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Problems set # 11	**Physics 400**	May 2, 2019

1. Show that $\Delta E \, \Delta t \geq \hbar/2$, where Δt is the shortest time, during which the average value of a certain quantity is changed by an amount equal to the standard deviation of this quantity.

2. Calculate the eigenfunctions and energy levels for a free particle, enclosed in a box with edges of lengths a, b, and c. [Hint: The presence of the box (because of continuity) requires the wave function to vanish at the edges.]

3. Consider the squared length of the angular momentum vector $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + L_z^2$. Show that $[\hat{L}^2, \hat{L}_i] = 0$, for $i = x, y, z$.

4. Show that the allowed values for l and m_z are integers such that $l = 0, 1, 2, \cdots$ and $m_z = l, \cdots, l-1, l$. [*Hint:* This result can be inferred from the commutation relationship.]

SOLUTIONS

1. For nonrelativistic quantum mechanics, it is not so surprising that time and space are treated differently, with position being an operator and *not time*. After all, this is also what happens in Newtonian mechanics: time is absolute, and part of the background, and all other observables are functions of time. This paradigm underlies the formulation of the fundamental problem of Newtonian physics: to determine how a system evolves in time. Time cannot be an observable because an observable is a function of what we consider the system's "state", but the state is considered a function of time in the first place (so time is the independent variable). In deriving the time-energy uncertainty principle one should be careful in defining the meaning of the standard deviation Δt. It is well known that the total energy of an isolated quantum mechanical system in distinction to a classical one, does not, in general, have a definite constant value. Instead of this the probability to obtain in a measurement any specified value of the energy of the system remains constant in time. The energy can only be determined exactly in the special case of a stationary state. But in this case, as easily seen, all dynamical variables or, more exactly, their distribution functions, remain constant in time. In other words, the *definiteness* of the total energy of the system entails the *constancy* with respect to the time of all dynamical variables. It can be concluded that there must exist a general connection between the dispersion of the total energy of the system and the time variation of coordinates, momenta, etcetera. The uncertainty relation with which are concern gives a quantitative formulation of this connection. Let A and and B denote any two quantities and at the same time the corresponding Hermitian operators. From

$$\Delta A \Delta B \geq \tfrac{1}{2}|\langle[\hat{A},\hat{B}]\rangle| \tag{1}$$

(relation derived in Problems set #6) we have

$$\Delta A\,\Delta B \geq \frac{1}{2}\langle AB - BA\rangle \tag{2}$$

where ΔA and ΔB are the standards of the quatities A and B and $\langle\cdot\rangle$ denotes as usual the quantum mechanical average. In addition, it is easily seen that

$$\frac{\hbar}{2}\frac{\partial\langle B\rangle}{\partial t} = i(\langle HB - BH\rangle) \tag{3}$$

where H is the Hamiltonian of the system not depending explicitely on time. Putting in (2) $A \equiv H$ we obtain, with the help of (3) the desired uncertainty relation for energy, in the form of the follwoing inequality:

$$\Delta H\,\Delta B \geq \frac{\hbar}{2}\left|\frac{\partial\langle B\rangle}{\partial t}\right| . \tag{4}$$

This relation gives, thus, the connection between the standard ΔH of the total energy of an isolated system, the standard ΔB of some other dynamical quantity and the rate of change of the average value of this quantity. The relation (4) can be put in a different form. The absolute value of an integral cannot exceed the integral of the absolute value of the integral. Thus, integrating (4) from t to $t+\delta t$ and taking into account that ΔH is constant one gets

$$\Delta H\,\delta t \geq \frac{\hbar}{2}\frac{|\langle B_{t+\delta t}\rangle - \langle B_t\rangle|}{\Delta B} , \tag{5}$$

where the denominator of the right-hand side denotes the average value of the standard ΔB during the time δt. Sometimes (especially in the case of a continuous spectrum of eigenvalues) it is convenient to refer the variations of the average value of a dynamical quantity to its standard. In such a case it is convenient to introduce a special notation Δt for the shortest time, during which the average value of a certain quantity is changed by an amount equal to the standard of this quantity. Δt can be called the standard time. With the help of this notation we can rewrite (5) in the form of an uncertaity relation

$$\Delta H \, \Delta t \equiv \Delta E \, \Delta t \geq \hbar/2 \,. \tag{6}$$

2. The time-independent Schrödinger equation of a particle of mass m, which is constrained to remain within a finite region of space ("a box") is given by

