Massachusetts Institute of Technology
Physics Department

Physics 8.322 **Spring 2007**
Quantum Theory II **March 12, 2007**
Assignment 6

DUE APRIL 6, 2007, AT THE END OF THE DAY

Announcements

- This problem set counts as TWO.
- Note the due date. The next problem set will be due April 13.
- Several sets of supplementary notes have appeared on the 8.322 website. There titles are:
  - Perturbation Theory Summary
  - Notes on WKB Connection Formulas
  - Summary of WKB Connection Formulas
  - Notes on WKB Approximation for

    Reflection above a Barrier and The Transition Amplitude in the Adiabatic Approximation

Reading topics for this period

- The adiabatic approximation. We will discuss the adiabatic theorem and derive the transition rate (*ie.* the failure of the theorem) for smooth time variation.
- Quantum adiabatic ("Berry's") phase
- The Born-Oppenheimer approximation.

Reading Recommendations 6

- Adiabatic approximation
  - Sakurai pays little attention to the adiabatic theorem, but has a good discussion of Berry's phase in Supplement I.
  - Griffith's treatment of the adiabatic approximation (§10) is similar to Sakurai's.

- Landau and Lifschitz §41 introduces the adiabatic approximation and §53 describes the transition amplitude in the adiabatic approximation.
- Schiff has a good treatment of the Born-Oppenheimer approximation (pages 445-455), although he misses the (Berry phase related) vector potential.
- See J. Moody, A. Shapere, and F. Wilczek, Phys. Rev. Lett. **56** (1986) 893, for a discussion of the Born-Oppenheimer approximation including effects associated with the Berry phase.

Problem Set 6

Topics covered in the problems

- The adiabatic approximation
- The quantum adiabatic phase
- Hannay's angle
- Born-Oppenheimer approximation

Problems

1. **Reflection above the barrier**

   A particle of mass m and zero total energy is incident on a barrier of the form: $V(x) = -V_0\sqrt{1+x^2/a^2}$.

   (a) Compute the probability that it will be reflected in the WKB approximation. Answer:

   $$|R|^2 = \exp\left(-\frac{\sqrt{2\pi}\,\Gamma(1/4)}{2\Gamma(7/4)}\sqrt{\frac{mV_0a^2}{\hbar^2}}\right)$$

   (b) Approximate the potential by a parabola near $x = 0$, $V(x) \approx -V_0 - \frac{V_0x^2}{2a^2}$ and use the result derived in the notes for the WKB reflection probability from an inverted oscillator. Compare your result with the answer to part (a).

2. **A slow field reversal**

   How to transform a spin state adiabatically at low cost.

   An electron is held in a spin up state along the $\hat{z}$-axis by a 5 kilogauss magnetic field, $\vec{B} = B_0\hat{z}$. An experimenter would like to reverse the electron spin adiabtically.

   (a) Explain why, if she had the choice, she would slowly *rotate* the magnetic field until it pointed in the $-\hat{z}$ direction, as opposed to slowly *reversing* the field.

(b) However it is expensive to rotate a magnet, and cheap to just reverse the current. Having taken 8.322 the experimenter decides it's almost as good just to reverse the field, provided she places the apparatus in a weak permanent magnet with its field pointing some direction in the xy-plane. What is her reasoning?

(c) If her permanent magnet is 5 gauss, estimate how long she should take to reverse the field if she wants to have less than a 10^{-6} probability that the spin will flip. You can assume that the process is carried out smoothly enough that the WKB approximation applies.

3. **Quantum Adiabatic Engineering**

The object of this problem is to find a way to shift the state of a spin-1 particle as you wish.

A spin-1 particle has three eigenstates, $|+\rangle$, $|0\rangle$, and $|-\rangle$, corresponding to $S_z = +1, 0, -1$ respectively.

