SOLUTIONS for Homework #9

1. *Exercise 5.4.* Obviously, $P_{n-1} \equiv H'_n$ is a polynomial of the $(n-1)^{\text{th}}$ order. Taking the derivative of the Hermite equation

$$H''_n - 2\xi H'_n + 2nH_n = 0, \tag{1}$$

we obtain

$$H'''_n - 2(\xi H''_n + H'_n) + 2nH'_n = 0, \tag{2}$$

or

$$P''_{n-1} - 2\xi P'_{n-1} + 2(n-1)P_{n-1} = 0. \tag{3}$$

This should be compared with the Hermite equation of the $(n-1)^{\text{th}}$ order,

$$H''_{n-1} - 2\xi H'_{n-1} + 2(n-1)H_{n-1} = 0. \tag{4}$$

We see that the polynomials H_{n-1} and P_{n-1} should be proportional,

$$\frac{dH_n}{d\xi} \equiv P_{n-1} = C_n H_{n-1}. \tag{5}$$

To find the coefficient of proportionality, we use the property

$$\frac{d^n H_n}{d\xi^n} = 2^n n!. \tag{6}$$

Taking $(n-1)$ times the derivative of eq. (5), we find

$$2^n n! = C_n 2^{n-1}(n-1)! \quad \rightsquigarrow \quad C_n = 2n. \tag{7}$$

Finally,

$$\frac{dH_n(\xi)}{d\xi} = 2nH_{n-1}(\xi). \tag{8}$$

Exercise 5.5. The normalized harmonic oscillator wave functions are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-\xi^2/2} H_n(\xi), \quad x = \sqrt{\frac{\hbar}{m\omega}}\xi. \tag{9}$$

A matrix element of an operator $\hat{\mathcal{O}}$,

$$\langle n|\hat{\mathcal{O}}|k\rangle = \int_{-\infty}^{\infty} dx\, \psi_n(x)\hat{\mathcal{O}}\psi_k(x), \tag{10}$$

can be written as

$$\langle n|\hat{\mathcal{O}}|k\rangle = \frac{1}{\sqrt{\pi 2^{k+n} k! n!}} \int_{-\infty}^{\infty} d\xi\, e^{-\xi^2/2} H_n(\xi)\hat{\mathcal{O}} e^{-\xi^2/2} H_k(\xi). \tag{11}$$

In particular, for $\hat{\mathcal{O}} = x^p$,

$$\langle n|x^p|k\rangle = \left(\frac{\hbar}{m\omega}\right)^{p/2} \frac{1}{\sqrt{\pi 2^{k+n} k! n!}} I_{n,k;p}, \tag{12}$$

where we have borrowed the notation

$$I_{n,k;p} = \int d\xi \, e^{-\xi^2} H_n(\xi) H_k(\xi) \xi^p \tag{13}$$

from eq. (5.36), *Merzbacher*, p. 87. According to the generating equation [*Merzbacher*, (5.37)],

$$\sum_{nkp} I_{n,k;p} \frac{s^n t^k (2\lambda)^p}{n!k!p!} = \sqrt{\pi} e^{\lambda^2 + 2[st + \lambda(s+t)]}. \tag{14}$$

We need to find $I_{n,k;1}$. To do this, we equate the coefficients in front of (2λ):

$$\sum_{nk} I_{n,k;1} \frac{s^n t^k}{n!k!} = \sqrt{\pi} e^{2st}(s+t). \tag{15}$$

The right hand side can be presented as a series,

$$\sqrt{\pi} e^{2st}(s+t) = \sqrt{\pi} \sum_r \frac{2^r}{r!} (s^{r+1} t^r + s^r t^{r+1}). \tag{16}$$