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E\psi. \tag{7}$$

Let $k^2 = 2mE/\hbar^2$, and note that it is real. This equation can be solved with the help of the separation of variables technique. Start out by trying a solution of the following form $\psi(x,y,z) = X(x)\,Y(y), Z(z)$. Substitution of this solution into the time-independent Schrödinger equation yields: $YZX'' + XZY'' + XYZ'' = -k^2 XYZ$. Then divide both sides of the equation by ψ, obtain $X''/X + Y''/Y + Z''/Z = -k^2$, and note that each of the three terms on the right-hand side is independent of the others, because x, y, z are independent variables. In order for their sum to be equal to a constant, $-k^2$, each of those terms must be independently equal to a constant, such that the sum of all three constants is equal to $-k^2$. Denote those three constants by $-k_x^2$, $-k_y^2$, $-k_z^2$, respectively, such that Schrödinger equation now translates into three ordinary differential equations: $X'' = -k_x^2 X$, $Y'' = -k_y^2 Y$, $Z'' = -k_z^2 Z$. The solutions to these equations are: $X(x) = A\sin(k_x x) + B\cos(k_x x)$, $Y(y) = C\sin(K_y y) + D\cos(k_y y)$, $Z(z) = F\sin(k_z x) + G\cos(k_z x)$, where A, B, C, D, F, and G are (complex) undetermined parameters. Since the infinitely high walls do not allow the particle to leave the box, the wave function is zero at all times for $(x,y,z) < (0,0,0)$ and $(x,y,z) > (a,b,c)$, and hence $\psi(0,0,0) = \psi(a,b,c) = 0$, because the wave function needs to be continuous. Imposing $\psi(0,0,0) = 0$ implies $B = D = G = 0$, whereas applying the second boundary condition $\psi(a,b,c) = 0$ yields $k_x a = n\pi$, $k_y b = m\pi$, and $k_z c = l\pi$, with $n, m, l \in \mathbb{Z}$. The particle is equally likely to be found everywhere, $\int_0^a \int_0^b \int_0^c |\psi(x,y,z)|^2 dxdydz = 1$, and so $N = ACF$ can be determined from the requirement that the wave function is normalized, i.e.

$$|N|^2 \int_o^a \int_0^b \int_0^c \sin^2(n\pi x/a)\sin^2(m\pi y/b)\sin^2(l\pi z/c)\, dx\, dy\, dz = \frac{1}{8}|N|^2 abc \Rightarrow |N| = \sqrt{\frac{8}{abc}}. \tag{8}$$

All in all, the stationary states of a particle in a 3-dimensional box are given by

$$\psi_{nlm}(x,y,z) = \sqrt{\frac{8}{abc}} \sin(n\pi x/a)\, \sin(m\pi y/b)\, \sin(l\pi z/c), \tag{9}$$

and the corresponding energy levels are

$$E_{n,m,l} = \frac{\hbar^2\pi^2}{2m}(\frac{n^2}{a^2} + \frac{m^2}{b^2} + \frac{l^2}{c^2}). \tag{10}$$

3. Consider the commutator $[\hat{L}^2, \hat{L}_z]$:

$$\begin{aligned} [\hat{L}^2, \hat{L}_z] &= [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_z] \quad \text{from the definition of } \hat{L}^2 \\ &= [\hat{L}_x^2, \hat{L}_z] + [\hat{L}_y^2, \hat{L}_z] + [\hat{L}_z^2, \hat{L}_z] \\ &= [\hat{L}_x^2, \hat{L}_z] + [\hat{L}_y^2, \hat{L}_z] \quad \text{since } \hat{L}_z \text{ commutes with itself} \\ &= \hat{L}_x\hat{L}_x\hat{L}_z - \hat{L}_z\hat{L}_x\hat{L}_x + \hat{L}_y\hat{L}_y\hat{L}_z - \hat{L}_z\hat{L}_y\hat{L}_y \,. \end{aligned} \tag{11}$$