Consider a spin-1 particle nailed down at $\vec{x} = 0$ so it cannot move, but with its spin is left free. In the absence of any external perturbations all three states of the spin would have the same energy, E_0. An external magnetic field splits the states by means of the magnetic interaction energy, $H_B = -\mu_0 \frac{1}{\hbar}\vec{S} \cdot \vec{B}$. The environment of the particle generates a small constant magnetic field in the $\hat{x}$ direction, $\delta\vec{B} = B_x\hat{x}$. In addition, the environment generates a small quadrupole interaction that tends to align the spin in the $|\pm\rangle$ direction. This contribution to the Hamiltonian has the form, $H_Q = -c\{\frac{1}{\hbar^2}\}S_z^2$ $(c > 0)$. The entire Hamiltonian is therefore

$$H = E_0 I - \mu_0\{\frac{1}{\hbar}\vec{S}\} \cdot \vec{B} - c\{\frac{1}{\hbar^2}\}S_z^2 \tag{1}$$

Remember the spin operators for $S = 1$ and their algebra,

$$\begin{aligned} S_x &= \hbar \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\ S_y &= \hbar \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \\ S_z &= \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \end{aligned} \tag{2}$$

obey the usual commutation relations of angular momentum, $[S_x, S_y] = i\hbar S_z$, etc.

(a) Suppose the particle is placed in an external time-dependent magnetic field, $\vec{B}(t) = (B_0 - \beta t)\hat{z}$. Assume the following hierarchy of energies:

$$\mu_0 B_0 \gg c \gg \mu_0 B_x \gg \hbar\beta \tag{3}$$

Sketch the energy levels of this system as a function of time in the adiabatic approximation.

(b) Suppose the system starts out in the state $|+\rangle$ at $t = 0$. Show that this state evolves adiabatically to a state that is approximately equal to $|0\rangle$ and then to $|-\rangle$. By altering the time dependence of $\vec{B}(t)$ you can transform the initial state $|+\rangle$ into either of these final states. Explain how you would do this.

You have several tools at your disposal: You could choose *not* to run through the entire time dependence of B as proposed in part (a), or you could choose to change B *very rapidly*, so suddenly that the state of the system could not respond (the sudden approximation).

4. **Simplifying Degeneracies in the Adiabatic Approximation**

Even though a quantum system may depend on a large number of parameters, near the crossing of two energy levels the important physics is summarized by a two state problem depending on three parameters, $\vec{B}(t)$. In effect, near where two states become degenerate, the system looks like a spin $\frac{1}{2}$ particle in an external magnetic field!

Consider a quantum system described by a Hamiltonian, $H(\alpha)$, that depends on a set of parameters $\{\alpha_j(t), j = 1, 2, \ldots, N\}$ that can vary with time. Suppose that H has only discrete eigenvalues.

Consider the eigenvalues of H as functions of the parameters $\{\alpha_j\}$. In general, no two eigenvalues are the same (we assume H has no symmetries). For some specific value of the parameters suppose two energy levels cross. To be specific, suppose that states $|a_1\rangle$ and $|a_2\rangle$ are degenerate for $\alpha_j = \alpha_j^0, j = 1, 2, \ldots, N$.

$$\begin{aligned} H(\alpha^0)|a_1\rangle &= E_0|a_1\rangle \\ H(\alpha^0)|a_2\rangle &= E_0|a_2\rangle. \end{aligned} \tag{4}$$

Consider parameter choices close to α^0, $\alpha_j - \alpha_j^0 = \delta\alpha_j$. Show that the mixing of states a_1 and a_2 can be described by the Hamiltonian

$$H = \sum_{k=1}^{3} B_k \sigma_k \equiv \vec{B} \cdot \vec{\sigma} \tag{5}$$

where $\{\sigma_k, k = 1, 2, 3\}$ are the Pauli matrices, and

$$B_k = \frac{1}{2} \sum_{n,m=1,2} \sigma^k_{mn} \sum_{j=1}^{N} \langle a_m | \delta\alpha_j \left. \frac{\partial H}{\partial \alpha_j} \right|_{\alpha_j = \alpha_j^0} |a_n\rangle \tag{6}$$

Thus, when we study a spin $\frac{1}{2}$ particle in an external magnetic field, we are actually studying the most general case!

