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UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part I

[1] A massless spring of zero unstretched length and spring constant k connects particles with masses m_1 and m_2. The whole system rests on a frictionless table. The masses are free to move in x and y on the table.

(a) Write the Lagrangian for the system choosing a set of coordinates which are optimized to have the most cyclic coordinates.

(b) What are the generalized momenta associated with the cyclic coordinates?

(c) Write the Hamiltonian for the system using the same coordinates.

(d) Determine Hamilton's equations of motion.

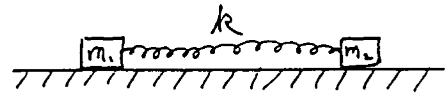
(e) Reduce the problem to a single differential equation in one variable plus conserved momenta.

1

PROBLEM ~~(3)~~ 2 (15 points)

A massless spring of unstretched length b and spring constant k connects particles with masses m_1 and m_2. The whole system rests on a frictionless table. The masses are free to move in x and y on this table.

a) Write the Lagrangian for the system in any set of coordinates. How many coordinates are needed to describe the system.



$$L = T - U = \overset{+1}{\tfrac{1}{2} m_1 (\dot{x}_1^2 + \dot{y}_1^2)} + \overset{+1}{\tfrac{1}{2} m_2 (\dot{x}_2^2 + \dot{y}_2^2)}$$

$$- \tfrac{1}{2} k \Big[\overset{+1}{\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}} - b\Big]^2$$

b) Now write the Lagrangian for the system choosing a set of generalized coordinates which are optimized to have the most cyclic coordinates. (A coordinate q is cyclic if $\frac{\partial L}{\partial q} = 0$.)

$$L = \overset{+1}{\tfrac{1}{2} \underbrace{(m_1 + m_2)}_{M} (\dot{X}_{cm}^2 + \dot{Y}_{cm}^2)} + \overset{+1}{\tfrac{1}{2} \underbrace{\frac{m_1 m_2}{m_1 + m_2}}_{\mu} (\dot{r}^2 + r^2 \dot{\theta}^2)} - \overset{+1}{\tfrac{1}{2} k (r - b)^2}$$

$$r = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

$$\tan\theta = \frac{(y_1 - y_2)}{(x_1 - x_2)} \quad = \quad X_{cm}, Y_{cm}, \theta \text{ are cyclic}$$

c) What are the generalized momenta associated with the cyclic coordinates?

$$P_j = \frac{\partial L}{\partial \dot{q}_j} \longrightarrow \text{const. for cyclic coordinate}$$

$$P_{X_{cm}} = M \dot{X}_{cm} \quad +1$$

$$P_{Y_{cm}} = M \dot{Y}_{cm} \quad +1$$

$$P_\theta = \mu r^2 \dot{\theta} \quad +1$$

d) Write the Hamiltonian for the system using your optimized coordinates.

$$H = T + U = \frac{1}{2}M\left(\dot{X}_{cm}^2 + \dot{Y}_{cm}^2\right) + \frac{1}{2}\mu\left(\dot{r}^2 + r^2\dot{\theta}^2\right) + \frac{1}{2}kr^2$$

$$P_r = \mu\dot{r}$$

$$H = \frac{P_{xcm}^2 + P_{ycm}^2}{2M} + \frac{P_r^2}{2\mu} + \frac{P_\theta^2}{2\mu r^2} + \frac{1}{2}k(r-\cancel{b})^2$$

+1 +1 +1 +1

e) Determine Hamilton's equations of motion.

$$\dot{X}_{cm} = \frac{\partial H}{\partial P_{xcm}} = \frac{P_x}{M} \checkmark$$

$$\dot{Y}_{cm} = \frac{\partial H}{\partial P_{ycm}} = \frac{P_y}{M} \checkmark$$

$$\dot{\theta} = \frac{\partial H}{\partial P_\theta} = \frac{P_\theta}{\mu r^2} \checkmark$$

$$\dot{r} = \frac{\partial H}{\partial P_r} = \frac{P_r}{\mu} \checkmark$$

$$\left.\begin{aligned} \dot{P}_{xcm} &= \frac{-\partial H}{\partial X_{cm}} = 0 \Rightarrow P_{xcm} = \text{const} \\ \dot{P}_{ycm} &= \frac{-\partial H}{\partial Y_{cm}} = 0 \Rightarrow P_{ycm} = \text{const} \\ \dot{P}_\theta &= \frac{-\partial H}{\partial \theta} = 0 \Rightarrow P_\theta = \text{const.} \end{aligned}\right\} +$$

$$\dot{P}_r = \frac{-\partial H}{\partial r} = \frac{+P_\theta^2}{\mu r^3} - k(r-\cancel{b})$$

$$\Rightarrow \boxed{\mu\ddot{r} = \frac{P_\theta^2}{\mu r^3} - k(r-\cancel{b})} +1$$

equation of motion in r

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UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part I

[2] An interstellar mission is sent from earth to a solar system which is at a distance of 20 light years from the earth. The spaceship is rapidly accelerated to a velocity (relative to the earth) of $0.99c$ toward its objective. Upon reaching the distant solar system, the crew takes some pictures as the ship is rapidly accelerated to $0.99c$ heading back toward the earth. The pictures are immediately transmitted by radio to those waiting on earth.

(a) How long does the round trip take according to people waiting on earth?

(b) How long does the round trip take for people on the spaceship?

(c) After how many years since takeoff do the people on earth see the first pictures from the distant solar system?

(d) In those pictures, they see the wonders of the distant solar system as well as the clocks on the spaceship. What time do those clocks read (in years)?

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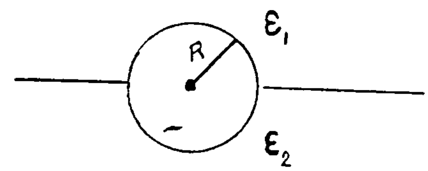
DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part I

[3] The center of a conducting sphere of radius R resides on a plane that is the interface between two large dielectric slabs (see figure). The upper slab is characterized by dielectric constant ϵ_1 and the lower by dielectric constant ϵ_2, and both slabs are very thick compared to R. Given that the total charge on the sphere is Q, determine the electric field in the vicinity of the sphere.



2

2

PROBLEM ~~4~~ 2 (10 points)

A spaceship is sent from earth to another solar system which is at a distance of 20 light years from the earth. The spaceship is rapidly accelerated to a velocity (relative to the earth) of 0.99c toward its objective. Upon reaching the distant solar system, the crew takes some pictures as the ship is rapidly accelerated to 0.99c heading back toward the earth. The pictures are immediatly transmitted by radio to those waiting on earth.

