

Quantum Physics(量子物理) 習題 Robert Eisberg (Second edition) CH 07: One-electron atoms

7-01 \cdot Using the technique of separation of variable, show that there are solutions to the three-dimensional Schröedinger equation for a time-independent potential, which can be written $\Psi(x, y, z, t) = \psi(x, y, z)e^{\frac{iEt}{\hbar}}$ where $\psi(x, y, z)$ solution to the time-independent Schröedinger equation. <P> The time-dependent equation is $-\frac{\hbar^2}{2\mu}(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}) + V_{\mu}$ Let $\Psi(x, y, z, t) = \psi(x, y, z)T(t)$ Putting this into the first equation gives $-\frac{\hbar^2}{2\mu}T(t)(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}) + V(x, y, z)\psi(x, y, z)T(t) = i\hbar\psi(x, y, z)\frac{dT}{dt}$ Assuming that V does not depend on t explicitly Dividing the above by the wave function yields $-\frac{\hbar^2}{2\mu}\frac{1}{\psi}(\nabla^2\psi) + V = \frac{1}{2\mu}\frac{dT}{dt} = constant = E$ There are two equation: $\nabla^2 \psi \psi = 0$ For the space dependent part of the wave function, and $\frac{i\hbar}{T}\frac{dT}{dt} = E \; ; \; \frac{dT}{dt} = E \; ; \; \frac{dT}{dt} = -\frac{iE}{\hbar}dt \; ; \; T = e^{-\frac{iEt}{\hbar}}$ For the time dependent part.....## 7-02 Verify that $\Phi(\varphi) = e^{im_i\varphi}$ is the solution to the equation for $\Phi(\varphi)$, (7-15).

7-03 • Hydrogen, deuterium. And singly ionized helium are all examples of one-electron atoms. The deuterium nucleus has the same charge as the hydrogen nucleus, and almost exactly twice the mass. The helium nucleus has twice the charge of the hydrogen nucleus, and almost exactly four times the mass. Make an accurate prediction of the ratios of the ground state energies of these atoms. (Hint : Remember the variation in the reduced mass.)

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<解>:

7-04 \cdot (a) Evaluate, in electron volts, the energies of the three levels of the hydrogen atom in the states for n = 1, 2, 3. (b) Then calculate the frequencies in hertz, and the wavelengths in angstroms, of all the photons that can be emitted by the atom in transitions between these levels. (c) In what range of the electromagnetic spectrum are these photons?

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7-05 • Verify by substitution that the ground state eigenfunction E_{100} , and the ground state eigenvalue E_1 , satisfy the time-independent Schroedinger equation for the hydrogen atom.

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 $7-06 \cdot$ (a) Extend Example 7-4 to obtain from the uncertainty principle a predication of the total energy of the ground state of the hydrogen atom. (b) Compare with the energy predicted by (7-22).

<解>:

(b) $5a_0$

7-07 · (a) Calculate the locating at which the radial probability density is a maximum for the n=2, l=1 state of the hydrogen atom. (b) Then calculate the expectation value of the radial coordinate in this state. (c) Explain the physical significance of the difference in the answer to (a) to (b). (Hint : See Figure 7-5.) <##>: (a) $4a_0$

7-08 \cdot (a) Calculate the expectation value \overline{V} for the potential energy in the ground state





of the hydrogen atom. (b) Show that in the ground state $E = \frac{\overline{V}}{2}$, where *E* is the total energy. (c) Use the relation E = K + V to calculate the expectation value \overline{K} of the kinetic energy in the ground state, and show that $\overline{K} = -\frac{\overline{V}}{2}$. These relations are obtained for any state of motion of any quantum mechanical (or classical) system with a potential in the form $V(r) \propto -\frac{1}{r}$. They are sometimes called the virial theorem.