5. **Berry Phase for Spin-J**

   A quantum particle of spin J is at rest in a magnetic field. It is initially in the state $\left|J, M_J\right\rangle$. The magnetic field is changed adiabatically as a function of time such that $\vec{B}(0)=\vec{B}(T)$ and the cone described by the function $\vec{B}(t)$ subtends solid angle Ω. What is the adiabatic phase accumulated by the particle during this adiabatic transport? [This is the generalization of the result derived in lecture for spin-1/2.]

6. **An adiabatic excursion**

   A electron (g-factor 2) is held in a magnetic field, that varies slowly with time. ($H=-\vec{\mu}\cdot\vec{B}$ and $\vec{\mu}=-e\vec{s}/mc$.) The magnetic field has a large constant component in the $\hat{e}_3$ direction, and its component in the $\hat{e}_1-\hat{e}_2$ plane varies on an elliptical trajectory,

$$\vec{B}(t)=\hat{e}_3 B_0+\hat{e}_1 B\cos\lambda\cos\omega t+\hat{e}_2 B\sin\lambda\sin\omega t$$

   with $B_0 \gg B$ and $0<\lambda<\frac{\pi}{4}$. It may be useful to denote $\omega_L=eB_0/mc$.

   (a) What are the conditions on the parameters of the problem so that the adiabatic approximation would provide a good description of the time development of the system? Use the criteron introduced in lecture.

   (b) A particle is initially in the eigenstate with spin $-\hbar/2$ along $\hat{B}$. After a long time any transients have settled down. Use the WKB approximation to the adiabatic transition probability to estimnate the time average probability per unit time that it makes a transition to the state with spin $+\hbar/2$. Hint: The transition probability is dominated by times when the energy difference between the two levels is minimum. For those times the energy difference varies approximately quadratically with time.

   For the rest of this problem, assume the validity of the adiabatic approximation and ignore any transitions between eigenstates of the instantaneous hamiltonian, $H(t)$. Suppose at $t=0$ a particle is prepared initially in a the state

$$\left|\psi(0)\right\rangle=\frac{1}{\sqrt{2}}\left(\left|+\hat{B}(0)\right\rangle+\left|-\hat{B}(0)\right\rangle\right)$$

   where $\left|+\hat{B}(0)\right\rangle$ and $\left|-\hat{B}(0)\right\rangle$ are the eigenstates with spin $\pm\hbar/2$ along the direction defined by $\hat{B}(t)$ at $t=0$.

   (c) Ignoring the adiabatic phase the state $\left|\psi(t)\right\rangle$ will return to its original form (up to an irrelevant phase) after a time T. Estimate T in the approximation $B_0 \gg B$. Make sure your approximation is accurate enough to capture the leading λ dependence.

   (d) Now include the effects of the adiabatic phase. This will change the time necessary for the state to return to its original form. What is the change in T? Remember to assume $B_0 \gg B$.

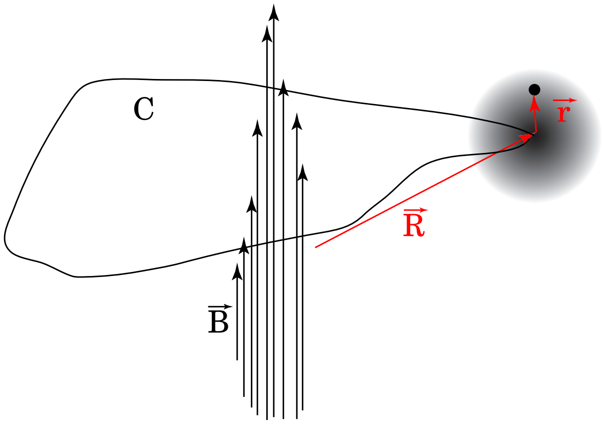

Figure 1: An electron localized in a potential at $\vec{R}$ which is then carried on a curve C around a region containing a magnetic field, $\vec{B}$.

