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Exam in TFY4205 Quantum Mechanics
Saturday June 10, 2006
9:00–13:00

Allowed help: Alternativ C
Approved Calculator.
K. Rottman: *Matematische Formelsammlung*
Barnett and Cronin: *Mathematical formulae*

At the end of the problem set some relations are given that might be helpful.

This problem set consists of 9 pages.

Problem 1. Spin

A system of two particles with spin 1/2 is described by an effective Hamiltonian

$$H = A\,(s_{1z} + s_{2z}) + B\mathbf{s}_1 \cdot \mathbf{s}_2\,, \tag{1}$$

where $\mathbf{s}_1$ and $\mathbf{s}_2$ are the two spins, s_{1z} and s_{2z} are their z-components, and A and B are constants. Find the energy levels of this Hamiltonian.

Solution

We choose χ_{S,M_S} as the common eigenstate of $\mathbf{S}^2 = (\mathbf{s}_1 + \mathbf{s}_2)^2$ and $S_z = s_{1z} + s_{2z}$. For $S = 1$, $M_S = 0, \pm 1$, it is a triplet and is symmetric when the two electrons are exchanged. For $S = 0$, $M_S = 0$, it is a singlet and is antisymmetric. For stationary states we use the time-independent Schrödinger equation

$$H\chi_{S,M_S} = E\chi_{S,M_S} \tag{2}$$

Using

$$\mathbf{S}^2\chi_{1,M_S} = S(S+1)\hbar^2\chi_{1,M_S} = 2\hbar^2\chi_{1,M_S} \tag{3}$$

$$\mathbf{S}^2\chi_{0,M_S} = S(S+1)\hbar^2\chi_{1,M_S} = 0 \tag{4}$$

and

$$\mathbf{S}^2 = (\mathbf{s}_1 + \mathbf{s}_2)^2 = \mathbf{s}_1^2 + \mathbf{s}_2^2 + 2\mathbf{s}_1 \cdot \mathbf{s}_2 \tag{5}$$

$$= \frac{3\hbar^2}{4} + \frac{3\hbar^2}{4} + 2\mathbf{s}_1 \cdot \mathbf{s}_2 \tag{6}$$

we have

$$\mathbf{s}_1 \cdot \mathbf{s}_2 \chi_{1,M_S} = \left(\frac{S^2}{2} - \frac{3\hbar^2}{4} \right) \chi_{1,M_S} \tag{7}$$

$$= \frac{\hbar^2}{4} \chi_{1,M_S}\,, \tag{8}$$

$$\mathbf{s}_1 \cdot \mathbf{s}_2 \chi_{0,0} = \left(\frac{S^2}{2} - \frac{3\hbar^2}{4} \right) \chi_{0,0} \tag{9}$$

$$= -\frac{3\hbar^2}{4} \chi_{0,0}\,, \tag{10}$$

and

$$S_z \chi_{1,M_S} = (s_{1z} + s_{2z})\, \chi_{1,M_S} = M_S \hbar \chi_{1,M_S} \tag{11}$$

$$S_z \chi_{0,0} = 0\,. \tag{12}$$

Hence for the triplet state, the energy levels are

$$E_{1,M_S} = M_S \hbar A + \frac{\hbar^2}{4} B\,, \text{ with } M_S = 0, \pm 1 \tag{13}$$

comprising three lines

$$E_{1,1} = \hbar A + \frac{\hbar^2}{4} B\,, \tag{14}$$

$$E_{1,0} = \frac{\hbar^2}{4} B\,, \tag{15}$$

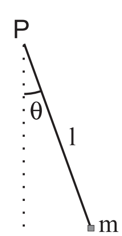
$$E_{1,-1} = -\hbar A + \frac{\hbar^2}{4} B\,. \tag{16}$$

For the singlet state, the energy level consists of only one line

$$E_{0,0} = -\frac{3\hbar^2}{4} B\,. \tag{17}$$

Problem 2. Perturbation Theory

A mass m is attached by a massless rod of length l to a pivot P and swings in a vertical plane under the influence of gravity, see the figure below.



a) In the small angle approximation find the energy levels of the system.

Solution

We take the equilibrium position of the point mass as the zero point of potential energy. For small angle approximation, the potential energy of the system is

$$V = mgl\,(1 - \cos\theta) \approx \frac{1}{2}mgl\theta^2\,, \tag{18}$$

and the Hamiltonian is

$$H = \frac{1}{2}ml^2\left(\frac{d\theta}{dt}\right)^2 + \frac{1}{2}mgl\theta^2\,. \tag{19}$$

By comparing it with the one-dimensional harmonic oscillator ($\theta \to x/l$), we obtain the energy levels of the system

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{20}$$

where $\omega = \sqrt{g/l}$.

b) Find the lowest order correction to the ground state energy resulting from the inaccuracy of the small angle approximation.