<解>:

- 7-09 \cdot (a) Calculate the expectation value \overline{V} of the potential energy in the n=2, l=1 state of the hydrogen atom. (b) Do the same for the m=2, l=0 state. (c) Discuss the results of (a) and (b), in connection with the virial theorem of Problem 8, and explain how they bear on the origin of the *l* degeneracy.
- < $# < : (a) 2E_2$ (b) $2E_2$
- 7-10 Bt substituting into the equation for R(r), (7-17), the form $R(r) \propto r^{l}$, show that it is a solution for $r \rightarrow 0$. (Hint : Ignore terms that become negligible relative to others as $r \rightarrow 0$.)

$$l(l-1)r^{l-2} + \frac{2\mu}{\hbar^2} \{Er^l - Vr^l\}^2 = l(l+1)r^{l-2}$$

Now E is a constant independent of r, and $V = \frac{k}{r}$; thus the two terms in $\{\}$ are proportional to r^{l} , r^{l-1} . As r approaches zero, $r^{l-2} >> r^{l}$, r^{l-1} ; hence, $\{\} \rightarrow 0$, and the equation is satisfied.....##





7-11 • Consider the probability of finding the electron in the hydrogen atom somewhere inside a cone of semiangle 23.5° of the +z axis ("arctic polar region"). (a) If the electron were equally likely to be found anywhere in space, what would be the probability of finding the electron in the arctic polar region? (b) Suppose the atom is in the state n = 2, l = 1, $m_l = 0$; recalculate the probability of finding the electron in the arctic polar region.

<解>:(a) 4.147% (b) 11.44%



7-12 \cdot (a) Sketch a polar diagram of the directional dependence of the one-electron atom probability density for l = 2, $m_l = 0$. (b) At what angle θ does the angular probability density have its minimum value? (c) Where does the angular probability density have a value one-fourth its maximum value?

<解>:(a)







7-13 \cdot Consider the hydrogen atom eigenfunction ψ_{432} . What are (a) the total energy in eV; (b) the expectation value of the radial coordinate in Å; (c) the total angular momentum; (d) the z component of the angular momentum; (e) the uncertainty in the angular momentum; (f) the uncertainty in the z component of the angular momentum?

<解>:(a) -0.85eV

- (b) 9.52Å
- (c) 3.46ħ
- (d) 2ħ
- (e) zero
- (f) zero
- 7-14 \cdot Show that the sum of hydrogen atom probability densities for the n=3 quantum states, analogous to the sum in Example 7-5, is spherically symmetrical.
- <解>:
- 7-15 Show that $\Phi(\varphi) = \cos m_l \varphi$, and $\Phi(\varphi) = \sin m_l \varphi$, are particular solutions to the equation for $\Phi($

<解>:

Evaluate $L_{x_{op}}\psi_{21-1}$ for the hydrogen atom. (b) Why does the result indicate

that ψ_{21-1} is not an eigenfunction of $L_{x_{op}}$?

(a)
$$L_{x_{op}} = i\hbar(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi})$$

$$\psi_{21-1} = \frac{1}{8\sqrt{\pi}} a_0^{-\frac{5}{2}} r e^{-\frac{r}{2}a_0} \sin \theta e^{-i\phi}$$

第5頁/ 與10頁





$$\frac{\partial \psi_{21-1}}{\partial \theta} = \psi_{21-1} \cot \theta ; \quad \frac{\partial \psi_{21-1}}{\partial \phi} = -i\psi_{21-1}$$

Therefore, $L_{x_{op}}\psi_{21-1} = \hbar(i\cot\theta\sin\phi + \cot\theta\cos\phi)\psi_{21-1}$

$$L_{x_{1}}\psi_{21-1} = \hbar \cot \theta (\cos \phi + i \sin \phi)\psi_{21-1} = \hbar \cot \theta e^{i\phi}\psi_{21-1}$$

(b) This result cannot be put into the form $L_{x_{op}}\psi_{21-1} = C\psi_{21-1}$, with C

independent of $r, \theta, \phi \dots \#$

7-17 • Prove that $L_{op}^2 \psi_{nlm_l} = l(l+1)\hbar^2 \psi_{nlm_l}$. (Hint : Use the differential equation satisfied

by $\Theta_{lm_l}(\theta)$,(7-16).)