1

a) How long does the round trip take according to people waiting on earth?

$$t = \frac{40}{.99} \approx 40.4 \text{ years}$$

3

b) How long does the round trip take for people on the spaceship?

$$\gamma = \frac{1}{\sqrt{1-(.99)^2}} \approx \frac{1}{\sqrt{.02}} \approx \frac{1}{.14}$$

$$\ell' = \ell/\gamma = .14\,\ell$$

$$t' = (.14)(40)/.99 = (40.4)(.14) = 5.7 \text{ years}$$

3

c) After how many years since takeoff do the people on earth see the first pictures from the distant solar system.

$$t = \frac{20}{.99} + 20 = 40.2 \text{ years}$$

3

d) In those pictures, they see the wonders of the distant solar system as well as the clocks on the the spaceship. What time do those clocks read (in years)? Show that this is consistent with the Doppler shifted clock frequency.

$$\text{time} = \frac{5.7}{2} \text{ years} \approx 2.8 \text{ y.}$$

$$\nu = \sqrt{\frac{1-\beta}{1+\beta}}\,\nu_0 = \sqrt{\frac{.01}{1.99}}\,\nu_0 = \frac{\nu_0}{10\sqrt{2}} \approx \frac{\nu_0}{14}$$

$$\text{time} = \frac{40.2 \text{ y}}{14} \approx 2.8 \text{ y}$$

(3)

Sol'n

boundary conditions

E_t vanish on sphere and be continuous at interfaces

D_n be continuous at interfaces

Also require $\nabla^2\phi = 0$, in each dielectric.

These conditions are satisfied by radial electric field

$$\underline{E} = \frac{Q'}{r^2}\hat{r}$$

charge on sphere is given by

$$4\pi Q = \int \underline{D}\cdot d\underline{S} = \frac{Q'}{R^2}\left[\epsilon_1 2\pi R^2 + \epsilon_2 2\pi R^2\right]$$

$$\therefore Q = Q'\left(\frac{\epsilon_1+\epsilon_2}{2}\right)$$

$$\therefore \underline{E} = \frac{2Q}{(\epsilon_1+\epsilon_2)}\frac{\hat{r}}{r^2}$$

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UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part I

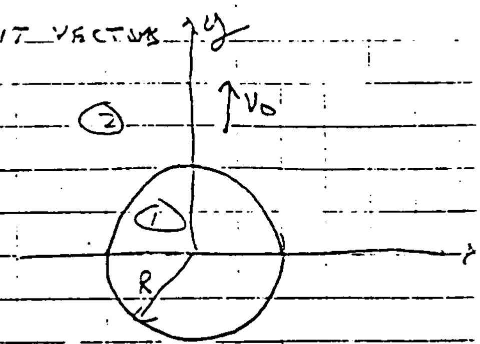
[4] A thin conducting sheet of thickness t and conductivity g moves with a constant speed v between the poles of a magnet. The magnet makes a uniform field B perpendicular to the sheet over a circular area of radius R. Calculate the electric field, the current density j, and hence the drag force on the sheet. This is the basis of the eddy current damping used in many applications such as chemical beam balances.

Note: Let the velocity be in the y direction and the magnetic field B be in the z direction. The problem is two dimensional, best solved in cylindrical coordinates. Ignore the field made by currents in the conducting sheet.

4

TAKE $\vec{v} = V_0 \hat{j}$ $\quad$ $\hat{i},\hat{j},\hat{k}$ UNIT VECTORS

$\vec{B} = B_0 \hat{k}$



THEN $\vec{v}\times\vec{B} = V_0 B_0 \hat{i}$

$\nabla\cdot\vec{j} = 0$

$$\vec{j} = g(\vec{E}+\vec{v}\times\vec{B}) = g\vec{E} \qquad r>R$$

$$= g(\vec{E}+V_0B_0\hat{i}) \qquad r<R$$

SO $\nabla\cdot\vec{E} = 0$ EXCEPT AT $r=R$

$\nabla\times\vec{E} = 0 \rightarrow \vec{E} = -\nabla\phi$

$\nabla^2\phi = 0$ EXCEPT AT $r=R$

BOUNDARY CONDITIONS AT $r=R$

j_r IS CONTINUOUS $\quad$ ϕ IS CONTINUOUS

$$\phi_1 = Ar\cos\theta \qquad \phi_2 = \frac{C}{r}\cos\theta$$

$$AR\cos\theta = \frac{C}{R}\cos\theta$$

$$g(-A\cos\theta + V_0B_0\cos\theta) = g\frac{C}{R^2}\cos\theta$$

SOLVE TO GET $A = \frac{V_0B_0}{2}$ $\quad$ $C = \frac{V_0B_0R^2}{2}$

$$\phi_1 = \frac{V_0B_0}{2}r\cos\theta \qquad \phi_2 = \frac{VB_0R^2}{2r}\cos\theta$$

$$E_{r1} = -\frac{V_0B_0}{2}\cos\theta \qquad E_{r2} = \frac{V_0B_0R^2}{2r^2}\cos\theta$$

$$E_{\theta 1} = \frac{V_0B_0}{2}\sin\theta \qquad E_{\theta 2} = \frac{V_0B_0R^2}{2r^2}\sin\theta$$

$$\vec{j}_1 = \frac{gV_0B_0}{2}\hat{i} \qquad j_{r2} = \frac{gV_0B_0R^2}{2r^2}\cos\theta$$

$$j_{\theta 2} = \frac{gV_0B_0R^2}{2r^2}\sin\theta$$

$$\vec{F}_D = \int \vec{j}\times\vec{B}\,dV$$

$$= t\,\frac{gV_0B_0}{2}B_0(-\hat{j})\int da$$

$$= -\frac{1}{2}\pi R^2 t g V_0 B_0^2\,\hat{j}$$ (IN $-y$ DIRECTION)

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DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part I

[5] *Five Easy Pieces.* Each answer must be supported by reasoning.

Possibly useful information:

- 1 Rydberg $= \frac{m_e e^4}{2\hbar^2} = 13.6$ eV
- Bohr radius: $a_B = \frac{\hbar^2}{me^2} \sim 0.5$Å
- Nucleon mass $m_N \approx 2000 m_e$

(a) A proton and an electron form a bound pair with a mean distance of about 0.5 Å. Estimate the order of magnitude of their interaction energy in electron volts.

(b) A deuteron has a radius of about 1 Fermi ($= 10^{-15}$ m). Estimate the order of magnitude of the strong interaction energy of the nucleons in electron volts.

