PHYS3022 Applied Quantum Mechanics   Problem Set 7 (Revised)
Due: 18 April 2019 (Thursday)   "T+4 = 23 April 2019"

All problem sets should be handed in not later than 5pm on the due date. Drop your assignments in the PHYS3022 box outside Rm.213.
Please work out the steps of the calculations in detail. Discussions among students are highly encouraged, yet it is expected that we do your homework independently.

7.0 **Reading Assignment.** The electronic part of a molecular problem gives chemical bonding. The motions of the nuclei give rise to vibrational levels and rotational levels. Molecules are usually in their electronic ground state and vibrational ground state. But room temperature can distribute them among the rotational levels. Molecular spectrum originates from transitions between molecular levels. In the microwave/far IR range, we have rotational spectrum. In the IR range, we have vibrational or vibrational-rotational spectrum. With QM of molecules, molecular spectrum gives us useful information, including the bond length R_0 and the force constant of the bond (thus the strength of the bond). Behind this application is the knowledge about harmonic oscillator and rigid rotor. For the physics contents, see the chapter on molecules in *Modern Physics* (e.g. by Taylor, Zafiratos, Dubson; and by Harris). We use more QM in our treatment in typical modern physics and quantum physics books. If you would like to learn more about molecules, e.g. anharmonic effect, polyatomic molecules, see *Physical Chemistry* and *Quantum Chemistry* by McQuarrie, *Quantum Chemistry and Spectrocopy* by Thomas Engel. For those only want to read "physics" books, see *Physics of Atoms and Molecules* by Bransden and Joachain, which takes you from the undergraduate level to the postgraduate level both in quantum mechanics and in atomic/molecular physics.

The last part of the course discusses Tunnelling and its applications. The problem is motivated by phenomena in α-particle decays in heavy nuclei. For tunnelling (and more generally transport properties of matter), we need to consider **travelling waves** in quantum mechanics. There is an issue of normalization. We discussed three possible ways out. One is to extend the definition of orthonormality using Dirac δ-functions. Another way is to form wave packets. In solid state physics, one mimics an infinite system by a finite (but big) system and imposes the periodic boundary condition. The concept of **Probability Current Density** is then introduced. These concepts are essential for an understanding of the tunnelling formulation. Although we use the single (square) barrier as the example, we discussed the proper and formal definitions of the **Transmission Coefficient** and **Reflection Coefficient**. Our discussion is meant to prepare you for many other transport (tunnelling) problems that you may encounter in courses/research in the future. To put the application to α-particle decays and to nuclear fusion into a proper context, we will do a "Crash Module on the Physics of Nuclei". The aims here are to get cross the point that the quantum mechanics we know can be readily applied to understand many pieces of nuclear physics, and to introduce two important figures in nuclear physics. They are the binding energy per nucleon versus the mass number of nucleon and the Segre Chart. Other applications of tunnelling, including Scanning Tunnelling Microscope, writing using atoms, field emission, and quantum cascade lasers are discussed briefly.

For reading on tunnelling, sections in Griffiths' book and Rae's book provide the standard discussion. Shankar's book (higher level than our courses intended to be) has a discussion using wave packets. Well beyond the level of our course, *Quantum Theory of Tunnelling* by Razavy gives a 550-page discussion on the topics. For textbook chapters on nuclear physics, read for example Chapters 13 and 14 of *Modern Physics* by Serway *et al.*, and TDZ Chapters 16 and 17 of *Modern Physics for Scientists and Engineers* by Taylor *et al.*. They cover the standard undergraduate nuclear physics contents (some of which you met in PHYS1122). Two other books are reserved in the University Library specifically for nuclear physics. They are: A pictorial book with clear descriptions (but no equations) entitled *Nucleus - A trip to the heart of matter* by MacKintosh *et a;.* and a standard textbook on nuclear and particle physics entitled *Nuclear and Particle Physics* by Williams.

Part A: Standard Problems on Molecular Spectrum

7.1 **(See class notes: rotational spectrum.)** The microwave spectrum of KI (to be specific, ^{39}K^{127}I) consists of a series of lines whose spacing is almost constant at 3634 MHz. **Calculate the bond length** of ^{39}K^{127}I. [Hint: Think like a physicist! You should get used to the following way of approaching a problem: (i) In which range does the frequency belong to? (ii) What leads to a series of equally spaced lines? (iii) Which kind of excitation/transitions will that be? (iv) What is the physical parameters involved in such excitation?]