Thus, the only nonvanishing coefficients among $I_{n,k;1}$ are those for $k = n \pm 1$,

$$I_{r,r+1;1} = I_{r+1,r:1} = \sqrt{\pi} 2^r (r+1)!. \tag{17}$$

The resulting expressions follow now from (12) and (17),

$$\langle n|x|n+1\rangle = \sqrt{\frac{\hbar}{2m\omega}(n+1)}, \tag{18}$$

$$\langle n|x|n-1\rangle = \sqrt{\frac{\hbar}{2m\omega} n}, \tag{19}$$

In an analogous fashion we find that x^2 has nonvanishing diagonal elements, $n = k$, and off-diagonal with $k = n \pm 2$:

$$\langle n|x^2|n\rangle = \frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right), \tag{20}$$

$$\langle n|x^2|n+2\rangle = \frac{\hbar}{2m\omega}\sqrt{(n+1)(n+2)}, \tag{21}$$

$$\langle n|x^2|n-2\rangle = \frac{\hbar}{2m\omega}\sqrt{n(n-1)}, \tag{22}$$

2. *Exercise 5.8.* The calculation can be performed with the use of (8) or more general result (23). The matrix elements of the momentum operator, similarly to the coordinate matrix elements (18) and (19), do not vanish only for $\Delta n = \pm 1$,

$$\langle n|\hat{p}|n+1\rangle = -i\sqrt{\frac{m\omega\hbar}{2}(n+1)}, \tag{23}$$

$$\langle n|\hat{p}|n-1\rangle = i\sqrt{\frac{m\omega\hbar}{2}n}. \tag{24}$$

Of course, Hermiticity holds,

$$\langle n|\hat{p}|n+1\rangle = \langle n+1|\hat{p}|n\rangle^*. \tag{25}$$

The wave packet

$$\Psi(x,0) = \sum_n c_n \psi_n(x) \tag{26}$$

evolves in time according to

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-i\omega t(n+1/2)}. \tag{27}$$

Then the time-dependent expectation value of the momentum can be found as

$$\langle \hat{p}\rangle_t = \sum_{nk} c_n^* c_k e^{i(n-k)\omega t} \langle n|\hat{p}|k\rangle. \tag{28}$$

Using our previous results for the matrix elements $\langle n|\hat{p}|n \pm 1\rangle$ we obtain

$$\langle \hat{p}\rangle_t = \sum_n c_n^* \{c_{n+1} e^{-i\omega t} \langle n|\hat{p}|n+1\rangle + c_{n-1} e^{i\omega t} \langle n|\hat{p}|n-1\rangle$$

$$= -i\sqrt{\frac{m\omega\hbar}{2}} \sum_n \sqrt{n} \{c_{n-1}^* c_n e^{-i\omega t} - c_n^* c_{n-1} e^{i\omega t}\}. \tag{29}$$

The comparison with eq. (5.55), *Merzbacher*, p. 90, shows that the equation of motion is valid,

$$\frac{d}{dt}\langle \hat{x}\rangle_t = \frac{\langle \hat{p}\rangle_t}{m}. \tag{30}$$

Exercise 5.9 follows as a straightforward consequence of found equations for $\langle \hat{x}\rangle$ and $\langle \hat{p}\rangle$.

3. The distribution of the oscillator coordinate in the thermal ensemble is given by

$$f(x) = \sum_n \rho_n(T) \psi_n^2(x). \tag{31}$$

Note that, due to the normalization of ρ_n, this distribution is normalized as well,

$$\int dx\, f(x) = 1. \tag{32}$$

With the explicit form of the oscillator eigenfunctions,

$$f(x) = \frac{1}{Z} e^{-(n+1/2)\hbar\omega/T} \sqrt{\frac{m\omega}{\pi\hbar}} \frac{1}{2^n n!}\, e^{-\xi^2} H_n^2(\xi), \quad \xi = \sqrt{\frac{m\omega}{\hbar}} x. \tag{33}$$

Here we can use the integral representation of Hermite polynomials [eq.(5.43), *Merzbacher*],

$$H_n(\xi) = \frac{2^n}{\sqrt{\pi}} \int_{-\infty}^{\infty} dv(\xi + iv)^n e^{-v^2}, \tag{34}$$

Because of the normalization (32), we can ignore constant factors and write down eq. (33) in the form

$$f(x) = \text{const}\, e^{-\xi^2} \sum_n \frac{(2\eta)^n}{n!} \int dv\, dv'\, (\xi + iv)^n (\xi + iv')^n e^{-(v^2+v'^2)}, \tag{35}$$

where

$$\eta = e^{-\hbar\omega/T}. \tag{36}$$

First we carry out the summation over n,

$$\sum_n \frac{(2\eta)^n}{n!} (\xi + iv)^n (\xi + iv')^n = e^{2\eta(\xi+iv)(\xi+iv')}. \tag{37}$$

