SOLUTIONS for Homework #7

1. In the coordinate representation the eigenfunctions $\psi(x)$ of $\hat{F}$ satisfy the differential equation

$$\hat{F}\psi(x) = \left(\alpha x - i\hbar\beta\frac{d}{dx}\right)\psi(x) = f\psi(x), \tag{1}$$

where f is the corresponding eigenvalue. Solving this equation we obtain

$$\psi(x) = Ae^{-i(\alpha/2\hbar\beta)x^2 + i(f/\hbar\beta)}x, \tag{2}$$

where A is a normalization constant.

To find the conditions for this function to be *physically acceptable*, we calculate the probability density

$$|\psi(x)|^2 = |A|^2 e^{(1/\hbar)\mathrm{Im}[(\alpha/\beta)x^2 - 2(f/\beta)x]}. \tag{3}$$

This quantity will not have an unphysical growth at $x \to \pm\infty$ only if

$$\mathrm{Im}\left(\frac{\alpha}{\beta}\right) < 0. \tag{4}$$

In particular, the operator $\hat{x}+i\hat{p}$ has reasonable eigenfunctions $(\alpha/\beta = -i)$ while $\hat{x} - i\hat{p}$ has not $(\alpha/\beta = i)$. Later, studying the harmonic oscillator, we will understand this difference in more physical terms.

An observable quantity corresponds to a *Hermitian* operator. On the class of functions we consider acceptable, $\hat{x}$ and $\hat{p}$ are Hermitian operators. Therefore $\hat{F}$ is *observable* if α and β are *real* numbers. Then $\mathrm{Im}(\alpha/\beta) = 0$, and the probability density (3) becomes

$$|\psi|^2 = |A|^2 e^{-(2/\hbar\beta)x\,\mathrm{Im}\,f}. \tag{5}$$

This result is again unacceptable since the probability density exponentially increases in one direction of the x-axis. The only allowed case corresponds to $\mathrm{Im}\,f = 0$. This means that allowed eigenvalues f are *real*, as it should be for a Hermitian operator. We conclude that, for an observable $\hat{F}$, the physical spectrum consists of all real numbers f, and each eigenvalue corresponds to a unique eigenfunction (2) (no degeneracy).

For two eigenfunctions (2) corresponding to the real eigenvalues f, f' and real parameters α, β we find

$$\int_{-\infty}^{\infty} dx\,\psi_f^*\psi_{f'} = A_f^* A_{f'} \int dx\, e^{(i/\hbar\beta)(f'-f)x} = 2\pi\hbar|\beta|\delta(f'-f). \tag{6}$$

Here we have used a standard formula

$$\delta(ax) = \frac{1}{|a|}\delta(x), \tag{7}$$

which follows from the limiting process of defining the δ-function as an *even* function of its argument. As it should be for an Hermitian operator, the eigenfunctions corresponding to different eigenvalues are *orthogonal*. It is easy to see that for complex values of the parameters it would be no orthogonality. Now we can choose for all f

$$A_f = \frac{1}{\sqrt{2\pi\hbar|\beta|}} \quad \rightsquigarrow \quad \int_{-\infty}^{\infty} dx\, \psi_f^* \psi_{f'} = \delta(f' - f). \tag{8}$$

With this normalization we can check the *completeness* of the continuous spectrum of the eigenvalues $\{f\}$:

$$\int_{-\infty}^{\infty} df\, \psi_f(x)\psi_f^*(x') = \frac{1}{2\pi\hbar|\beta|} e^{(i\alpha/\hbar\beta)(x^2 - x'^2)} \int df\, e^{(i/\hbar\beta)(x-x')f}. \tag{9}$$

The integral here equals $2\pi\hbar|\beta|\delta(x - x')$; with $x = x'$ the exponential factor in front of the integral becomes 1, and

$$\int_{-\infty}^{\infty} df\, \psi_f(x)\psi_f^*(x') = \delta(x - x'), \tag{10}$$

as required for completeness.