7. **Bohm-Aharonov Effect**

   Read §10.2.4 in Griffiths on the Aharonov-Bohm Effect (Scanned and posted on the 3.222 website.)

   Consider a potential centered at position $\vec{R}$ with an electron in a localized eigenstate $\psi_n(r - R)$, shown in Fig. (1). (For our purposes, it doesn't matter whether this potential is a box with hard walls, a harmonic oscillator, or any other confining potential.)

   Now, assume this system moves adiabatically such that the location of the potential $\vec{R}$ moves around a closed path C, entirely within a region outside of an external magnetic field characterized by a vector potential, $\vec{A}(\vec{r})$, as shown in the figure. Show that the Berry phase $\gamma_n(C) = \frac{e}{\hbar c}\Phi_B$, where Φ_B is the flux enclosed by the path C.

8. **Hannay's Angle**

   Hannay's angle is the classical analog of Berry's phase. This problem leads you through the discovery of Hannay's angle for a very simple system similar to the system in which we studied Berry's phase. This is not a general discussion of Hannay's angle or a derivation of its relation to Berry's phase. Also the problem is entirely geometry and classical mechanics.

   Consider the physical system shown in Fig. (2). It consists of a wheel with spokes mounted on a rigid rod. The wheel is attached by a *frictionless* sleeve so the torque exerted by the rod on the wheel has no component parallel to the rod. (That's the definition of frictionless.) The wheel is mounted perpendicular to the rod. One spoke on the wheel is painted orange so we can keep track of its orientation. Initially the rod and wheel are at rest. Then the rod is rotated to sweep out a right circular cone of opening angle β. At the end, the rod and wheel have returned to their original configuration, except the orange spoke has rotated through an angle $\theta = -2\pi \sin\alpha = -2\pi\cos\beta$. Note that this is simply related to the solid angle subtended by the cone,

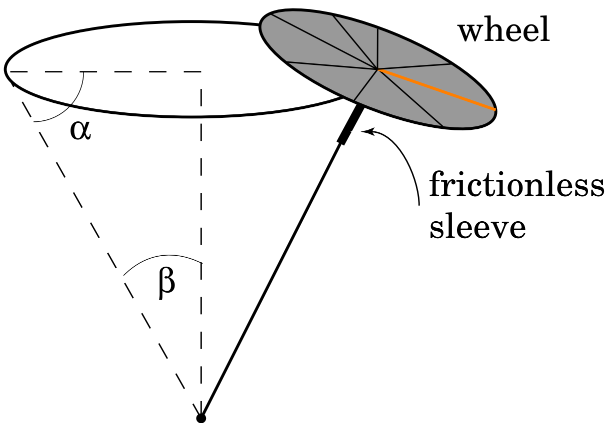

Figure 2: Wheel mounted frictionlessly on a rod which then executes a cone in configuration space. Follow the orange spoke.

$\Omega = 2\pi(1-\cos\beta) = 2\pi - \theta.$

Now put this system aside and consider instead the same wheel mounted on a rigid helical wire as shown in Fig. (3). Again the wheel is attached by a frictionless sleeve and held at right angles to the wire. The parametric equation of the helix is

$$\vec{x}(s) = (x(s), y(s), z(s)) = (\cos\alpha\cos s, \cos\alpha\sin s, s\sin\alpha)$$

One step of the helix corresponds to $s \to s + 2\pi$. α is the "pitch angle" of the helix.

(a) Explain why the problem of the wheel sliding along the helix is equivalent to the problem of the wheel mounted on the rod.