(c) An electron is trapped by an electric field on a helium surface. By means of the uncertainty principle or otherwise, deduce the electric field dependence of the electron ground state energy.

(d) Determine the degeneracy of the first excited state of a simple harmonic oscillator of frequency ω in three dimensions.

(e) Let T be the operator representing a rotation of 120° about the axis joining two possible positions of the nitrogen atom in NH_3. Clearly $T^3 = 1$. Find the eigenvalues of the operator T.

(5)

Solution L. J. Sham

1. (a) $V \sim -\frac{e^2}{a_B} \sim -\frac{me^4}{\hbar^2} \sim -30\,\text{eV}$

(b) $V \sim E \sim \frac{\hbar^2}{m_N r^2} \sim \frac{m_e}{m_N}\left(\frac{a_B}{r}\right)^2 \frac{\hbar^2}{m_e a_B^2}$

$\sim \frac{1}{2000} \times \left(\frac{10^{-10}}{2\times 10^{-15}}\right)^2 \times 30\,\text{eV}$

$\sim 10^7\,\text{eV} \sim 10\,\text{MeV}$

(c) $H = \frac{p^2}{2m} + eFx$ $\quad F$ = electric field

Energy $E \sim \frac{\hbar^2}{2m(\Delta x)^2} + eF\Delta x$

$\frac{\partial E}{\partial \Delta x} \sim -\frac{\hbar^2}{m(\Delta x)^3} + eF$

$\Delta x \propto F^{1/3}$

$E \propto F^{2/3}$

(d) $H = H_x + H_y + H_z$ $\quad H_j = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_j^2} + \frac{1}{2}m\omega^2 x_j^2$

First excited state $\Psi(x,y,z) = \psi_1(x)\,\psi_0(y)\,\psi_0(z)$ etc

$\therefore$ Degeneracy $= 3$.

(e) $T\psi = \alpha\psi$ $\quad T^3\psi = \alpha^3\psi$

$\alpha^3 = 1$

$\alpha = 1, e^{i2\pi/3}, e^{i4\pi/3}$.

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UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part I

[6] Consider a system of two non-identical particles, 1 and 2, which have the same mass μ. The potential energy of the system is given by

$$V(\vec{r}_1, \vec{r}_2) = -\frac{A}{\sqrt{r_1^2 + r_2^2 - 2\vec{r}_1 \cdot \vec{r}_2}} + B(r_1^2 + r_2^2 + 2\vec{r}_1 \cdot \vec{r}_2) \qquad A, B > 0.$$

Find the ground state energy of this quantum mechanical system.

MLG (gwL)(?)

6

2. Consider a system of two non-identical particles, 1 and 2, which have the same mass μ The potential energy of the system is given by

$$V(\vec{r}_1, \vec{r}_2) = -\frac{A}{\sqrt{r_1^2 + r_2^2 - 2\vec{r}_1\cdot\vec{r}_2}} + B(r_1^2 + r_2^2 + 2\vec{r}_1\cdot\vec{r}_2)$$

$$A, B > 0.$$

Find the ground state energy of this quantum mechanical system.

Solution to 2:

Introduce $\vec{r} = \vec{r}_1 - \vec{r}_2$

$$\vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{2}$$

Find $\nabla_1^2 + \nabla_2^2 = 2\nabla_r^2 + \frac{1}{2}\nabla_R^2$

$$H = \frac{p_r^2}{2m} - \frac{e^2}{r} + \frac{P^2}{2M} + \frac{1}{2} M\omega^2 R^2$$

$$m = \frac{\mu}{2}, \quad M = 2\mu$$

Thus Hamiltonian is the sum of a coulomb atom and a harmonic oscillator.

$$E_{grd} = -\frac{me^4}{2\hbar^2} + \frac{3}{2}\hbar\omega$$

where $e^2 = A$, $\frac{1}{2}M\omega^2 = 4B$

$$E_{grd} = -\frac{\mu A^2}{4\hbar^2} + 3\hbar\sqrt{\frac{B}{\mu}}$$

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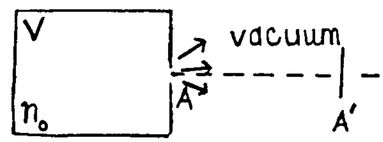
UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part I

[7] Gas molecules of mass m effuse from a hole of area A in a cubic box of volume V at temperature T. They bounce elastically off of a target of cross sectional area A', as shown. The density of molecules in the box is held constant at n_0, and a vacuum is maintained in the surrounding area.



(a) Calculate the work required to bring the target from infinity to a distance L from the target, assuming that $A'/L^2 \ll 1$.

(b) Now suppose that the initial density of molecules in the box is n_0 at time $t = 0$, but that the molecules are not replaced as they leave the box. Outline the argument leading to an approximate expression for the flux of molecules leaving the box in terms of the density, $n(t)$, of molecules in the box at time t. You may express your answer in terms of the mean speed, $\bar{v}$, of a molecule. Use this expression to calculate the density of molecules in the box, $n(t)$, and hence the time, τ_ϵ, for the gas density to drop to $1/\epsilon$ of its initial value. Your answer should be good to a factor of 2 or so, depending on the crudeness of your estimate of the flux through the hole.

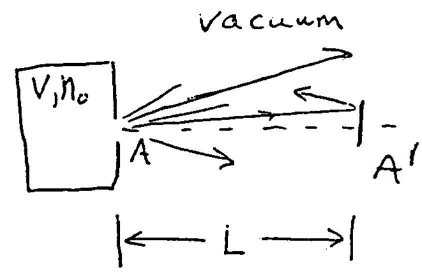
7

Solution (good)

Graduate Exam Problem in Statistical Mechanics

Cliff Surko Spring '94

A. Gas molecules of mass m effuse from a hole of area A in a cubical box of volume V at temperature T. They bounce elastically off of a target of cross sectional area A', as shown. The density of molecules in the box is held constant at n_0, and a vacuum is maintained in the surrounding area.



(a) Calculate the work required to bring the target from infinity to a distance L from the target, assuming that $A'/L^2 << 1$.