2. *a*. Let us denote by a tilde the transformed functions,

$$\tilde{\psi}(\mathbf{r}) = \hat{\mathcal{P}}\psi(\mathbf{r}) = \psi(-\mathbf{r}), \tag{11}$$

and transformed operators

$$\tilde{\hat{\mathcal{O}}} = \hat{\mathcal{P}}\hat{\mathcal{O}}\hat{\mathcal{P}}^{-1}. \tag{12}$$

The new operators have the same physical amplitudes (matrix elements) between new functions as the old operators between old functions,

$$\int d^3r\, \tilde{\psi}_1^*(\mathbf{r})\tilde{\hat{\mathcal{O}}}\tilde{\psi}_2(\mathbf{r}) = \int d^3r\, \psi_1^*(\mathbf{r})\hat{\mathcal{O}}\psi_2(\mathbf{r}). \tag{13}$$

Here we use the coordinate representation of the wave functions. For $\hat{\mathcal{O}} \Rightarrow \hat{\mathbf{r}}$ we find

$$\int d^3r\, \tilde{\psi}_1^*(\mathbf{r})\tilde{\hat{\mathbf{r}}}\tilde{\psi}_2(\mathbf{r}) = \int d^3r\, \psi_1^*(-\mathbf{r})\tilde{\hat{\mathbf{r}}}\psi_2(-\mathbf{r}) = -\int d^3r\, \psi_1^*(\mathbf{r})\tilde{\hat{\mathbf{r}}}\psi_2(\mathbf{r}). \tag{14}$$

On the other hand, according to eq. (13), this integral has to be equal to

$$\int d^3r\, \psi_1^*(\mathbf{r})\hat{\mathbf{r}}\psi_2(\mathbf{r}).$$

The comparison shows that

$$\hat{\mathcal{P}}\hat{\mathbf{r}}\hat{\mathcal{P}}^{-1} \equiv \tilde{\hat{\mathbf{r}}} = -\hat{\mathbf{r}}, \tag{15}$$

as it must be for spatial inversion. Analogously we find for the momentum operator $\hat{\mathbf{p}}$:

$$\int d^3r\, \psi_1^*(\mathbf{r})\hat{\mathbf{p}}\psi_2(\mathbf{r}) = \int d^3r\, \psi_1^*(-\mathbf{r})\tilde{\hat{\mathbf{p}}}\psi_2(-\mathbf{r}). \tag{16}$$

Changing the integration variable $\mathbf{r} \to -\mathbf{r}$ in the left hand side, we obtain

$$\int d^3r\, \psi_1^*(-\mathbf{r}) \left(-i\hbar\frac{\partial}{\partial(-\mathbf{r})}\right) \psi_2(-\mathbf{r}) = -\int d^3r\, \psi_1^*(-\mathbf{r})\hat{\mathbf{p}}\psi_2(-\mathbf{r}), \tag{17}$$

and the comparison with (16) shows that

$$\hat{\mathcal{P}}\hat{\mathbf{p}}\hat{\mathcal{P}}^{-1} \equiv \tilde{\hat{\mathbf{p}}} = -\hat{\mathbf{p}}, \tag{18}$$

in agreement with the classical definition $\mathbf{p} = m\dot{\mathbf{r}}$, which is valid also for quantum equations of motion. Vectors, such as $\mathbf{r}$ and $\mathbf{p}$, which change sign under spatial inversion, are called *polar vectors*. On the other hand, the orbital momentum vector $\mathbf{L} = [\mathbf{r} \times \mathbf{p}]$ behaves in an opposite way: its components do not change sign under inversion:

$$\hat{\mathcal{P}}\hat{\mathbf{L}}\hat{\mathcal{P}}^{-1} = [(\hat{\mathcal{P}}\hat{\mathbf{r}}\hat{\mathcal{P}}^{-1}) \times (\hat{\mathcal{P}}\hat{\mathbf{p}}\hat{\mathcal{P}}^{-1}] = \hat{\mathbf{L}}. \tag{19}$$

Such vectors are called *axial vectors*, or *pseudovectors*.

b. Using the relation between the coordinate, $\psi(\mathbf{r})$, and momentum, $\phi(\mathbf{p})$, wave functions, we require that the two forms of the operator, $\hat{\mathcal{O}}_{\rm coord}$ and $\hat{\mathcal{O}}_{\rm mom}$, acting onto $\psi(\mathbf{r})$ and $\phi(\mathbf{p})$, respectively, would keep intact the connection between the two functions via the Fourier-transformation:

$$\hat{\mathcal{O}}_{\rm coord}\psi(\mathbf{r}) = \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{(i/\hbar)(\mathbf{p}\cdot\mathbf{r})}\hat{\mathcal{O}}_{\rm mom}\phi(\mathbf{p}). \tag{20}$$

For the *inversion* operator this gives

$$\int \frac{d^3p}{(2\pi\hbar)^3}\, e^{-(i/\hbar)(\mathbf{p}\cdot\mathbf{r})}\phi(\mathbf{p}) = \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{(i/\hbar)(\mathbf{p}\cdot\mathbf{r})}\hat{\mathcal{P}}_{\rm mom}\phi(\mathbf{p}). \tag{21}$$

Changing the integration variable $\mathbf{p} \to -\mathbf{p}$, we see that

$$\hat{\mathcal{P}}_{\rm mom}\phi(\mathbf{p}) = \phi(-\mathbf{p}). \tag{22}$$

The inversion operator acts identically in the coordinate and momentum representations.