Sometimes (quite often, actually), the spacing is expressed in terms of a number called the **rotational constant** of a molecule. In units of Hz, the spacing is given by $2B$. However, it is also given in units of cm^{-1} (wavenumber). In this case, the spacing is given by $2\overline{B}$. **Find an expression** for B and $\overline{B}$ (they represent the same quantity only in different units). Hence, **find** B and $\overline{B}$ for ^{39}K^{127}I.

7.2 Consider the molecules HCl and DCl, where D denotes the deuterium (a heavier isotope of hydrogen) atom.

(a) **Explain why** the force constant k and bond length R_0 should be about the same for DCl as for HCl. [Hint: Think about the reason of bonding.]

(b) Adjacent vibrational levels in HCl are separated by $\hbar\omega_c \approx 0.37$ eV. **Estimate** the corresponding value in DCl?

7.3 (Revised) Consider the molecule ^{6}LiF. The bond has an equilibrium separation (bond length) of $R_0 = 1.56 \times 10^{-10}$ m and a spring constant $k = 250$ N·m^{-1}.

(a) **Sketch (taking into consideration of the given numbers)** an energy-level diagram showing the first five rotational levels in the $n = 0$ and $n = 1$ vibrational states.

(b) **Illustrate by arrows** in the sketch in part (a) the allowed transitions in an IR absorption experiment between the rotational levels in $n = 0$ and the rotational levels in $n = 1$.

(c) Hence, **illustrate** how the vibrational-rotational spectrum will look like by a sketch and **mark** some key features with numbers.

Part B: Probability Current Density and Standard Tunnelling Problems

7.4 **Probability current density**

The Probability Current Density $\vec{J}$ is generally given by

$$\vec{J} = \frac{\hbar}{2mi}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) \qquad (1)$$

where Ψ is the shorthand notation of $\Psi(\vec{x},t)$.

(a) For the wavefunction

$$\Psi(\vec{x},t) = A\; e^{i\vec{k}\cdot\vec{x}-i\omega t} + B\; e^{-i\vec{k}\cdot\vec{x}-i\omega t} \qquad (2)$$

evaluate the probability current density starting from the definition. [Recall that the gradient of Ψ is a vector.]

(b) For the wavefunction

$$\psi(\vec{x}) = |\psi(\vec{x})| \, e^{i\delta(\vec{x})} \tag{3}$$

where $\delta(\vec{x})$ is a phase that has **spatial dependence**, **calculate** the probability current density.

7.5 Tunnelling through a single barrier - Filling in the steps

(a) Read class notes on tunnelling through a potential barrier. Some steps are missing in the mathematics when we solved for the transmission coefficient $T(E)$ and reflection coefficient $R(E)$ for $E < U$. Here, we will fill in the steps. **Set up** the equations and **fill in the steps to solve** for $T(E)$ and $R(E)$ **separately**. [Meaning: Don't use $R + T = 1$, solve R and T separately.] Hence, **obtain** $R + T$ from your results.

(b) **Turn your answer** for $T(E)$ into one for the case of $E > U$.

(c) **What is** $T(E)$ when it is NOT a potential energy barrier with $U > 0$ but a potential energy well with $U < 0$ instead?

[Remarks: If you have done the EM problems of EM waves incident normally (analogous to our 1D problem) onto a slab of medium of thickness L, you will see an analogous answer to part (b) for the air-slab-air system. Part (c) is like a medium-air-medium system. The Quantum Mechanical version of the water-glass-air problem is that of a single barrier with the V on each side being different.]

Part C: Some Essential Nuclear Physics

7.6 Binding Energy and Binding Energy per Nucleon

Estimate the binding energy and the **binding energy per nucleon** of a helium nucleus based on the missing mass. We may use data of atomic mass of helium, etc. from textbooks e.g., Appendix B of SMM (Serway *et al.*, Modern Physics) or from websites. Cite the source of the numbers in your answer.]

7.7 Mass of force carrier and range of interaction.

Experimental (scattering) results point to a rather uniform mass density inside the nucleus. Thus, there is some preferred separation between two neighboring nucleons. If we are to interpret the result by a repulsive interaction that prevents two nucleons from getting too close, say 10^{-17} m, to each other, **what** would the mass of the carrier of this repulsive interaction be?