If $f(v)$ is Maxwell Boltzmann velocity distribution, where $\int f(v)\, d^3v = n$, then

the Force on the target at distance x will be:

$$F = A \int \underbrace{f(v)\, v \cos\theta\, d^3v}_{\text{flux}} \; \underbrace{(2mv\cos\theta)}_{\text{momentum transfer}} \; ;$$

where θ is $\angle$ between normal to target (and the hole) and the particle trajectory,

where $d^3v = v^2 dv\, \delta\Omega$; $\delta\Omega \simeq \dfrac{A'}{X^2}$; $\cos\theta \simeq 1$

Thus the work done will be:

$$W = -\int_{\infty}^{L} F\,dx = \frac{AA'}{L} \int f(v)\, v^2 dv\, (2mv^2)$$

Now, $\displaystyle\int f(v)\, v^2 dv\, (mv^2) = \frac{n}{4\pi}\, \overline{mv^2} = \frac{1}{4\pi}(3k_BT)$ ← By the equipartition theorem

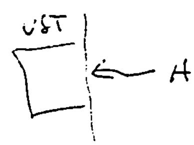
Thus $$\underline{\underline{W = \frac{3}{2\pi} \frac{AA' n k_B T}{L}}}$$

(b) Now suppose that the initial density of molecules in the box is n_0 at time $t = 0$, but that the molecules are not replaced as they leave the box. Outline the arguement leading to an approximate expression for the flux of molecules leaving the box in terms of the density, $n(t)$, of molecules in the box at time t. You may express your answer in terms of the mean speed, $\bar{v}$, of a molecule. Use this expression to calculate the density of molecules in the box, $n(t)$, and hence the time, τ_e, for the gas density to drop to $1/e$ of its initial value. Your answer should good to a factor of 2 or so, depending on the crudeness of your estimate of the flux through the hole.

Crude estimate:

$\sim \frac{1}{6}$ of molecules are travelling in any of the six cartesian directions $\pm x, \pm y, \pm z$

Thus the flux through the hole will be



$$\Phi \simeq \frac{1}{6}\frac{n\bar{v}\,\delta t\,A}{A\,\delta t} = \underline{\frac{1}{6}n\bar{v}}$$

$$\left\{ \begin{array}{l} \text{The exact answer is} \\ \Phi = \frac{1}{4}n\bar{v} \end{array} ; \quad \Phi = \int_{v_z>0} f(v)\,v\cos\theta\,d^3v \right\}$$

$$\frac{dN}{dt} = V\frac{dn}{dt} = -\frac{1}{4}n\bar{v}A$$

$$n = n_0 e^{-\frac{\bar{v}A}{4V}t}$$

$$\underline{\tau_e = \frac{4V}{\bar{v}A}}$$

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UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part I

[8] In his 1934 article entitled "Food and the Theory of Probability" (*United States Naval Institute Proceedings* **60**, 75 (1934)), E. Condon employs a statistical analysis to explain the following empirical rule found by U.S. Navy cooks: In a mess of over 1000 soldiers, one should prepare approximately twelve per cent less food *per soldier* than in a mess of 100 soldiers (*The Cook Book of the United States Navy*, U.S. Government Printing Office (1932), page 9).

(a) Suppose that an individual soldier eats on average $\bar{f}$ kilograms of food (per mess) with a standard deviation σ. Compute the average amount of food $\bar{F}_N$ needed to feed N soldiers. Further assuming that the soldiers' appetites are uncorrelated, compute the standard deviation Σ_N of the total amount of food required.

(b) Suppose that N is large. What is the distribution function $P_N(F)$ of the total amount of food consumed in a mess of N soldiers?

Condon's explanation of "Cook's Law" is that one should very rarely run out of food. Assume, then, that the high standards of the U.S. Navy call for enough food on 99.73% of all messes, which can be accomplished by preparing a total amount of food three standard deviations above the mean in each mess.

(c) Suppose that a recipe for 64 soldiers calls for X kilograms of beans, and that a recipe for 1024 soldiers calls for 16Y kilograms of beans. Using "Cook's Law," determine the average $\bar{f}$ and standard deviation of the individual soldier's bean consumption. If $X =$ 14.4 kg and $Y = 0.9X$ (so that 10 percent fewer beans per soldier is used in the 1024 person mess as compared with the 64 person mess), compute the numerical values of $\bar{f}$ and σ.

Solution

(a) The total amount of food consumed in a mess of N soldiers is $F_N = \sum_{i=1}^N f_i$, where f_i is the amount of food consumed by the i^{th} soldier. Thus,

$$\begin{aligned}
\langle F_N \rangle &= \langle \sum_{i=1}^{N} f_i \rangle \\
&= N \bar{f} \\
\langle (F_N)^2 \rangle &= \langle \sum_{i=1}^{N} \sum_{j=1}^{N} f_i f_j \rangle \\
&= \sum_{i \neq j} \langle f_i f_j \rangle + \sum_i \langle (f_i)^2 \rangle \\
&= N(N-1)\bar{f}^2 + N(\bar{f}^2 + \sigma^2) \\
&= \langle F_N \rangle^2 + N\sigma^2
\end{aligned}$$

from which we read off $\bar{F}_N = N\bar{f}$ and $\Sigma_N = \sqrt{N}\,\sigma$.

(b) From the central limit theorem, we have that the distribution $P_N(F)$ becomes a Gaussian in the large N limit. Thus,

$$P_N(F) \underset{N\to\infty}{=} \frac{1}{\sqrt{2\pi N\sigma^2}} \exp\left(-\frac{(F - N\bar{f})^2}{2N\sigma^2}\right) .$$

(c) Assuming that the amount of food prepared in each mess is three standard deviations above the mean, we have $A(N) = N\bar{f} + 3\sqrt{N}\,\sigma$. Let X represent the amount of food prepared in a mess of 64 soldiers, and $16Y$ the amount of food prepared in a mess of 1024 soldiers. Then

$$\begin{aligned}
64\bar{f} + 24\sigma &= X \\
1024\bar{f} + 96\sigma &= 16Y
\end{aligned}$$

which can be inverted to give

$$\bar{f} = \frac{4Y - X}{192}$$

$$\sigma = \frac{X - Y}{18} .$$

If $Y = 0.9X$, then $\bar{f} = X/180$ and $\sigma = 26X/1920$, so with $X = 14400\,\mathrm{g}$ one obtains $\bar{f} = 195\,\mathrm{g}$ and $\sigma = 80\,\mathrm{g}$ (of beans).

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UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part II

[9] Consider a particle, of mass m, moving under the influence of a potential $V(\vec{r})$. The particle is in a bound state (i.e., confined to a finite region of space).

(a) Show, using classical nonrelativistic mechanics, that $2\overline{T} = \overline{+\vec{r}\cdot\vec{\nabla}V(\vec{r})}$ where $T = \frac{1}{2}m\dot{r}^2$ is the kinetic energy and the bar means long-time average over the orbit. This is called the Virial Theorem.

(b) Show that the same relation holds in quantum theory where the average is replaced by the quantum mechanical expectation value.