For the *translation* operator the same procedure gives

$$\hat{\mathcal{D}}_{\rm coord}(\mathbf{a})\psi(\mathbf{r}) = \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{-(i/\hbar)\mathbf{p}\cdot(\mathbf{r}-\mathbf{a})}\phi(\mathbf{p}) = \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{(i/\hbar)(\mathbf{p}\cdot\mathbf{r})}\hat{\mathcal{D}}_{\rm mom}\phi(\mathbf{p}). \tag{23}$$

Thus, in the momentum representation the spatial displacement induces the phase transformation,

$$\hat{\mathcal{D}}_{\rm mom}(\mathbf{a})\phi(\mathbf{p}) = e^{-(i/\hbar)(\mathbf{p}\cdot\mathbf{a})}\phi(\mathbf{p}). \tag{24}$$

This agrees with the general definition of the translation operator

$$\hat{\mathcal{D}}(\mathbf{a}) = e^{-(i/\hbar)(\hat{\mathbf{p}}\cdot\mathbf{a})}, \tag{25}$$

which is valid in an arbitrary representation.

c. If a coordinate function has a certain parity $\Pi = \pm 1$,

$$\psi(\mathbf{r}) = \Pi\psi(-\mathbf{r}), \tag{26}$$

we find for its momentum counterpart

$$\phi(\mathbf{p}) = \int d^3r\, e^{(-i/\hbar)(\mathbf{p}\cdot\mathbf{r})}\psi(\mathbf{r}) = \Pi\int d^3r\, e^{(-i/\hbar)(\mathbf{p}\cdot\mathbf{r})}\psi(-\mathbf{r}) =$$

$$\Pi\int d^3r\, e^{(i/\hbar)(\mathbf{p}\cdot\mathbf{r})}\psi(\mathbf{r}) = \Pi\phi(-\mathbf{p}). \tag{27}$$

3. The normalized stationary wave functions for a particle confined to a potential box $0 \le x \le a$ are

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right), \quad n = 1, 2, ... \tag{28}$$

The distribution of coordinates is given by

$$w_n(x) = |\psi_n(x)|^2 = \frac{2}{a}\sin^2\left(\frac{n\pi}{a}x\right). \tag{29}$$

For the following calculations we need the integrals

$$\int dx\, x\sin^2 x = \frac{1}{4}\left[x^2 - x\sin(2x) - \frac{1}{2}\cos(2x)\right], \tag{30}$$

$$\int dx\, x^2\sin^2 x = \frac{x^3}{6} - \left(\frac{x^2}{4} - \frac{1}{8}\right)\sin(2x) - \frac{x\cos(2x)}{4}. \tag{31}$$

Obviously, the mean value of the coordinate is at the middle of the box,

$$\langle n|x|n\rangle = \int_0^a dx\, x w_n(x) = \frac{a}{2}. \tag{32}$$

The mean square value of the coordinate is equal to

$$\langle n|x^2|n\rangle = a^2 \left[\frac{1}{3} - \frac{1}{2(\pi n)^2}\right], \tag{33}$$

and the dispersion of the coordinate

$$(\Delta x)_n^2 = \langle n|x^2|n\rangle - \langle n|x|n\rangle^2 = \frac{a^2}{12}\left[1 - \frac{6}{(\pi n)^2}\right]. \tag{34}$$

b. The Fourier-transformation leads to the wave function in the momentum representation

$$\phi_n(p) = \int_0^a dx\, e^{-(i/\hbar)px}\psi_n(x) = \sqrt{2}a\left[1 - (-)^n e^{-(i/\hbar)pa}\right]\frac{(\pi n/a)}{(\pi n/a)^2 - (p/\hbar)^2}. \tag{35}$$

From here we find the distribution function for the momentum

$$w_n(p) = |\phi_n(p)|^2 = \frac{4}{a}[1 - (-)^n \cos(pa/\hbar)]\frac{(\pi n/a)^2}{[(\pi n/a)^2 - (p/\hbar)^2]^2}. \tag{36}$$

An apparent divergence at the points $p = \pm n\pi\hbar/a$ is compensated by the zeros of the square bracket.

