量子化学作业 第一章（2017-2018 学期）

1-4. Planck's principal assumption was that the energies of the electronic oscillators can have only the values $E = nh\nu$ and that $\Delta E = h\nu$. As $\nu \to 0$, then $\Delta E \to 0$ and E E is essentially continuous. Thus, we should expect the non-classical Planck distribution to go over to the classical Rayleigh-Jeans distribution at low frequencies, where $\Delta E \to 0$. Show that Equation 1.2 reduces to Equation 1.1 as $\nu \to 0$. (Recall that $e^x = 1 + x + (x^2/2!) + \cdots$, or, in other words, that $e^x \approx 1 + x$ when x is small.)

1-7. Sirius, one of the hottest known stars, has approximately a blackbody spectrum with $\lambda_{\max} = 260nm$. Estimate the surface temperature of Sirius.

1-9. We can use the Planck distribution to derive the Stefan- Boltzmann law, which gives the total energy density emitted by a blackbody as a function of temperature. Derive the Stefan-Boltzmann law by integrating the Planck distribution over all frequencies. Hint: You'll need to use the integral: $\int_0^\infty dx\, x^3/(e^x - 1) = \pi^4/15$

1-10. Can you derive the temperature dependence of the result in Problem l- 9 without evaluating the integral?

1-18. The threshold wavelength for potassium metal is 564 nm. What is its work function? What is the kinetic energy of electrons ejected if radiation of wavelength 410 nm is used?

1-20. When a clean surface of silver is irradiated with light of wavelength 230 nm, the kinetic energy of the ejected electrons is found to be 0.805 eV. Calculate the work function and the threshold frequency of silver.

1-22. Show that Planck's constant has dimensions of angular momentum.

1-30. Calculate the reduced mass of a nitrogen molecule in which both nitrogen atoms have an atomic mass of 14.00. Do the same for a hydrogen chloride molecule in which the chlorine atom has an atomic mass of 34.97. Hydrogen has an atomic mass of 1.008.

1-32. Derive the Bohr formula for $\tilde{v}$ for a nucleus of atomic number Z.

1-35. Show that the speed of an electron in the nth Bohr orbit is $v = e^2 / 2\varepsilon_0 nh$. Calculate the values of v for the first few Bohr orbits.

1-40. Through what potential must a proton initially at rest fall so that its de Broglie wavelength is $1.0 \times 10^{-10} m$?

1-42. One of the most powerful modern techniques for studying structure is neutron diffraction. This technique involves generating a collimated beam ofneutrons at a particular temperature from a high-energy neutron source and is accomplished at several accelerator facilities around the world. If the speed of a neutron is given by $v_n = (3k_B T / m)^{1/2}$, where m is the mass of a neutron, then what temperature is needed so that the neutrons have a de Broglie wavelength of 50 pm?

MATHCHAPTER A

A-4. Express the following complex numbers in the form $x+iy$:

(a) $e^{\pi/4i}$ (b) $6e^{2\pi i/3}$

(c) $e^{-(\pi/4)i+\ln 2}$ (d) $e^{-2\pi i}+e^{4\pi i}$

A-7. Use Equation A.6 to derive

$$z^n = r^n(\cos\theta + i\sin\theta)^n = r^n(\cos n\theta + i\sin n\theta)$$

and from this, the formula of de Moivre:

$$(\cos\theta + i\sin\theta)^n = \cos n\theta + i\sin n\theta$$

A-9. Consider the set of functions

$$\Phi_{\mathrm{m}}(\varphi) = \frac{1}{\sqrt{2\pi}}e^{im\varphi} \begin{cases} m = 0, \pm 1, \pm 2, \ldots \\ 0 \le \varphi \le 2\pi \end{cases}$$

First show that

$$\int_0^{2\pi} d\varphi\, \Phi_m(\varphi) = \begin{cases} 0 & \text{for all values of } m \neq 0 \\ \sqrt{2\pi} & m = 0 \end{cases}$$

Now show that

$$\int_0^{2\pi} d\varphi\, \Phi^*{}_m(\varphi)\, \Phi_n(\varphi) = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases}$$

A-16. The Schwartz inequality says that $z_1 = x_1 + iy_1$ and $z_2 = x_2 + iy_2$, then $x_1x_2 + y_1y_2 \le |z_1||z_2|$. To prove this inequality, start with its square:

$$(x_1x_2 + y_1y_2)^2 \le |z_1|^2 |z_2|^2 = (x_1^{\,2} + y_1^{\,2})(x_2^{\,2} + y_2^{\,2})$$

Now use the fact that $(x_1y_2 - x_2y_1)^2 \ge 0$ to prove the inequality.

A-17. The triangle inequality says that if z_1 and z_2 are complex numbers, then $|z_1 + z_2| \le |z_1| + |z_2|$. To prove this inequality, start with:

$$|z_1 + z_2|^2 = (x_1 + x_2)^2 + (y_1 + y_2)^2 = x_1^{\,2} + y_1^{\,2} + x_2^{\,2} + y_2^{\,2} + 2x_1x_2 + 2y_1y_2$$

Now use the Schwartz inequality (previous problem) to prove the inequality. Why do you think this is called the triangle inequality