Solution

The perturbation Hamiltonian is

$$\begin{aligned} H' &= mgl(1 - \cos\theta) - \frac{1}{2}mgl\theta^2 && (21)\\ &= -\frac{1}{24}mgl\theta^4 = -\frac{1}{24}\frac{mg}{l^3}x^4\,, && (22) \end{aligned}$$

where $x = l\theta$. The ground state wave function for a harmonic oscillator is

$$\psi_0 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\exp -\frac{1}{2}\frac{m\omega}{\hbar}x^2\,. \tag{23}$$

The lowest order correction to the ground state energy resulting from the inaccuracy of the samll angle approximation is

$$E' = \langle 0|H'|0\rangle = -\frac{1}{24}\frac{mg}{l^3}\langle 0|x^4|0\rangle\,. \tag{24}$$

Using

$$\begin{aligned} \langle 0|x^4|0\rangle &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2}\int_{-\infty}^{\infty} dx x^4 \exp -\frac{m\omega}{\hbar}x^2\,, && (25)\\ &= \frac{3}{4}\left(\frac{m\omega}{\hbar\pi}\right)^{-1} && (26) \end{aligned}$$

we find

$$E' = -\frac{\hbar^2}{32ml^2}\,. \tag{27}$$

Problem 3. Variational Method

An idealized ping pong ball of mass m is bouncing in its ground state on a recoilless table in a one-dimensional world with only a vertical direction.

a) Prove that the energy depends on the mass m, the constant of gravity g, and Planck's constant h according to $\epsilon = Kmg(m^2g/h^2)^\alpha$ and determine α.

Solution

The kinetic energy is

$$H_k = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \tag{28}$$

and the potential energy is (origin at the table)

$$V = mgx \,. \tag{29}$$

We assume that we measure the coordinate in a length scale l. We then find that the energy scales satisfy the scaling relation

$$\epsilon \propto \frac{\hbar^2}{m}\frac{1}{l^2} \propto mgl \tag{30}$$

which means that

$$l^3 \propto \frac{m^2 g}{\hbar^2} \tag{31}$$

so that we can write the energy as

$$\epsilon \quad \propto \quad mg\left(\frac{m^2 g}{\hbar^2}\right)^{-1/3} \quad . \tag{32}$$

The constant is thus $\alpha = -1/3$.

b) Give arguments for why a good guess for a trial function for the ground state energy is

$$\psi(x) = x\exp -\lambda x^2/2 \,, \tag{33}$$

where λ is a variational parameter.

Solution

In the ground state, it is reasonable to assume that the particle is located close to the table since a classical particle in its lowest energy state will be localized at $x = 0$. We also know that the wave function must vanish at $x = 0$ because the table is impenetrable. A reasonable trial function that satisfies these two criteria is of the form $\psi(x) = x\exp -\lambda x^2$ since

$$\psi(x = 0) = 0 \tag{34}$$

and

$$\psi(x \to \infty) = 0 \,. \tag{35}$$

The latter condition ensures that the particle cannot be too far off the table and that the norm of the wave function is finite.

c) By a variational method estimate the constant K for the ground state energy.

Solution

The Hamiltonian is

$$H = H_k + V\,. \tag{36}$$

$$\psi(x) = x \exp -\lambda x^2/2\,. \tag{37}$$

Consider

$$\langle H\rangle H = \frac{\int_0^\infty dx \psi^* H \psi}{\int_0^\infty dx \psi^* \psi} \tag{38}$$

The norm is

$$\begin{aligned}
\int_0^\infty dx\psi^*\psi &= \int_0^\infty dx x^2 \exp -\lambda x^2 && (39)\\
&= -\frac{d}{d\lambda}\int_0^\infty dx \exp -\lambda x^2 && (40)\\
&= -\frac{d}{d\lambda}\frac{1}{2}\sqrt{\frac{\pi}{\lambda}} && (41)\\
&= \frac{1}{4}\sqrt{\pi}\lambda^{-3/2}\,. && (42)
\end{aligned}$$

We use

$$\begin{aligned}
\frac{d^2}{dx^2}\psi(x) &= \frac{d^2}{dx^2} x \exp -\lambda x^2/2 && (43)\\
&= \frac{d}{dx}\left(1-\lambda x^2\right)\exp -\lambda x^2/2 && (44)\\
&= \left(-3\lambda x + \lambda^2 x^3\right)\exp -\lambda x^2/2 && (45)
\end{aligned}$$