Now we calculate the two-dimensional Gaussian integral

$$\int dv\, dv'\, e^{-(v^2+v'^2)+2\eta(\xi+iv)(\xi+iv')} = \text{const}\, e^{[2\eta/(1+\eta)]\xi^2}. \tag{38}$$

Together with the factor $\exp(-\xi^2)$ from eq. (35), this determines the Gaussian distribution

$$f(x) = \text{const}\, e^{-[(1-\eta)/(1+\eta)]\xi^2}. \tag{39}$$

The factor in the exponent here is

$$\frac{1-\eta}{1+\eta} = \frac{1 - e^{-\hbar\omega/T}}{1 + e^{-\hbar\omega/T}} = \tanh \frac{\hbar\omega}{2T}. \tag{40}$$

Going back to the coordinate variable x and adding the standard normalizing Gaussian factor, we obtain

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}, \tag{41}$$

where the width σ is determined by

$$\sigma^2 = \frac{\hbar}{2m\omega} \coth \frac{\hbar\omega}{2T}. \tag{42}$$

In the classical region of high temperature, $\hbar\omega \ll T$,

$$\coth \frac{\hbar\omega}{2T} \approx \frac{2T}{\hbar\omega}, \quad \sigma^2 \approx \frac{T}{m\omega^2}, \tag{43}$$

the Planck constant disappears, and we come to the classical Boltzmann distribution

$$f(x) \propto e^{-(m\omega^2/2T)x^2} = e^{-U(x)/T}. \tag{44}$$

In the opposite case of low temperature, $\hbar\omega \gg T$,

$$\coth \frac{\hbar\omega}{2T} \approx 1, \quad \sigma^2 \approx \frac{\hbar}{2m\omega}, \tag{45}$$

and the distribution becomes that of the ground quantum state,

$$f(x) = |\psi_0(x)|^2 \propto e^{-(m\omega/\hbar)x^2}. \tag{46}$$

Another derivation of the distribution (41) can be based on the found earlier matrix elements of the coordinate and momentum, for example combining the equations for $d\rho(x)/dx$ and $x\rho(x)$.

4. We solve the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\left(\frac{a}{x} - \frac{x}{a}\right)^2 \psi = E\psi. \tag{47}$$

The potential has a form of a well with the left wall asymptotically approaching the vertical axis and the parabolic right side. Near the classical equilibrium point $x = a$, the potential is close to that of the harmonic oscillator with the frequency which can be found by expanding the potential near this point and approximating it by $m\omega^2/2$. Here only the discrete spectrum is possible with $E > 0$. Introducing dimensionless positive variables

$$y = \frac{x}{a}, \quad v = \frac{2mU_0a^2}{\hbar^2}, \quad s = \frac{2mEa^2}{\hbar^2}, \tag{48}$$

we rewrite the equation for $\psi(y)$ as

$$\frac{d^2\psi}{dy^2} - v\left(y^2 + \frac{1}{y^2}\right)\psi + (2v + s)\psi = 0. \tag{49}$$

Now we are looking at the behavior near the singular points of the equation; obviously the dangerous regions are $y \to +\infty$ and $y \to 0$. At very large values of y we have an oscillator-like behavior,

$$\frac{d^2\psi}{dy^2} \approx vy^2\psi, \quad y \to +\infty. \tag{50}$$

The solution behaves like

$$\psi \sim e^{\alpha y^2}. \tag{51}$$

Then we find

$$\psi' = 2\alpha y\psi, \quad \psi'' = (2\alpha + 4\alpha^2 y^2)\psi \approx 4\alpha^2 y^2 \psi, \tag{52}$$

and the comparison with (50) shows that

$$4\alpha^2 = v \quad \rightsquigarrow \quad \alpha = -\frac{1}{2}\sqrt{v}, \tag{53}$$

where we choose the solution decaying at large distances. Near the origin, the main terms in the equation are