(9) Solution to 4

A. $$\frac{d\vec p}{dt} = -\vec\nabla V$$

$$\vec r\cdot\frac{d\vec p}{dt} = -\vec r\cdot\vec\nabla V$$

$$\vec r\cdot\frac{d\vec p}{dt} = \frac{d}{dt}\,\vec r\cdot\vec p - \dot{\vec r}\cdot\vec p = -\vec r\cdot\vec\nabla V$$

Average over a very long time τ : $\int_0^\tau \frac{dt}{\tau}$ & note

$$\frac{1}{\tau}\int_0^\tau dt\,\frac{d}{dt}\,\vec r\cdot\vec p = \frac{(\vec r\cdot\vec p)_\tau - (\vec r\cdot\vec p)_0}{\tau}$$

Since motion is bounded, as $\tau\to\infty$, this term $\Rightarrow 0$

so $$\overline{\dot{\vec r}\cdot\vec p} = \overline{\vec r\cdot\vec\nabla V}$$

$\vec p = m\dot{\vec r}$, so l.h.s $= 2T$; $\overline{2T} = \overline{\vec r\cdot\vec\nabla V}$

B. $\langle\psi|\,[\vec r\cdot\vec p, H]\,|\psi\rangle = 0$ if $H\psi = E\psi$:
and motion is bounded so that H is appropriately hermitian.
Since $H = \frac{\vec p^{\,2}}{2m} + V(\vec r) = T + V$

$$[\vec r\cdot\vec p, \vec p^{\,2}] = 2i\hbar\,\vec p^{\,2}$$
$$[\vec r\cdot\vec p, V] = -i\hbar\,\vec r\cdot\vec\nabla V$$

we have the result $2\langle\psi|\frac{\vec p^{\,2}}{2m}|\psi\rangle = \langle\psi|\vec r\cdot\vec\nabla V$

C. $\langle\psi|[\vec r\cdot\vec p, H_D]\,\psi\rangle = 0 = \langle\psi|\,i\hbar\, c\,\vec\alpha\cdot\vec p - i\hbar\,\vec r\cdot\vec\nabla V\,|\psi\rangle$

If $V \sim 1/r$, $\vec r\cdot\vec\nabla V = -V$. $\therefore$ $\langle\psi|c\vec\alpha\cdot\vec p|\psi\rangle = -\langle\psi|$

$E(\psi,\psi) = (\psi, H_D\psi) = (\psi, [c\vec\alpha\cdot\vec p + \beta mc^2 + V]\,\psi) = mc^2(\psi,$
as advertised.

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UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part II

[10] A particle orbits a center of attraction with a potential energy $V(r)$, in an almost circular orbit of radius r_0. Find the precession of the orbit, that is, the angular separation $\Delta\theta$ after one trip from r_{min} back to r_{min}, and show that it is a multiple of π for the two special cases of the Kepler problem $V(r) = -k/r$ and the harmonic oscillator $V(r) = \frac{1}{2}kr^2$.

(10) (good) (1)

Graduate Mechanics problem H Levine

A particle orbits a center of attraction with a potential energy $V(r)$, in an almost circular orbit of radius r_0. Find the precession of the orbit, that is the angular separation $\Delta\theta$ after one trip from r_{min} back to r_{min}, and show that it is a multiple of π for the two special cases of the Kepler problem $V(r) = -k/r$ and the harmonic oscillator $V(r) = \frac{1}{2}kr^2$

Solution

Conservation of energy

$$\frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\theta}^2 + V(r) = E$$

Angular momentum conserved

$$L = mr^2\dot{\theta} = \text{constant}$$

$$\Rightarrow \quad \dot{r} = \sqrt{(E-V)2m - L^2/2mr^2}$$

$$\dot{\theta} = L/mr^2$$

$$\frac{dr}{d\theta} = \frac{\sqrt{2m(E-V) - L^2/2mr^2)}}{L/mr^2}$$

2

$$\Delta\Theta = 2\int_{r_{min}}^{r_{max}} \frac{L\,dr/mr^2}{\sqrt{2m(E-V) - L^2/2mr^2}}$$

let $x = 1/r$

$$\Rightarrow \frac{2L}{m}\int_{x_{min}}^{x_{max}} \frac{dx}{\sqrt{2m(E-\tilde{V}(x)) - \frac{L^2}{2m}x^2)}} \qquad \tilde{V}(x) = V\left(\frac{1}{x}\right)$$

almost circular orbit at r_0 $\quad V_{eff}(x) = \tilde{V}(x) + \frac{L^2}{2m}x^2$

$$V'_{eff}(x_0) = 0$$

$$E = E_0 + \delta E \qquad (E_0 \text{ is energy of circular orbit})$$

so, integral is

$$\frac{2L}{m}\int \frac{dx}{\sqrt{2m(\delta E - \frac{1}{2}(x-x_0)^2\, V''(x_0))}} \quad ?$$

$$= \frac{2L}{m}\frac{1}{\sqrt{mV''(x_0)}}\ \sin^{-1}\frac{x-x_0}{(2\delta E/V'')}\Bigg|_{x_{min}}^{x_{max}} =$$

$$\pi \cdot \frac{2L}{m}\frac{1}{\sqrt{m\,V''_{eff}(x_0)}}$$

$$\tilde{V}''_{eff}(x_0) = \frac{L^2}{m} + \frac{\partial^2}{\partial x^2}V\left(\frac{1}{x}\right)$$

$$= \frac{L^2}{} + \left(r_0^4 V''(r) + 2r^3 V'(r\right.$$

but

$$\frac{L^2}{m r_o^3} = V'(r_o) \qquad \text{via} \quad V_{eff}' = 0$$

$$\Rightarrow 2\pi \sqrt{\frac{V'(r_o)}{3V'(r_o) + r_o V_o''(r_o)}}$$

if $\quad V \sim 1/r \qquad \Rightarrow \quad \Delta\Theta = 2\pi$

if $\; V \sim r^2 \qquad\qquad \Delta\Theta \sim \pi$

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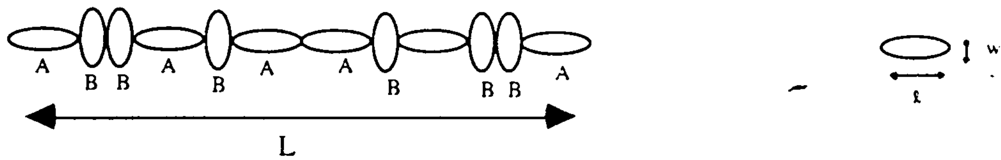
UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part II

[11] Consider a polymer consisting of N monomeric units shown in the figure below. Each unit has length ℓ and width w. All of the monomeric units may freely rotate between two allowed orientations, A or B, as indicated in the figure. Further suppose that the energy of the two orientations is equal and that the chain is immersed in an inert solvent with temperature T.