In order to calculate the expectation values of p and p^2 it is easier to use the coordinate representation and the corresponding operator $\hat{p} = -i\hbar(d/dx)$. Then we see immediately that

$$\langle n|\hat{p}|n\rangle = 0, \tag{37}$$

as expected for a *standing wave*. The mean square momentum is

$$\langle n|\hat{p}^2|n\rangle = (\Delta p)_n^2 = \left(\frac{\pi\hbar n}{a}\right)^2, \tag{38}$$

as it was easy to figure out from known energies (inside the box the total energy is kinetic one),

$$E_n = \langle n|\hat{K}|n\rangle = \frac{\pi^2\hbar^2 n^2}{2ma^2} = \frac{\langle n|\hat{p}^2|n\rangle}{2m}. \tag{39}$$

The uncertainty product can be found from (34) and (38):

$$(\Delta x)_n^2(\Delta p)_n^2 = \frac{\hbar^2}{12}\left[(\pi n)^2 - 6\right]. \tag{40}$$

The uncertainty relation holds: even for the minimum case, $n = 1$,

$$(\Delta x)_n(\Delta p)_n = \hbar\frac{\sqrt{\pi^2 - 6}}{2\sqrt{3}} > \frac{\hbar}{2}. \tag{41}$$

When one starts to think about the fluctuation of kinetic energy, the situation seems to be contradictory. Naively, one would say, as we did above, that inside the box the total Hamiltonian is reduced to kinetic energy, $\hat{H} \to \hat{K}$, the value of energy is fixed on the level E_n, and therefore kinetic energy does not fluctuate, $\langle n|\hat{K}^2|n\rangle = \langle n|\hat{K}|n\rangle^2$. On the other hand, if we use the momentum probability density (36) for calculating

$$\langle n|\hat{K}^2|n\rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} w_n(p)\frac{p^4}{4m^2}, \tag{42}$$

we would see that this integral *diverges* at large momenta. Indeed, at $|p| \to \infty$, the distribution density $w_n(p) \propto p^{-4}$, and the integral with p^4 from the operator $\hat{K}^2$ is divergent.

To resolve this controversy, we need to discuss the physical procedure of measuring the value of kinetic energy. To measure the content of kinetic energy for the state of a particle confined to a box, we need to instantly remove the walls and allow the particle to move freely. The wave function has no time to change. But now the momentum is a constant of motion (no potential walls any longer) so that each momentum component propagates independently and can be registered with the probability $w_n(p)$. Repeating the experiment many times, we can extract the distribution function of the momentum or kinetic energy. Then the result should agree with the calculation according to eq. (42) and give $\langle K^2\rangle \to \infty$. By the way, this is a real way of measuring the momentum distribution for atoms in a trap, for example in the studies of the *Bose-Einstein condensate*. The trap is suddenly removed, and the momenta are measured of free atoms (in those experiments the trap potential is close to that of a harmonic oscillator).

A correct consideration in the coordinate representation leads to the same conclusion of divergency. Indeed, having in mind the discussed above procedure of measurement, we need to consider the wave function in entire space. As we have seen in the derivation of the boundary conditions for an impenetrable wall, the condition $\psi = 0$ on the wall is a result of a limiting transition from a finite wall to the infinite one. In this consideration kinetic energy is not equal to the total Hamiltonian because of the presence of the walls. As a function in entire space, the wave function in the box is continuous at the wall, the first derivative has a finite discontinuity (zero outside and finite inside), and the second derivative is *infinite*, as a consequence of having the infinite potential. This infinity generates very high Fourier-components responsible for the divergence of the integral in the momentum representation. Therefore the calculation of $\langle \hat{p}^4 \rangle$ should go as follows:

$$\langle n|\hat{p}^4|n\rangle = \int_{-\infty}^{\infty} dx\, \psi_n^*(x)\hat{p}^4\psi_n(x) = \int_{-\infty}^{\infty} dx\, \left|\hat{p^2}\psi_n(x)\right|^2, \tag{43}$$

where we used the Hermiticity of the operator $\hat{p}^4$, and now we see that the integral contains the square of the second derivative of the wave function. The second derivative is infinite at the boundaries, i.e. contains contributions $\delta(x)$ and $\delta(x-a)$ proportional to the infinite potential. The integral $\int dx\, [\delta(x)]^2 = \delta(0)$ is infinite.