 $< || = 1 + 2^{2} \{r^{2} \nabla^{2} - \frac{\partial}{\partial r}(r^{2} - \frac{\partial}{\partial r})\}$ $< || = 1 + 2^{2} \{r^{2} \nabla^{2} - \frac{\partial}{\partial r}(r^{2} - \frac{\partial}{\partial r})\}$ $<math>
 < || = 1 + 2^{2} \{r^{2} \nabla^{2} - \frac{\partial}{\partial r}(r^{2} - \frac{\partial}{\partial r})\}$

But
$$\frac{\partial}{\partial r}(r^2 \frac{\partial \psi}{\partial r}) = \theta \phi \frac{d}{dr}(r^2 \frac{dR_3}{dr}) + \theta \phi \{l(l+1)R - \frac{2\mu}{\hbar^2}(E-V)Rr^2\}$$

 $\frac{d}{dr} + 2\frac{d\psi}{dr} = 10$

 $\frac{1}{dr} (r^2 - \frac{r}{dr}) = l(l+1)\psi^2 + \frac{r}{\hbar^2} (E-V)r^2 \psi$ By Eq. 7-17. Schreodinger's equation is $\nabla^2 \psi = \frac{2\mu}{\hbar^2} (V-E)\psi$

Substituting these last two results into the expression for L_{op}^2 gives

$$L_{op}^{2}\psi = l(l+1)\hbar^{2}\psi \dots \#$$

7-18 • We know that $\psi = e^{ikx}$ is an eigenfunction of the total energy operator e_{op} for the one-dimensional problem of the zero potential. (a) Show that it is also an eigenfunction of the linear momentum operator p_{op} , and determine the associated momentum eigenvalue. (b) Repeat for $\psi = e^{-ikx}$. (c) Interpret what the results of (a) and (b) mean concerning measurements of the linear

第6頁/袋10頁





momentum. (d) We also know that $\psi = \cos kx$ and $\psi = \sin kx$ are eigenfunctions of the zero potential e_{op} . Are they eigenfunctions of p_{op} ? (e) Interpret the results of (d).

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7-19 · All four of the function $e^{im_l\varphi}$, $e^{-im_l\varphi}$, $\cos m_l\varphi$ and $\sin m_l\varphi$ are particular solutions to the equation for $\Phi(\varphi)$, (7-15)(see Problem 15). (a) Find which are also eigenfunctions of the operator for the z component of angular momentum

 $L_{z_{op}}$. (b) Interpret your results.

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7-20 • A particle of mass μ is fixed at one end of a figid rod of negligible mass and length R. The other end of the rod notates in the x-y plane about a bearing located at the origin, whose taxts is in the z direction. This two-dimensional "rigid rotator" is illustrated in Figure 7-13. (a) Write an expression for the total energy of the system in terms of its angular momentum L. (Hint : Set the constant potential energy equal to zero, and then express te kinetic energy in term of L.) (b) By differentiate the appropriate operators into the energy equation, convert it into the Schroedinger equation $-\frac{\hbar^2}{2I}\frac{\partial^2\Psi(\varphi,t)}{\partial\varphi^2} = i\hbar\frac{\partial\Psi(\varphi,t)}{\partial t}$ where $I = \mu R^2$ is the rotational inertia, or moment of inertia, and $\Psi(\varphi,t)$ is the wave function written in terms of the angular coordinate φ and the time t. (Hint : Since the angular momentum is entirely in the z direction, $L = L_z$ and the corresponding operator is $L_{z_{op}} = -i\hbar\frac{\partial}{\partial\varphi}$.)







Figure 7-13 The rigid rotator moving in the x-y plane considered in Problem 20

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7-21 · By applying the technique of separation of variables, split the rigid rotator Schroedinger equation of Problem 20 to obtain $\Psi(a)$ the time-independent Schroedinger equation $-\frac{\hbar^2}{2I}\frac{d^2\Phi(\varphi)}{d\varphi^2} = E\Phi(\varphi)$ and (b) the equation for the time dependence of the wave function $\frac{dT(t)}{dt} = -\frac{iE}{\hbar}T(t)$. In these equation E = the separation constant, and $\Phi(\varphi)T(t) = \Psi(\varphi, t)$, the wave function.

$$\langle \widehat{\mathbf{H}} \rangle$$
: Let $\Psi(\phi, t) = \Phi(\phi)T(t)$

Substitute this into the energy equation of Problem 7-20(b) and divide by Ψ to obtain
 $-\frac{\hbar^2}{2t}T\frac{d}{d\phi^2}\Phi = i\hbar\Phi\frac{dT}{dt};
-\frac{\hbar^2}{2I}\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = i\hbar\frac{1}{T}\frac{dT}{dt} = E$