(a) Calculate the entropy $S(L)$ where L is the length of the partially stretched polymer.

(b) If tension τ is applied to both ends of the polymer. what will the equilibrium length L be?

(c) Rederive the result obtained in part (b) (i.e., $L(\tau, T)$) using the generalized ensemble method.

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Soln:

(a.) Calculate $S(T) = K_B \ln W$ where W is # of microstates of the chain with length L. Now

$$L = N_A \ell + N_B w$$

$$N = N_A + N_B$$

and $W = \dfrac{N!}{N_A!\, N_B!}$ is # of microstates

Now

$\ln(N!) \simeq N \ln N - N$ Stirlings formula

So

$$\ln W = N \ln N - N - N_A \ln N_A + N_A - N_B \ln N_B + N_B$$

$$= - N_A \ln \frac{N_A}{N} - N_B \ln \frac{N_B}{N}$$

Also need $\dfrac{N_A}{N} = \dfrac{L - Nw}{N(\ell - w)}$

$$\frac{N_B}{N} = - \frac{L - N\ell}{N(\ell - w)}$$

So

$$\boxed{S(L) = - \frac{K_B}{\ell - w} \left\{ (L - Nw) \ln \left[\frac{L - Nw}{N(\ell - w)} \right] - (L - N\ell) \ln \left[\frac{N\ell - L}{N(\ell - w)} \right] \right\}}$$

(b) Want to find tension τ. Use
$\tau = \left.\frac{\partial F}{\partial L}\right|_T$. But $F = E - TS = -TS$.
– Since we are assuming energy of microstates to be independent of monomer configuration, we have $\tau = -T\frac{\partial S}{\partial L}$.

Using result of part a, we have

$$\tau = \frac{k_B T}{\ell - w}\left\{ \ln(L - Nw) - \ln(N\ell - L)\right\}$$

or
$$\tau = \frac{k_B T}{\ell - w} \ln\left(\frac{L - Nw}{N\ell - L}\right)$$

or
$$\frac{L - Nw}{N\ell - L} = \exp \beta\tau(\ell - w) \equiv z$$

– Solve for L: $\quad L - Nw = (N\ell - L)z$

so

$$L(1 + z) = N(\ell z + w)$$

$$L = N\frac{\ell z + w}{1 + z} = N\left\{\frac{\ell + w}{2} + \frac{\ell - w}{2}\frac{z - 1}{z + 1}\right\}$$

So
$$\boxed{L = N\left\{\frac{\ell + w}{2} + \frac{\ell - w}{2}\tanh\left[\frac{\beta\tau}{2}(\ell - w)\right].\right\}}$$

(c.) Use generalized ensemble in which chain is in contact with a reservoir which exerts a constant tension τ. To write partition function introduce Ising-like variables S_i. $S_i = +1$ $\Rightarrow$ link i is in state A. $S_i = -1 \Rightarrow$ link i is in state B

Partition fcn is

$$\Xi_N = \sum_{[S_1 \cdots S_N]} \exp \beta\tau \sum_{i=1}^{N} \left\{ S_i \frac{\ell - W}{2} + \frac{\ell + W}{2} \right\}$$

$$= \Xi_1^N$$

where $\Xi_1 = e^{\beta\tau\ell} + e^{\beta\tau W}$

This partition function is related to the thermodynamic potential $\Omega \equiv F - \tau L$ according to

$$\Omega = -K_B T \ln \Xi_N$$

Now
$$d\Omega = dF - d(\tau L)$$
$$= \tau dL - L d\tau - \tau dL = -L d\tau.$$

So
$$L = -\left.\frac{\partial\Omega}{\partial\tau}\right|_T = +K_B T N \frac{\partial \ln \Xi_1}{\partial\tau}$$

$$= +K_B T N \left\{ \frac{\beta\ell\, e^{\beta\tau\ell} + \beta d\, e^{\beta\tau W}}{e^{\beta\tau\ell} + e^{\beta\tau W}} \right\}$$

$$= +N \left\{ \frac{\ell + W}{2} + \frac{\ell - W}{2} \frac{e^{\beta\tau\ell} - e^{\beta\tau W}}{e^{\beta\tau\ell} + e^{\beta\tau W}} \right\}$$

$$\boxed{L = +N \left\{ \frac{\ell + W}{2} + \frac{\ell - W}{2} \tanh \beta\tau\left(\frac{\ell - W}{2}\right) \right\}}$$

which is identical to the result obtained in part b.

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UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part II

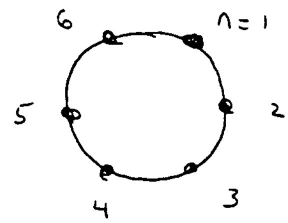
[12] Consider the following classical model of the Benzene molecule. Treat the $C - C$ bond as producing a nearest neighbor pair interaction $V(r) = \frac{1}{2}kr^2$ where r is the $C - C$ spacing. Further suppose that the C atoms are restricted to lie on a ring of radius R and that the ring remains in a plane.

(a) Find the frequencies and normal modes of oscillation for the benzene molecule.

(b) Repeat part (a) assuming that one of the carbon atoms is replaced by an infinitely heavy impurity atom I and that the $I - C$ interaction is the same as the $C - C$ interaction.

Normal Modes of Benzene

Solution:



(a.) Let x_n, $n=1,\cdots 6$ be clockwise displacement of n-th Carbon atom along ring. Constraint to lie on ring means NO transverse vibrations occur. For simplicity we will ignore difference between arc length, $x_n - x_{n-1}$, and the cord length between nearest neighbours.

Normal modes of form $e_n \propto e^{ikan}$ where $ka = \frac{m\pi}{3}$. $m=1,2,\cdots 6$ labels the 6 normal modes

$$\boxed{x_n \propto e^{imn\pi/3} \qquad m=1,\cdots 6}$$

To find ω_m write Newton's eqns

$$m_c \ddot{x}_n = -K(2x_n - x_{n-1} - x_{n+1})$$

So

$$-m_c w^2 e^{imn\pi/3} = -K(2 - e^{-im\pi/3} - e^{im\pi/3})e^{imn\pi/3}$$

So

$$\boxed{\omega_m^2 = \frac{2K}{m_c}\left(1 - \cos\frac{m\pi}{3}\right)}$$

where m_c is mass of Carbon atom.