We can use the commutation relation $[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$ to rewrite the first term on the right-hand side as $\hat{L}_x\hat{L}_x\hat{L}_z = \hat{L}_x\hat{L}_z\hat{L}_x - i\hbar\hat{L}_x\hat{L}_y$, and the second term as $\hat{L}_z\hat{L}_x\hat{L}_x = \hat{L}_x\hat{L}_z\hat{L}_x + i\hbar\hat{L}_y\hat{L}_z$. In a similar way, we can use $[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$ to rewrite the third term as $\hat{L}_y\hat{L}_y\hat{L}_z = \hat{L}_y\hat{L}_z\hat{L}_y + i\hbar\hat{L}_y\hat{L}_x$, and the fourth term $\hat{L}_z\hat{L}_y\hat{L}_y = \hat{L}_y\hat{L}_z\hat{L}_y - i\hbar\hat{L}_x\hat{L}_y$. Thus, on substituting in we find that

$$[\hat{L}^2, \hat{L}_z] = -i\hbar\hat{L}_x\hat{L}_y - i\hbar\hat{L}_y\hat{L}_x + i\hbar\hat{L}_y\hat{L}_x + i\hbar\hat{L}_x\hat{L}_y = 0 \,. \tag{12}$$

By performing a cyclic permutation of the indexes, we can show that this holds in general, i.e. $[\hat{L}^2, \hat{L}_i] = 0$, for $i = x, y, z$.

4. Assume that the eigenvalues of $\hat{L}^2$ and $\hat{L}_z$ are unknown and denote them λ and μ. We introduce two new operators, the raising and lowering operators $\hat{L}_+ = \hat{L}_x + i\hat{L}_y$ and $\hat{L}_- = \hat{L}_x - i\hat{L}_y$. The commutator with L_z is $[\hat{L}_z, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm$ (while they of course commute with L^2). Now consider the function $f_\pm = \hat{L}_\pm f$, where f is an eigenfunction of $\hat{L}^2$ and $\hat{L}_z$:

$$\hat{L}^2 f_\pm = \hat{L}_\pm\hat{L}^2 f = \hat{L}_\pm\lambda f = \lambda f_\pm \quad \text{and} \quad \hat{L}_z f_\pm = [\hat{L}_z, \hat{L}_\pm]f + \hat{L}_\pm\hat{L}_z f = \pm\hbar\hat{L}_\pm f + \hat{L}_\pm\mu f = (\mu \pm \hbar) f_\pm \,. \tag{13}$$

Then $f_\pm = \hat{L}_\pm f$ is also an eigenfunction of $\hat{L}^2$ and $\hat{L}_z$. Moreover, we can keep finding eigenfunctions of $\hat{L}_z$ with higher and higher eigenvalues $\mu' = \mu + \hbar + \hbar + \cdots$, by applying the $\hat{L}_+$ operator (or lower and lower with $\hat{L}_-$), while the $\hat{L}^2$ eigenvalue is fixed. Of course there is a limit, since we want $\mu' \leq \lambda$. Then there is a maximum eigenfunction such that $\hat{L}_+ f_M = 0$ and we set the corresponding eigenvalue to $\hbar l_M$. Now note that we can write $\hat{L}^2$ instead of using $\hat{L}_{x,y}$ by using $\hat{L}_\pm$:

$$\hat{L}^2 = \hat{L}_-\hat{L}_+ + \hat{L}_z^2 + \hbar\hat{L}_z \,. \tag{14}$$

Using this relationship on f_M we find:

$$\hat{L}^2 f_M = \lambda f_M \Rightarrow (\hat{L}_-\hat{L}_+ + \hat{L}_z^2 + \hbar\hat{L}_z) f_M = [0 + \hbar^2 l_M^2 + \hbar(\hbar l_M)] f_M \Rightarrow \lambda = \hbar^2 l_M(l_M + 1) \,. \tag{15}$$

In the same way, there is also a minimum eigenvalue l_m and eigenfunction such that $\hat{L}_- f_m = 0$ and we can find $\lambda = \hbar^2 l_m(l_m - 1)$. Since λ is always the same, we also have $l_m(l_m - 1) = l_M(l_M + 1)$, with solution $l_m = -l_M$ (the other solution would have $l_m > l_M$). Finally, we have found that the eigenvalues of L_z are between $+\hbar l$ and $-\hbar l$ with integer increases, so that $l = -l + N$ giving $l = N/2$: that is, l is either an integer or a half-integer. We thus set $\lambda = \hbar^2 l(l + 1)$ and $\mu = \hbar m$, with $m = -l, -l + 1, \cdots, l$.