The kinetic energy term is

$$\begin{aligned}
\int_0^\infty dx H_k \psi^*\psi &= \int_0^\infty dx \psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi(x) && (46)\\
&= -\frac{\hbar^2}{2m}\int_0^\infty dx\left(-3\lambda x^2 + \lambda^2 x^4\right)\exp -\lambda x^2 && (47)\\
&= -\frac{\hbar^2}{2m}\int_0^\infty dx\left(3\lambda\frac{d}{d\lambda} + \lambda^2\frac{d^2}{d\lambda^2}\right)\exp -\lambda x^2 && (48)\\
&= -\frac{\hbar^2}{2m}\left(3\lambda\frac{d}{d\lambda} + \lambda^2\frac{d^2}{d\lambda^2}\right)\frac{1}{2}\sqrt{\frac{\pi}{\lambda}} && (49)\\
&= \frac{\hbar^2}{2m}\frac{3}{8}\sqrt{\pi}\lambda^{-1/2}\,. && (50)
\end{aligned}$$

The potential energy term is

$$\begin{aligned}
\int_0^\infty dx V\psi^*\psi &= mg\int_0^\infty dx x^3 \exp -\lambda x^2 && (51)\\
&= -mg\frac{d}{d\lambda}\int_0^\infty dx x \exp -\lambda x^2 && (52)\\
&= -mg\frac{d}{d\lambda}\frac{1}{2\lambda} && (53)\\
&= mg\frac{1}{2\lambda^2}\,. && (54)
\end{aligned}$$

We thus find that

$$\langle H\rangle = \frac{3\hbar^2}{4m}\lambda + \frac{2mg}{\sqrt{\pi}\lambda^{1/2}}\,. \tag{55}$$

To minimize $\langle H\rangle$, we use

$$\frac{d}{d\lambda}\langle H\rangle = \frac{3\hbar^2}{4m} - \frac{mg}{\sqrt{\pi}}\lambda^{-3/2} = 0\,, \tag{56}$$

which gives

$$\lambda = \left(\frac{4m^2 g}{3\hbar^2\sqrt{\pi}}\right)^{2/3}\,. \tag{57}$$

The approximate ground state energy is then

$$\langle H\rangle = 3\left(\frac{3}{4\pi}\right)^{1/3} mg\left(\frac{m^2 g}{\hbar^2}\right)^{-1/3} \tag{58}$$

or, in other words, the constant

$$K = 3\left(\frac{3}{4\pi}\right)^{1/3}\,. \tag{59}$$

Problem 4. Motion in Electromagnetic Field

The Hamiltonian for a spinless charged particle in a magnetic field is

$$\hat{H} = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2\,, \tag{60}$$

where m is the electron mass, $\hat{\mathbf{p}}$ is the momentum operator, and $\mathbf{A}$ is related to the magnetic field by

$$\mathbf{B} = \nabla\times\mathbf{A}\,. \tag{61}$$

a) Show that the gauge transformation $\mathbf{A}(\mathbf{r}) \to \mathbf{A}(\mathbf{r}) + \nabla f(\mathbf{r})$ is equivalent to multiplying the wave function by a factor $\exp ief(\mathbf{r})/(\hbar c)$. What is the significance of this result?

Solution

The Schrödinger equation is

$$\frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2\psi(\mathbf{r}) = E\psi(\mathbf{r})\,. \tag{62}$$

Suppose we make the transformation

$$\begin{aligned} \mathbf{A}(\mathbf{r}) \to \mathbf{A}'(\mathbf{r}) &= \mathbf{A}(\mathbf{r}) + \nabla f(\mathbf{r}) && (63) \\ \psi(\mathbf{r}) \to \psi'(\mathbf{r}) &= \psi(\mathbf{r}) \exp ief(\mathbf{r})/(\hbar c) , && (64) \end{aligned}$$

and consider

$$\begin{aligned} \left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}'\right)\psi'(\mathbf{r}) &= \hat{\mathbf{p}}\psi'(\mathbf{r}) - \left[\frac{e}{c}\mathbf{A} + \frac{e}{c}\nabla f(\mathbf{r})\right] \exp\left[\frac{ie}{\hbar c} f(\mathbf{r})\right]\psi(\mathbf{r}) && (65) \\ &= \exp\left[\frac{ie}{\hbar c} f(\mathbf{r})\right]\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)\psi(\mathbf{r}) && (66) \end{aligned}$$