(b.) Normal mode e_n must obey $e_{n+6} = e_n$ (as before) and $e_6 = 0$ where $n=6$ is the label of the ∞ heavy impurity atom. So

$$\boxed{x_n \propto e^{imn\pi/3} - e^{-imn\pi/3}}$$

are new normal modes. There are only 5 of

these since $x_n = 0$ for $m = 6$ normal mode.
The replacement of C atom by ~~a~~ ∞ heavy impurity reduces # of degrees of freedom by 1.
Normal mode frequencies are

$$\boxed{\omega_m^2 = \frac{2K}{m_c}\left(1 - \cos\frac{m\pi}{3}\right)}$$

as in part a.

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UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part II

[13] A conducting sphere of radius R is immersed in a uniform magnetic field B and rotates with frequency ω about an axis through its center. Assuming that ω is parallel to B, determine the charge density in the sphere and on its surface. The net charge on the sphere is zero. (Hint: The first three Legendre polynomials are $P_0(x) = 1$, $P_1(x) = x$ and $P_2(x) = \frac{1}{2}(3x^2 - 1)$.)

Sol'n (13)

inside the sphere $\quad 0 = \underline{E} + \frac{\underline{v}}{c} \times \underline{B}$

$$\therefore \quad \underline{E} = -\frac{\underline{v} \times \underline{B}}{c} = \frac{\underline{B}}{c} \times (\omega \times r) = \underline{\omega}\frac{\underline{B} \cdot \underline{r}}{c} - \underline{r}\frac{(\underline{B} \cdot \underline{\omega})}{c}$$

$$\underline{E} = -\frac{\underline{\omega} \cdot \underline{B}}{c}(\hat{x}x + \hat{y}y) \quad , \text{ where } \underline{B} = \hat{z}B, \quad \underline{\omega} = \hat{z}\omega$$

$$4\pi\rho = \underline{\nabla} \cdot \underline{E} = -\frac{2\omega B}{c}$$

potential inside sphere

$$\varphi_1 = +\frac{\omega B}{2c}(x^2 + y^2) = +\frac{\omega B}{2c} r^2 \sin^2\theta$$

spherical coordinates

outside sphere

$$\varphi_2 = A + C\frac{1}{2}\underbrace{(3\cos^2\theta - 1)}_{2 - 3\sin^2\theta}\frac{1}{r^3} + \overset{=0}{\frac{D}{r}}$$

no net charge

$$\varphi_2 = A - C\frac{3}{2}\left(\sin^2\theta - \frac{2}{3}\right)\frac{1}{r^3}$$

ϕ_1 must match ϕ_2 at surface of sphere

$$\therefore\ -\frac{3}{2}\frac{C}{R^3} = \frac{\omega B}{2c}R^2 \quad , \quad C = -\frac{\omega B R^5}{3c}$$

$$A + \frac{C}{R^3} = 0 \quad , \quad A = +\frac{\omega B R^2}{3c}$$

$$\therefore\ \phi_2 = +\frac{\omega B R^2}{3c} + \frac{\omega B R^5}{2c}\left(\sin^2\theta - \frac{2}{3}\right)\frac{1}{r^3}$$

charge on surface of sphere

$$4\pi\sigma = \frac{\partial\phi_1}{\partial r} - \frac{\partial\phi_2}{\partial r} = +\frac{\omega B}{c}R\sin^2\theta + \frac{3}{2}\frac{\omega B R}{c} - \frac{\omega B R}{c}$$

$$= \frac{\omega B R}{c}\left[-1 + \frac{5}{2}\sin^2\theta\right]$$

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UNIVERSITY OF CALIFORNIA, SAN DIEGO

DEPARTMENT OF PHYSICS

Written Departmental Examination – Spring 1994, Part II

[14] The Helium atom.

(a) Approximately determine the energy of the ground state of the Helium atom treating the interaction between electrons as a perturbation.

(b) This result from perturbation theory needs to be improved. Find a simple, physically motivated, trial wave function that you could use for a variational calculation. Show what strategy you would use to perform the variational calculation.

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a)

Problem 1. Determine approximately the energy of the ground level of the helium atom and helium-like ions (a nucleus of charge Z and two electrons), regarding the interaction between the electrons as a perturbation.

Solution a

Solution. In the ground state of the ion, both electrons are in s states. The unperturbed value of the energy is twice the ground level of a hydrogen-like ion (because of the two electrons):

$$E^{(0)} = 2(-\tfrac{1}{2}Z^2) = -Z^2.$$

The correction in the first approximation is given by the mean value of the electron interaction energy in a state with wave function

$$\psi = \psi_1(r_1)\psi_2(r_2) = \frac{Z^3}{\pi}e^{-Z(r_1+r_2)} \tag{1}$$

(the product of two hydrogen functions with $l = 0$). The integral

$$E^{(1)} = \iint \psi^2 \frac{1}{r_{12}} dV_1 dV_2$$

is most simply calculated as

$$E^{(1)} = 2\int_0^\infty dV_2 \cdot \rho_2 \frac{1}{r_2}\int_0^{r_2} \rho_1 dV_1, \quad dV_1 = 4\pi r_1^2 dr_1,$$
$$dV_2 = 4\pi r_2^2 dr_2,$$

the energy of the charge distribution $\rho_2 = |\psi_2|^2$ in the field of the spherically symmetric distribution $\rho_1 = |\psi_1|^2$; the integrand with dV_2 is the energy of the charge $\rho_2(r_2)$ in the field of the sphere $r_1 < r_2$, and the factor 2 takes account of the contribution from configurations in which $r_1 > r_2$. Thus we find $E^{(1)} = 5Z/8$, and finally

$$E = E^{(0)} + E^{(1)} = -Z^2 + \tfrac{5}{8}Z.$$

For the helium atom ($Z = 2$) this gives $-E = 11/4 = 2{\cdot}75$; the actual value of the ground-state energy of this atom is $-E = 2{\cdot}90$ atomic units = ~~78.9~~ eV.
74.8 eV

§70. The Thomas-Fer

Numerical calculation
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b) This result in perturbation theory needs to be improved. To do that we use the variational method. What is the simplest trial wave function that you would use for this calculation? Also show what strategy you would use to perform this variational calculation.

Saluhan by

since $\psi_e^{(0)}$ is normalized. ~~Comparison with the perturbation-theory~~ expression (9.74) shows ~~that the variation method gives the same~~ result if we use $\psi_e^{(0)}$ as the trial function.