Where E is the separation constant. Thus two equations emerge:

(a)
 $\frac{\hbar^2}{2T}\frac{d^2\Phi}{d\phi^2} = E\Phi$
and

Where $E T;$
 $\frac{dT}{dt} = ET;$
 $\frac{dT}{dt} = \frac{E}{i\hbar}T = -\frac{iE}{\hbar}T \dots \#$

 $7-22 \cdot (a)$ Solve the equation for the time dependence of the wave function obtained in Problem 21. (b) Then show that the separation constant *E* is the total energy.

<\vec{FP}< : (a) From the preceding problem, $\frac{dT}{dt} = -\frac{iE}{\hbar}T$; $\frac{dT}{T} = -\frac{iE}{\hbar}dt$; $T = e^{-\frac{iEt}{\hbar}}$ The normalization constant will be incorporated into ϕ .

第8頁/袋10頁





- (b) The solution above represents an oscillation of frequency ω given by E = ħω. But this the de Broglie-Einstein relation. Hence E is the total energy.....##
- 7-23 Show that a particular solution to time-independent Schroedinger equation for the

rigid rotator of Problem 21 is $\Phi(\varphi) = e^{im\varphi}$ where $m = \frac{\sqrt{2IE}}{\hbar}$.

<P>First Problem 7-21(a): $\frac{d^2 \Phi}{d\phi^2} + \frac{2IE}{\hbar^2} \Phi = 0$

This is analogous to the classical simple harmonic oscillator equation

$$\frac{d^2x}{dt^2} + \omega^2 x = 0$$

The complex forms of the solution will therefore be

$$\Phi = c e^{im\phi} + c^* e^{-im\phi}, \quad m = \frac{\sqrt{2IE}}{\hbar}$$

7-24 \cdot (a) Apply the condition of single valuedness to the particular solution of Problem 23. (b) Then show that the allowed values of the total energy E for the two-dimensional quantum mechanical rigid rotator are $E = \frac{\hbar^2 m^2}{2I}$ |m| = 0, 1, 2, 3, ... (c) Compare the results of quantum mechanics with those of the old quantum theory obtained in Problem 42 of Chapter 4. (d) Explain why the two-dimensional quantum mechanical rigid rotator has no zero-point energy. Also explain why it is not a completely realistic model for a microscope system.

7-25 • Normalize the functions $\Phi(\varphi) = e^{im\varphi}$ found in Problem 24.

<解>: The complete wave function is, from the preceding problems, $\Psi = Ne^{im\phi}e^{\frac{iEt}{\hbar}}$ The wavefunction must be normalized at any time t: thus, $\int \Phi^* \Phi d\phi = 1$

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$$1 = \int_{0}^{2\pi} (N^* e^{-im\phi}) (N e^{im\phi}) d\phi = N^* N(2\pi)$$
$$\implies N^* N = \frac{1}{2\pi} \dots \# \#$$

7-26 \cdot (a) Calculate the expectation value of the angular momentum, \overline{L} , for two-dimensional rigid rotator in a typical quantum state, using the eigenfunctions found in Problem25. (b) Then calculate $\overline{L^2}$ and \overline{L}^2 , and interpret what your results have to say about the values of L that would be obtained in a series of measurements on the system. <P> Use $\Phi = (2\pi)^{-1/2} e^{im\phi}; L_z = -i\hbar \frac{\partial}{\partial \phi}$ $d\phi = \frac{m\hbar}{2\pi} \int_{0}^{2\pi} d\phi$ (a) $\overline{L} = \int_{0}^{2\pi} \Phi^*(-i\hbar \frac{\partial \Phi}{\partial \phi}) d\phi = -\frac{i\hbar}{2\pi} \int_{0}^{2\pi} e^{-im\phi}(im) e^{i\phi}$ $\overline{L} = m\hbar$ (b) $\overline{L}^2 = \frac{1}{2\pi} \int_0^{2\pi} e^{-im\phi}$ $d\phi = m^2 \hbar^2$ Also, from (a) $(L^2 = m^2 \hbar^2)$, measurements of L_z will yield $m\hbar$ exactly.....## Since

