x_0\) and \(y_0\) are individually conserved but cannot be measured simultaneously.

3. Show that by a suitable rescaling, the Hamiltonian for an electron moving essentially in the \(x, y\) plane in a time-independent magnetic field of strength \(\mathbf{B} = (0, 0, B(y))\) (i.e. depending on \(y\) but not \(x\)) can be reduced to

\[ H = -\left( \frac{\partial}{\partial x} - ia(y) \right)^2 - \left( \frac{\partial}{\partial y} \right)^2 + b(y)\sigma_3, \]

where \(\frac{da}{dy} = b(y)\). Use the Pauli matrix algebra to show that \(H\) can be written as \(Q^2\) where

\[ Q = i \left( \frac{\partial}{\partial x} - ia(y) \right) \sigma_2 - i \frac{\partial}{\partial y} \sigma_1. \]

Check that \(Q\) is hermitian and use this to deduce that any zero energy state is annihilated by \(Q\). Show that if there are spin down, zero energy states, they are of the form

\[ \left( \begin{array}{c} 0 \\ e^{-c(y)}f(x-iy) \end{array} \right) \]

where \(\frac{dc}{dy} = a(y)\). Show that if \(b(y) \geq b_0 > 0\), then \(c(y)\) grows at least quadratically as \(|y| \to \infty\).

4. A quantized particle of mass \(m\) moves in one dimension under the influence of a potential \(V(x) = -\frac{\hbar^2 \lambda}{m} \delta(x)\). Show that there is a bound state with energy \(-\hbar^2 \lambda^2/2m\). Now suppose the potential becomes

\[ V(x) = -\frac{\hbar^2 \lambda}{m} \sum_{l=-\infty}^{\infty} \delta(x - la). \]
Show that in this case there is (for $\lambda$ not too small) a negative energy band 

$$-\frac{\hbar^2}{2m} \kappa_L^2 \leq E \leq -\frac{\hbar^2}{2m} \kappa_U^2$$

where $\kappa_L$ is determined by $1 = \cosh \kappa_L a - \frac{\lambda}{\kappa_L} \sinh \kappa_L a$ and $\kappa_U$ satisfies a similar equation. Show that when $a \to \infty$ the band narrows down to the bound state energy.

[Hint: Use the obvious basis of negative energy solutions in the interval $-a < x < 0$, extend these to $0 < x < a$, and hence find the Floquet matrix and its trace.]

5. A quantized particle of mass $m$ moves in the one-dimensional potential

$$V(x) = -\frac{\hbar^2\lambda}{m} \sum_{l=-\infty}^{\infty} \delta(x-la), \quad \lambda > 0,$$

with energy $E = -\frac{\hbar^2 \kappa^2}{2m}$. Show that Bloch wave solutions, with Bloch wave vector $q$, are obtained by considering $C(q)\chi_\pm = e^{\pm iqa}\chi_\pm$ where $C(q)$ is the $2 \times 2$ Floquet matrix, and $\chi_\pm$ are 2-vectors.

Assume now that the Floquet matrix is defined with respect to the basis states $e^{\pm i\kappa x}$ on the interval $0 < x < a$. A model for a crystal with an impurity atom is given by

$$V(x) = -\frac{\hbar^2\lambda}{m} \sum_{l \neq 0} \delta(x-la) - \frac{\hbar^2\mu}{m} \delta(x).$$

Show that a bound-state-like solution with $\psi(x) = \psi(-x)$, satisfying $\psi(x+a) = e^{i\phi(x)}$ with $|e| < 1$ for $x > 0$ is possible if $C(\kappa - \mu) = e^{i\phi(\kappa + \mu)}$ and that this has energy outside the original negative energy band.

6. A simple model of a crystal consists of an infinite linear array of equally spaced sites. The probability amplitude at time $t$ for an electron to be at the $n$-th site is $c_n$, $n = 0, \pm 1, \pm 2, \ldots$. Given that the Schrödinger equation for the $c_n$ is

$$E c_n = E_0 c_n - A (c_{n-1} + c_{n+1}) \quad (n = 0, \pm 1, \pm 2, \ldots),$$

show that the energy $E$ of the electron must lie in a band $|E - E_0| \leq 2A$. Here $E_0 = E_0 + \alpha$ where $E_0$ is the energy of the electron on an isolated site, $\alpha$ is an additive constant and $-A$ is the (A real and positive) amplitude to jump between neighbouring sites.

Now suppose that a defect in the crystal results in the amplitude for jumping between sites 0 and 1 is changed from $-A$ to $-B$ with $B > A$. Obtain the new Schrödinger equation for $c_0$ and $c_1$. By considering solutions of the form

$$c_n = \begin{cases} \alpha s^{n-1}, & n \geq 1, \\ \beta s^{-n}, & n \leq 0, \end{cases}$$

show that $s = \pm A/B$ and hence that the electron may be trapped near the origin. Obtain the energies of the corresponding states.

7. Show how, for a general one-dimensional periodic potential,

$$V(x) = \sum_{n=1}^{\infty} \alpha_n \left( e^{2\pi i n x/a} + e^{-2\pi i n x/a} \right),$$

the nearly-free electron model leads to a band structure for the energy levels. Determine, in this approximation, the energy gap between adjacent energy bands.

8. Consider the scaled Schrödinger equation

$$-\frac{d^2\psi}{dx^2} + \lambda \cos 2x \psi = E \psi$$

where $|\lambda|$ is small. Using the nearly-free electron approximation, determine the energies at the bottom and top of the lowest energy band, and also the Bloch states at these energies.

9. Show that the tight binding wavefunction

$$\Psi_k(x) = \sum_{a \in \Lambda} \psi(x-a) e^{i \mathbf{k} \cdot \mathbf{a}},$$

where $\Lambda$ is a Bravais lattice in three dimensions and $\psi(x)$ is a state localized around an atom at the origin, is a Bloch state.