With this discussion as background, we consider variation functions for the helium ground state. If we used $\psi_e^{(0)}$ [Eq. (9.60)] for the trial function, we would get the first-order perturbation result -74.8 eV. To improve on this result, we use a trial function of the form of (9.60) but having a variational parameter. We try the normalized function

trial A

$$\varphi = \frac{1}{\pi}\left(\frac{\zeta}{a_0}\right)^3 e^{-\zeta r_1/a_0} e^{-\zeta r_2/a_0} \tag{9.77}$$

which is obtained from (9.60) by replacing the true atomic number Z by a variational parameter ζ (zeta). ζ has a simple physical interpretation. Since one electron tends to screen the other from the nucleus, each electron is subject to an effective nuclear charge somewhat less than the full nuclear charge Z. If one electron fully shielded the other from the nucleus, we would have an effective nuclear charge of $Z - 1$; since both electrons are in the same orbital, they will be only partly effective in shielding each other. We thus expect ζ to lie between $Z - 1$ and Z.

We now evaluate the variational integral. To expedite things, we rewrite the Hamiltonian (9.49) as

$$\hat{H} = \left[-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\zeta e'^2}{r_1} - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{\zeta e'^2}{r_2}\right] + (\zeta - Z)\frac{e'^2}{r_1} + (\zeta - Z)\frac{e'^2}{r_2} + \frac{e'^2}{r_{12}} \tag{9.78}$$

where we have added and subtracted the terms involving zeta. The terms in brackets in (9.78) are the sum of two hydrogenlike Hamiltonians for nuclear charge ζ; moreover, the trial function (9.77) is the product of two hydrogenlike $1s$ functions for nuclear charge ζ. Therefore, when these terms operate on φ, we will have an eigenvalue equation, the eigenvalue being the sum of two hydrogenlike $1s$ energies for nuclear charge ζ:

$$\left[-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\zeta e'^2}{r_1} - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{\zeta e'^2}{r_2}\right]\varphi = -\zeta^2(2)\frac{e'^2}{2a_0}\varphi \tag{9.79}$$

Using (9.78) and (9.79), we have

set int B

$$\int \varphi^* \hat{H}\varphi\, d\tau = -\zeta^2\frac{e'^2}{a_0}\int \varphi^*\varphi\, d\tau + (\zeta - Z)e'^2\int\frac{\varphi^*\varphi}{r_1}\,d\tau$$
$$+ (\zeta - Z)e'^2\int\frac{\varphi^*\varphi}{r_2}\,d\tau + e'^2\int\frac{\varphi^*\varphi}{r_{12}}\,d\tau \tag{9.80}$$

Let f_1 be a normalized $1s$ hydrogenlike orbital for nuclear charge ζ, occupied by electron 1; let f_2 be the same function for electron 2:

$$f_1 = \frac{1}{\pi^{1/2}}\left(\frac{\zeta}{a_0}\right)^{3/2} e^{-\zeta r_1/a_0}, \qquad f_2 = \frac{1}{\pi^{1/2}}\left(\frac{\zeta}{a_0}\right)^{3/2} e^{-\zeta r_2/a_0} \tag{9.81}$$

Noting that $\varphi = f_1 f_2$, we now evaluate the integrals in (9.80):

$$\int \varphi^*\varphi\, d\tau = \iint f_1^* f_2^* f_1 f_2\, d\tau_1\, d\tau_2 = \int f_1^* f_1\, d\tau_1 \int f_2^* f_2\, d\tau_2 = 1$$

$$\int \frac{\varphi^*\varphi}{r_1}\,d\tau = \int\frac{f_1^* f_1}{r_1}\,d\tau_1 \int f_2^* f_2\, d\tau_2 = \int\frac{f_1^* f_1}{r_1}\,d\tau_1$$

$$\int \frac{\varphi^*\varphi}{r_1}\,d\tau = \frac{1}{\pi}\frac{\zeta^3}{a_0^3}\int_0^\infty e^{-2\zeta r_1/a_0}\frac{r_1^2}{r_1}\,dr_1 \int_0^\pi \sin\theta_1\, d\theta_1 \int_0^{2\pi} d\varphi_1 = \frac{\zeta}{a_0}$$

where the Appendix integral (A.4) was used. Also

$$\int\frac{\varphi^*\varphi}{r_2}\,d\tau = \int\frac{f_2^* f_2}{r_2}\,d\tau_2 = \int\frac{f_1^* f_1}{r_1}\,d\tau_1 = \frac{\zeta}{a_0} \tag{9.82}$$

since it doesn't matter whether we use the label 1 or 2 on the dummy variables in the definite integral. Finally we must evaluate

$$e'^2\int\frac{\varphi^*\varphi}{r_{12}}\,d\tau \tag{9.83}$$

We recognize (9.83) as the same integral (9.63) that occurred in the perturbation treatment, except that Z is replaced by ζ; hence from (9.67)

$$e'^2\int\frac{\varphi^*\varphi}{r_{12}}\,d\tau = \frac{5\zeta e'^2}{8a_0} \tag{9.84}$$

The variational integral (9.80) thus has the value

$$\int \varphi^* \hat{H}\varphi\, d\tau = \left(\zeta^2 - 2Z\zeta + \tfrac{5}{8}\zeta\right)\frac{e'^2}{a_0} \tag{9.85}$$

As a check, if we set $\zeta = Z$ in (9.85), we get the first-order perturbation-theory result, (9.61) plus (9.67).

We now vary ζ to minimize the variational integral:

minimize C

$$\frac{\partial}{\partial\zeta}\int\varphi^*\hat{H}\varphi\, d\tau = \left(2\zeta - 2Z + \tfrac{5}{8}\right)\frac{e'^2}{a_0} = 0$$

$$\zeta = Z - \tfrac{5}{16} \tag{9.86}$$

As anticipated, the effective nuclear charge lies between Z and $Z - 1$. Using (9.86) and (9.85), we get

$$\int\varphi^*\hat{H}\varphi\, d\tau = \left(-Z^2 + \tfrac{5}{8}Z - \tfrac{25}{256}\right)\frac{e'^2}{a_0} = -\left(Z - \tfrac{5}{16}\right)^2\frac{e'^2}{a_0} \tag{9.87}$$

Putting $Z = 2$, we get as our approximation to the ground-state energy $-(27/16)^2 e'^2/a_0 = -(729/256)27.21$ eV $= -77.5$ eV, as compared to the true value -79.0 eV. Use of ζ instead of Z has reduced the error from 5.3 percent to 1.9 percent. In accord with the variation theorem, the true ground-state energy is less than the variational integral.