$$\frac{d^2\psi}{dy^2} \approx \frac{v}{y^2}\psi, \quad y \to 0. \tag{54}$$

This is an equation of *Euler type* with a solution as a power of the variable (then both terms lower the power by 2):

$$\psi \sim y^\gamma, \quad \gamma(\gamma - 1) = v. \tag{55}$$

In this quadratic equation we need to select the positive root for γ avoiding the infinite growth of the wave function at small y,

$$\gamma = \frac{1}{2}[\sqrt{4v + 1} + 1]. \tag{56}$$

Finally, we introduce the variable

$$\xi = \sqrt{v}y^2, \tag{57}$$

and look for the full solution in the form which accounts for the behavior near singularities,

$$\psi = e^{-\xi/2}\xi^{\gamma/2}u(\xi), \tag{58}$$

where $u(\xi)$ should be a regular function which does not change that behavior. We substitute this form into eq. (49), after some algebra verify that the singular terms cancel out, and we arrive at the equation for $u(\xi)$:

$$\xi u'' + (A - \xi)u' - B\,u = 0, \tag{59}$$

where

$$A = \gamma + \frac{1}{2}, \quad B = \frac{\gamma}{2} + \frac{1}{4} - \frac{s + 2v}{4\sqrt{v}}. \tag{60}$$

Without singularities in eq. (59) we are looking for the solution in the form of a power series,

$$u(\xi) = \sum_k c_k \xi^k. \tag{61}$$

The coefficients c_k must satisfy the recurrence relation

$$c_{k+1} = \frac{k+B}{k(k+1+A)} c_k. \tag{62}$$

If the series is infinite, the behavior of high order terms, $c_{k+1} \sim c_k/k$ coincides with that of the exponential series $\exp(\xi)$. That would win against the decaying exponent in (58) and, whence, lead to an unacceptable growth of the wave function. This means that the series in fact has to be a finite polynomial. We have a polynomial of power n in $\xi \propto x^2$ if $c_n \neq 0$ but $c_{k>n} = 0$. This requires $B = -n$, which is the quantization condition for energies, $s = s_n$,

$$\frac{s_n + 2v}{4\sqrt{v}} = n + \frac{\gamma}{2} + \frac{1}{4}, \tag{63}$$

or, returning to the original notations for s and γ,

$$E_n = \hbar\omega \left(n + \frac{1}{2} + \frac{1}{4}\sqrt{1+4v} - \frac{\sqrt{v}}{2} \right). \tag{64}$$

The spectrum of the problem is that of the *harmonic oscillator* with frequency

$$\omega = \sqrt{\frac{8mU_0}{\hbar^2}} \tag{65}$$

and the ground state shifted from $(\hbar\omega/2)$ by

$$\Delta E = \frac{1}{4}\sqrt{1+4v} - \frac{\sqrt{v}}{2}. \tag{66}$$

This shift is always positive; it vanishes only at $v \to \infty$. The frequency (65) exactly coincides with that of classical oscillations near the equilibrium point $x = a$.

The wave functions can be explicitly constructed with the use of the consecutive polynomials $u_n(\xi)$. The general expression for the wave functions can be written as

$$\psi_n(x) = N_n x^\gamma e^{-(\sqrt{v}/2a^2)x^2} F\left(-n, \gamma + \frac{1}{2}; \sqrt{v}\frac{x^2}{a^2}\right). \tag{67}$$

Here N_n is the normalization factor; F is the so-called *confluent hypergeometric function* which satisfies eq. (59), and in general is expressed as an infinite series,

$$F(B, A; \xi) = 1 + \frac{B}{A}\frac{\xi}{1!} + \frac{B(B+1)}{A(A+1)}\frac{\xi^2}{2!} + \frac{B(B+1)(B+2)}{A(A+1)(A+2)}\frac{\xi^3}{3!} + \dots \tag{68}$$

The series becomes a finite polynomial for $B = -n$ where $n \geq 0$ is an integer. Many known special functions can be expressed as particular cases of the confluent hypergeometric function, for example:

Bessel functions,	$A = 2B$
functions of parabolic cylinder,	$A = \frac{1}{2}$
incomplete gamma-functions,	$B = 1$
Laguerre polynomials,	$B = -n,$

the last case is just our solution.