The wheel is a rigid body, so the motion of the orange spoke relative to the center of the wheel, as it moves along the helix is determined by its instantaneous angular velocity, $\vec{\omega}(s)$. (This is a familiar result from rigid body mechanics.)

$$\frac{d\vec{v}}{dt} = \vec{\omega}(s) \times \vec{v}.$$

where $\vec{v}$ is a vector parallel to the orange spoke. The requirement for frictionless motion is that $\hat{t}\cdot\frac{d\vec{\omega}}{dt} = 0$. Here $\hat{t}$ is the tangent to the helix and $d\vec{\omega}/dt$ is proportional to the torque (by Newton's laws). Note that the torque is not zero — torque is required to twist the wheel as it moves along the wire. However the frictionless sleeve ensures that the torque has no component tangent to the wire. Since the wheel starts at rest ($\vec{\omega}(0) = 0$), the equation for frictionless transport (known to mathematicians as parallel transport) is

$$\hat{t}(s)\cdot\vec{\omega}(s) = 0 \text{ for all } s$$

It is useful to define a standard reference frame moving along the curve. This frame consists of the unit tangent, $\hat{t} = d\vec{x}/ds$ (we have chosen s so that $|\hat{t}| = 1$); the unit

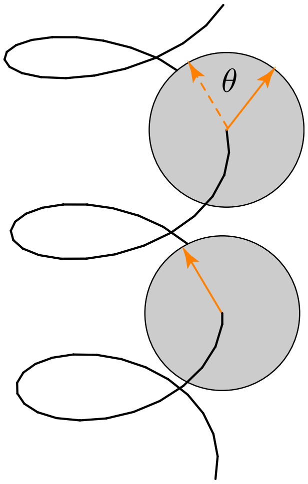

Figure 3: The equivalent problem on a helical wire. The wheel is shown at two times separated by arc length $s = 2\pi$. Only the orange spoke is shown. It has rotated through an angle θ relative to its position at $s = 0$.

normal, proportional to $d\hat{t}/ds$, and the unit "binormal", $\hat{b} = \hat{t} \times \hat{n}$. This is known as the Frenet frame. It is a general feature of the differential geometry of curves, but we are only concerned with the helix here. So for example,

$$\hat{t} = (-\cos\alpha \sin s, \cos\alpha \cos s, \sin\alpha) \tag{7}$$

The Frenet frame mounted on the helix is shown in Fig. (4).

(b) Derive expressions for $\hat{n}$ and $\hat{b}$ similar to eq. (7).

(c) Derive the Frenet formulas for the helix,

$$\begin{aligned} \frac{d\hat{t}}{ds} &= \kappa(s)\hat{n}(s) \\ \frac{d\hat{n}}{ds} &= -\kappa(s)\hat{t}(s) + \tau(s)\hat{b}(s) \\ \frac{d\hat{b}}{ds} &= -\tau(s)\hat{n}(s) \end{aligned} \tag{8}$$

κ and τ are the "curvature" and "torsion" of the helix respectively. What are κ and τ in terms of the pitch angle α? Note that the helix is a very special curve.

(d) The three unit vectors that define the Frenet frame can be thought of as a rigid body traveling along the curve. Its orientation changes as a function of s.

The s-dependence of $\hat{t}$, $\hat{n}$, and $\hat{b}$ can be described in terms of an angular velocity, $\omega_{\text{Frenet}}(s)$,

$$\frac{d\hat{u}}{ds} = \vec{\omega}_{\text{Frenet}}(s) \times \hat{u}$$

for $\vec{u} = \hat{t}, \hat{n}, \hat{b}$. Find $\vec{\omega}_{\text{Frenet}}$ and show that $\hat{t} \cdot \vec{\omega}_{\text{Frenet}} \neq 0$.

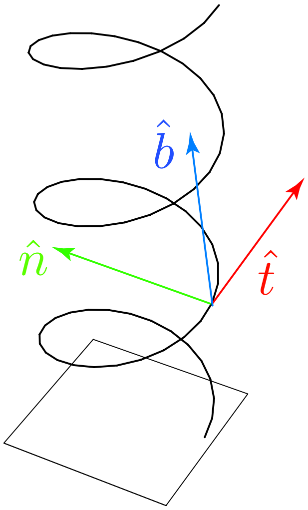

Figure 4: The Frenet frame on a helix. Note that the normal, $\hat{n}$, always lies in the (x, y)-plane. So it returns to its original orientation when $s \rightarrow s + 2\pi$.