4. *a*. Due to the symmetry of the potential with respect to the middle point $x = 0$, solutions can be classified by their *parity*. This classification appears naturally in the process of the standard solution, and the even and odd solutions have rather different properties. In the left half of the box we need to apply the boundary condition $\psi(-a) = 0$. Then the appropriate standing wave can be written as

$$\psi(x) = A\sin[k(x+a)], \quad -a < x < 0. \tag{44}$$

Similarly, in the right half of the box

$$\psi(x) = B\sin[k(x-a)], \quad 0 < x < a; \tag{45}$$

in both cases

$$k = \sqrt{\frac{2mE}{\hbar^2}}. \tag{46}$$

Matching the functions in the middle we obtain

$$A\sin(ka) = -B\sin(ka). \tag{47}$$

There are two ways to satisfy this condition. First, we can have $B = -A$. In this case, as it easy to see, $\psi(-x) = \psi(x)$, the solution is an *even* function. Second, we can have $\sin(ka) = 0$. In this case, the wave function vanishes at the origin, $\psi(0) = 0$, which corresponds to an *odd* solution. The odd case is trivial: a particle never sees the partition because the probability to be at this point is zero. Therefore these levels are exactly the same as if it were in a box of width $2a$ without a partition,

$$\psi_n^{\text{odd}} = \sqrt{\frac{2}{2a}}\sin\left(\frac{\pi\hbar}{2a}nx\right), \quad E_n = \frac{\pi^2\hbar^2}{2m(2a)^2}n^2, \quad n = 2, 4, \ldots \tag{48}$$

The *even* case, $B = -A$, requires a special treatment.The matching condition for the derivative of the wave function at the point $x = a$ of the δ-wall gives

$$kB\cos(ka) - kA\cos(ka) = \frac{2mg}{\hbar^2}A\sin(ka). \tag{49}$$

With $B=-A$ we find a transcendental equation for the bound states

$$\tan\xi=-\xi y, \quad \xi=ka, \quad y=\frac{\hbar^2}{mag}. \tag{50}$$

This gives an infinite series of the roots, see the drawing. The origin $\xi=ka=0$ is not a solution since here $\psi\equiv 0$.

b. In this special case $y\ll 1$, and the straight line has a small negative slope. For low-lying levels, the intersection with the curve $\tan\xi$ occurs close to the points $\tan\xi=0$, $\xi=n\pi$, $n=1,2,...$, but slightly below those points:

$$\xi_n=n\pi-\alpha_n, \quad \tan\xi_n\approx-\alpha_n, \quad \rightsquigarrow \quad \alpha_n\approx n\pi y. \tag{51}$$

These solutions are close to the corresponding odd roots (48),

$$E_n^{\text{even}}=\frac{\xi_n^2\hbar^2}{2ma^2}\approx\frac{\pi^2\hbar^2}{2ma^2}n^2(1-2y), \tag{52}$$

so that the splitting can be written as

$$\Delta_n\equiv E_n^{\text{even}}-E_n^{\text{odd}}\approx-2y\frac{\pi^2\hbar^2}{2ma^2}n^2, n=1,2,... \tag{53}$$

The level come in pairs with the splitting smaller than the distance to the next pair $E_{n+1}-E_n$ for not very large $n\ll 1/y$. The ground state function is always even. Here the coupling between the left and right parts is weak, and we have the system of levels in a half-well mirrored in an even or odd fashion in the second half. For the odd case there is no coupling at all; the presence of the attractive coupling for the even states lowers the energy.

*c.*The spectrum of the even states at high energies, $\xi\gg 1/y$, corresponds to the point near the infinite values of $\tan\xi$,

$$\xi_n=\pi\left(n-\frac{1}{2}\right)+\beta_n, \quad \beta_n\ll 1, \quad n=1,2,... \tag{54}$$

Here

$$\tan\xi_n\approx 1/\beta_n=\xi_n y\approx\pi y\left(n-\frac{1}{2}\right), \tag{55}$$

and the energies are

$$E_n^{\text{even}}\approx\frac{\hbar^2}{ma^2}\left[\pi^2\frac{(2n-1)^2}{8}+\frac{1}{y}\right], \tag{56}$$

being close to the even levels in an empty box of width $2a$. The correction $1/y$ describes a small shift of high levels due to the partition.