$$\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}'\right)^2 \psi'(\mathbf{r}) = \exp\left[\frac{ie}{\hbar c} f(\mathbf{r})\right]\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2 \psi(\mathbf{r}) \quad (67)$$

where we have used

$$\begin{aligned} \hat{\mathbf{p}}\psi'(\mathbf{r}) &= \frac{\hbar}{i}\nabla\left\{\exp\left[\frac{ie}{\hbar c} f(\mathbf{r})\right]\psi(\mathbf{r})\right\} && (68) \\ &= \exp\left[\frac{ie}{\hbar c} f(\mathbf{r})\right]\left[\frac{e}{c}\nabla f(\mathbf{r}) + \hat{\mathbf{p}}\right]\psi(\mathbf{r}) . && (69) \end{aligned}$$

Substitution in the Schrödinger equation gives

$$\frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}'\right)^2 \psi'(\mathbf{r}) = E\psi'(\mathbf{r}) . \quad (70)$$

This shows that under the gauge transformation $\mathbf{A}' = \mathbf{A} + \nabla f$, the Schrödinger equation remains the same and that there is only a phase difference between the original and the new wave functions. Thus the systm has gauge invariance.

b) Consider the case of a uniform field $\mathbf{B}$ directed along the z-axis. Show that the energy levels can be written as

$$E = \left(n + \frac{1}{2}\right)\frac{|e|\hbar}{mc}B + \frac{\hbar^2 k_z^2}{2m} , \quad (71)$$

where $n = 0, 1, 2, \ldots$ is a discrete quantum number and $\hbar k_z$ is the (continous) momentum in the z-direction.

Discuss the qualitative features of the wave functions.

Hint: Use the gauge where $A_x = -By,\ A_y = A_z = 0$.

Solution

We consider the case of a uniform magnetic field $\mathbf{B} = \nabla \times \mathbf{A} = B\mathbf{e}_z$, for which we have $A_x = -By$ and $A_y = A_z = 0$. The Hamiltonian can be written as

$$\hat{H} = \frac{1}{2m}\left[\left(\hat{p}_x + \frac{eB}{c}y\right)^2 + \hat{p}_y^2 + \hat{p}_z^2\right] \quad (72)$$

Since $[\hat{p}_x, \hat{H}] = [\hat{p}_z, \hat{H}] = 0$ as $\hat{H}$ does not depend on x, z explicitly, we may choose the complete set of mechanical variables (p_x, p_z). The corresponding eigenstate is

$$\psi(x, y, z) = \exp i(p_x x + p_z z)/\hbar\chi(y) . \quad (73)$$

Substituting it into the Schrödinger equation, we have

$$\frac{1}{2m}\left[\left(p_x+\frac{eB}{c}y\right)^2-\hbar^2\frac{\partial^2}{\partial y^2}+p_z^2\right]\chi(y)=E\chi(y)\,. \tag{74}$$

Let $cp_x/eB=-y_0$. Then the above equation becomes

$$-\frac{\hbar^2}{2m}\chi''+\frac{m}{2}\left(\frac{eB}{mc}\right)^2(y-y_0)^2\chi=\left(E-\frac{p_z^2}{2m}\right)\chi\,, \tag{75}$$

which is the equation of motion of a harmonic oscillator. Hence the energy levels are

$$E=\frac{\hbar^2k_z^2}{2m}+\left(n+\frac{1}{2}\right)\hbar\frac{|e|\hbar}{mc}\,, \tag{76}$$

where $n=0,1,2,\ldots$, $k_z=p_z/\hbar$, and the wave functions are

$$\psi_{p_xp_zn}(x,y,z)=\exp i(p_xx+p_zz)/\hbar\chi_n(y-y_0)\,, \tag{77}$$

where $\chi_n(y-y_0)$ are the eigenstates for the harmonic oscillator, e.g. products of quadratic exponentials and Hermite polynomials. As the expressions for the energy does not depend on p_x and p_z excplitily, there are infinite degeneracies with respect to p_x and p_z.

The following information might be useful in solving the problem in this exam:

a) The Hamiltonian for a one-dimensional harmonic oscillator is

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \,, \tag{78}$$

where x is the position, m is the mass, and ω is the oscillator frequency. The energy levels are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \,. \tag{79}$$

The ground state wave function for a harmonic oscillator is

$$\psi_0 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp -\frac{1}{2}\frac{m\omega}{\hbar}x^2 \,. \tag{80}$$

b) The integral

$$\int_0^\infty dx \exp -\lambda x^2 = \frac{1}{2}\sqrt{\frac{\pi}{\lambda}} \,. \tag{81}$$