Thus if the wheel were affixed to the Frenet frame, torque parallel to the wire would be required to keep it at rest. So the orange spoke is not a rest in the Frenet frame.

(e) $\hat{n}(s)$ and $\hat{b}(s)$ form a basis for any vector in the plane perpendicular to $\hat{t}(s)$, so the vector defining a spoke on the wheel must be a linear superposition of $\hat{n}(b)$ and $\hat{b}(s)$.

$$\vec{v}(s) = \cos\theta(s)\hat{n}(s) + \sin\theta(s)\hat{b}(s)$$

Find a differntial equation for the angle $\theta(s)$ from the requirement that the angular velocity of $\vec{v}$ has no component along $\hat{t}$.

(f) What is $\theta(2\pi) - \theta(0)$ and why is it the quantity we are interested in?

(g) [Not Required] Generalize this result to an arbitrary (closed) motion of the rod.

9. **The Born Oppenheimer Approximation for a Diatomic Molecule**

The Born-Oppenheimer (B-O) Approximation is a version of the adiabatic approximation where the slowly varying parameters are actually associated with variables that are themselves quantized. Although the B-O approximation was developed for molecular physics, the general idea permeates much of modern physics: Suppose there are two energy or time scales in a problem. A short time (or high energy) scale and a long time (or low energy) scale. If the separation of scales is large enough, the slow variables, changing over a long time scale, do not have enough energy to induce transitions among the eigenstates of the fast variables. Instead the eigenstate and eigenenergy describing the fast variables changes adiabatically with the slow variables. Colloquially, the fast variables remain "frozen" in a particular state as the slow variables evolve. You will hear condensed matter, particle and nuclear theorists refer to this approach as "integrating out" the high energy effects in a system. This term originates in the path history approach.

This problem is really a short set of supplementary notes on the B-O approximation leaving several sections for you to work out.

As we will see, effects related to Berry's phase appear in the effective Hamiltonian for the slow variables. This was not fully realized until Berry's work in 1984.

Consider a diatomic molecule. Let the coordinate separation of the two atoms be given by the three component vector, $\mathbf{R}$. Let the coordinates of the electrons be described by a multicomponent vector $\mathbf{r}$. (This is really a shorthand for $\mathbf{r}_1, \mathbf{r}_2..., \mathbf{r}_n$ for n-electrons.) Ignore spin. The Hamiltonian (in coordinate space) can be written,

$$H = -\frac{1}{2\tilde{M}_N}\nabla^2_{\mathbf{R}} - \frac{1}{2m_e}\nabla^2_{\mathbf{r}} + V_N(\mathbf{R}) + V_e(\mathbf{r}, \mathbf{R}) \tag{9}$$

The first term is the kinetic energy of the nuclei ($\tilde{M}_N$ is the reduced mass). The second is the kinetic energy of the electrons. The third is the Coulomb potential energy of the two nuclei,

$$V_N(\mathbf{R}) = \frac{Z_1 Z_2 e^2}{|\mathbf{R}|}$$

And the fourth term is the Coulomb interaction among the electrons and between the electrons and the nuclei, which does not have to be written explicitly.

The first step in the B-O approximation is to decompose the Schrödinger wave function for the molecule into electron and nuclear components,

$$\Psi(\mathbf{r}, \mathbf{R}) = \sum_m \Phi_m(\mathbf{R})\psi_m(\mathbf{r}, \mathbf{R}) \tag{10}$$

where $\psi_m(\mathbf{r}, \mathbf{R})$ is a solution to the Schrödinger equation for the electrons *with the nuclear coordinates fixed*,

$$\left(-\frac{1}{2m_e}\nabla^2_{\mathbf{r}} + V_N(\mathbf{R}) + V_e(\mathbf{r}, \mathbf{R})\right)\psi_m(\mathbf{r}, \mathbf{R}) = \varepsilon_m(\mathbf{R})\psi_m(\mathbf{r}, \mathbf{R}) \tag{11}$$

Note that it is consistent to treat the nuclear coordinate, $\mathbf{R}$, as fixed in eq. (11) because it commutes with all the other operators in the equation. (In particular, $\nabla_{\mathbf{R}}$ does not appear.) Note also that the electron eigenenergy, $\varepsilon_m(\mathbf{R})$ depends on the nuclear coordinate, $\mathbf{R}$.