7.8 Fermi gas model of nuclei illustrated in 1D and degenerate pressure due to many non-interacting (independent) fermions.

When we invoke the independent particle model for a many-nucleon nucleus, we first solve a single-nucleon in a well problem and then fill in the protons/neutrons according to the Pauli Exclusion Principle as protons/fermions are fermions. This is the Fermi gas model. The Fermi gas model is very useful, as it can be applied to nuclei (10^{-14} m scale), metals (1 cm scale), and stars (astronomical scale).

To illustrate the key physics, let's work on the 1D version of the model. Consider 1D particle-in-a-box of size L. The single-particle states are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \tag{4}$$

Let's say there are $\mathcal{N} \gg 1$ spin-half fermions and they are non-interacting. So the question is to fill them into the states according to the Pauli Exclusion Principle. [If you are very strict, yes take $\mathcal{N}$ to be an even number.] [Remark: Even if we ignore the fermions' spin – the results to be obtained remains the same qualitatively.]

(a) With the single-particle states, we fill in the fermions to achieve the ground state. Eventually we run out of fermions. There is a highest state labelled by n_{max} that is filled. All states above it are empty and all below it are filled. The highest energy filled is called the **Fermi energy** E_F, after the famous Enrico Fermi. **Find** a relation between the Fermi energy E_F and the ratio $(\mathcal{N}/L)$. [Remark: Note that $\mathcal{N}/L$ has the following physical meaning. There are $\mathcal{N}$ fermions in the box of size L. Thus, $\mathcal{N}/L \equiv \rho$ is the number of particles per unit length or the (linear) particle number density. It is a property of the system.]

(b) The result in part (a) says that E_F remains the same as long as $\mathcal{N}/L$ is a constant. For example, a certain metal (e.g. copper) wire (pretending to be 1D) has 10^7 electrons per cm. Then for wires of 2m long and 1 millimeter "short", they have the same E_F. For this metal, **find** the Fermi energy E_F in units of eV. Hence, **find** a corresponding temperature $T_F = E_F/k$, where k is the Boltzmann constant. The quantity is called the Fermi temperature.

(c) But we know from Eq. (1) that if we double the size L of the well, the single-particle energies drop! **Give a physical picture** why E_F can be maintained fixed when a system is doubled in size (L to $2L$, say).

(d) Thus, **argue** that the **total energy** E_{tot} is proportional (actually smaller than) to $\mathcal{N}E_F$.

(e) (Optional: NO bonus) Try to derive E_{tot} exactly and express the answer in terms of E_F and N.

(f) If we now squeeze the box a bit so that the length becomes $L - \Delta L$, **find** out how the energy changes. In analogy to the idea of a pressure, $-\partial E_{tot}/\partial L$ corresponds to a pressure (in 1D). **How** does this "pressure" scale with the number density $\rho = \mathcal{N}/L$ in 1D.

Important Remarks: Although the number of protons/neutrons in a nucleus is just a few tens, the basic results here are valid. In part (e), you see the famous **degenerate pressure** due to a **gas of fermions**. The fermions need not be interacting. The resulting pressure is entirely a quantum effect due to the Pauli Exclusion Principle (anti-symmetric wavefunction). A collection of fermions confined in a box (1D here) leads to a pressure against squeezing the box. Note that we only considered $T = 0$ ground state physics here. Even so, the pressure is there. In astrophysics, the gravitation force tends to squeeze a dying star and yet the fermions inside it exerts an opposing pressure against the pull due to gravity. Depending on the mass of the star, sometimes a balance can be achieved. In some cases, gravity will win though. Similarly, the degenerate pressure is there in a neutron star. You will learn more about Fermi gas and Bose gas in your Thermodynamics and Statistical Physics course.

3D Fermi gas: If we do this exercise in 3D, we will get

$$E_{tot} \propto \mathcal{N}E_F \propto \mathcal{N}\left(\frac{\mathcal{N}}{V}\right)^{2/3}, \tag{5}$$

when $\mathcal{N}$ identical fermions are confined in a box of volume V, where $V = L^3$. You need not work this out. But you should know the result and carry it to future courses on solid state physics, astrophysics, and statistical mechanics.