The solutions to eq. (11) form a complete orthonormal set for fixed $\mathbf{R}$,

$$\int d\mathbf{r}\psi^*_m(\mathbf{r}, \mathbf{R})\psi_n(\mathbf{r}, \mathbf{R}) = \delta_{mn}$$

(a) Now consider the full Schrödinger equation, $H\Psi(\mathbf{r}, \mathbf{R}) = E\Psi(\mathbf{r}, \mathbf{R})$, where H is given by eq. (9) and $\Psi(\mathbf{r}, \mathbf{R})$ by eq. (10). Multiply through by $\psi^*_l(\mathbf{r}, \mathbf{R})$ and integrate over $\mathbf{r}$ to obtain an "effective" Schrödinger equation in the space of nuclear wavefunctions,

$$H_{lm}(\mathbf{R})\Phi_m(\mathbf{R}) = E\Phi_l(\mathbf{R}) \tag{12}$$

where $H_{lm}(\mathbf{R}) \equiv \int d\mathbf{r} \psi_l^*(\mathbf{r}, \mathbf{R}) H \psi_m(\mathbf{r}, \mathbf{R})$.
Show

$$\begin{aligned} H_{lm}(\mathbf{R}) &= -\frac{1}{2\tilde{M}_N} \delta_{lm} \nabla_{\mathbf{R}}^2 + 2\big\langle l(\mathbf{R}) \big| \vec{\nabla}_{\mathbf{R}} \big| m(\mathbf{R}) \big\rangle \cdot \vec{\nabla}_{\mathbf{R}} \\ &+ \big\langle l(\mathbf{R}) \big| \nabla_{\mathbf{R}}^2 \big| m(\mathbf{R}) \big\rangle + \delta_{lm} \left(V_N(\mathbf{R}) + \varepsilon_m(\mathbf{R}) \right) \end{aligned} \tag{13}$$

where $\big|m(\mathbf{R})\big\rangle$ is the electron eigenstate with wavefunction, $\psi_m(\mathbf{r}, \mathbf{R}) = \big\langle \mathbf{r} \big| m(\mathbf{R}) \big\rangle$ and eigenvalue $\varepsilon_m(\mathbf{R})$.

Assume *that the nuclei move slowly compared to the electrons*, slow enough that the quantum state of the electrons remains fixed as functions of the nuclear coordinates. This is the essence of the Born-Oppenheimer approximation, and it conceptually the same as the adiabatic approximation.

(b) In this limit

$$H_{lm}(\mathbf{R}) \to \delta_{lm} H_m(\mathbf{R})$$

Show that in the Born-Oppenheimer approximation, eq. (13) can be written

$$\begin{aligned} H_m(\mathbf{R}) \Phi_m(\mathbf{R}) &= E_m \Phi(\mathbf{R}), \text{ with} \\ H_m(\mathbf{R}) &= -\frac{1}{2\tilde{M}_n} \left(\vec{\nabla}_{\mathbf{R}} - i \vec{A}_m(\mathbf{R}) \right)^2 + V_m(\mathbf{R}) \end{aligned} \tag{14}$$

(c) What is the Born-Oppenheimer "effective potential", $V_m(\mathbf{R})$?

(d) What is the Born-Oppenheimer "effective vector potential", $\vec{A}_m(\mathbf{R})$? Show that it is real. How is it related to the Berry phase $\gamma_m(\mathbf{R})$?

(e) Explain in words how you would go about solving for the vibrational and rotational states of the hydrogen molecular ion, H_2^+.