

SOLUTIONS

1. In *Problem 1, Homework 9*, we have calculated the matrix elements of the operator \hat{x}^2 for the harmonic oscillator, eqs. (??, ??) and (??). They have selection rules $\Delta n = 0, \pm 2$. Using the matrix multiplication $\hat{x}^4 = \hat{x}^2 \cdot \hat{x}^2$, we can write

$$\langle n | \hat{x}^4 | n \rangle = \sum_{n'} \langle n | \hat{x}^2 | n' \rangle \langle n' | \hat{x}^2 | n \rangle. \quad (1)$$

Now the selection rules show that only three terms in this sum remain:

$$(x^4)_{nn} = (x^2)_{nn}^2 + (x^2)_{n,n-2}(x^2)_{n-2,n} + (x^2)_{n,n+2}(x^2)_{n+2,n}, \quad (2)$$

or, taking into account the Hermiticity of \hat{x}^2 ,

$$(x^4)_{nn} = (x^2)_{nn}^2 + (x^2)_{n,n-2}^2 + (x^2)_{n,n+2}^2. \quad (3)$$

With the explicit values of the matrix elements of \hat{x}^2 , we find

$$\begin{aligned} (x^4)_{nn} &= \left(\frac{\hbar}{m\omega} \right)^2 \left[\left(n + \frac{1}{2} \right)^2 + \frac{1}{4} n(n-1) + \frac{1}{4} (n+1)(n+2) \right] \\ &= \left(\frac{\hbar}{m\omega} \right)^2 \frac{3}{4} (2n^2 + 2n + 1). \end{aligned} \quad (4)$$

2. a. The given function $\Psi(x, 0)$ is the result of the displacement of the ground state wave function $\psi_0(x)$,

$$\Psi(x, 0) = \hat{\mathcal{D}}(a)\psi_0(x) = \psi_0(x - a). \quad (5)$$

It is a superposition of all stationary states of the unperturbed oscillator,

$$\Psi(x, 0) = \sum_{n=0}^{\infty} C_n \psi_n(x), \quad (6)$$

where the amplitudes C_n are matrix elements of the shift operator,

$$C_n = \int dx \psi_n(x) \hat{\mathcal{D}}(a) \psi_0(x) \equiv \langle n | \hat{\mathcal{D}}(a) | 0 \rangle. \quad (7)$$

There are various ways to evaluate these amplitudes. We can use the explicit form of the harmonic oscillator eigenfunctions

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-(m\omega/2\hbar)x^2} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right). \quad (8)$$

With the dimensionless variables

$$\xi = \sqrt{\frac{m\omega}{\hbar}} x, \quad b = \sqrt{\frac{m\omega}{\hbar}} a, \quad (9)$$

we write the amplitudes (7) as

$$C_n = \frac{1}{\sqrt{\pi 2^n n!}} e^{-b^2/2} \int d\xi H_n(\xi) e^{-\xi^2 + b\xi}. \quad (10)$$

Since the Hermite polynomials are

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}, \quad (11)$$

we integrate by parts n times in (10):

$$C_n = \frac{1}{\sqrt{\pi 2^n n!}} e^{-b^2/2} \int d\xi e^{b\xi} (-1)^n \frac{d^n}{d\xi^n} e^{-\xi^2} = \frac{1}{\sqrt{\pi 2^n n!}} e^{-b^2/2} b^n \int d\xi e^{-\xi^2 + b\xi}. \quad (12)$$

The last Gaussian integral is easily evaluated by forming the complete square in the exponent which leads to the final result

$$C_n = \frac{1}{\sqrt{2^n n!}} b^n e^{-b^2/4}. \quad (13)$$

The probability of finding the n^{th} stationary state is given by

$$P_n = C_n^2 = \frac{1}{2^n n!} b^{2n} e^{-b^2/2}. \quad (14)$$

The probabilities are normalized correctly:

$$\sum_{n=0}^{\infty} P_n = e^{-b^2/2} \sum_n \left(\frac{b^2}{2}\right)^n \frac{1}{n!} = 1. \quad (15)$$

The average degree of excitation of the original oscillator is the mean number of excited quanta

$$\langle n \rangle = \sum_n n P_n = \frac{b^2}{2}, \quad (16)$$

and we came to the *Poisson distribution*

$$P_n = \frac{\langle n \rangle^n e^{-\langle n \rangle}}{n!}. \quad (17)$$

b . For $a < (\hbar/m\omega)^{1/2}$, $b < 1$, and $\langle n \rangle < 1$, the probabilities P_n rapidly fall off as n increases. For $b = 1$, we have

$$P_0 = 0.6065, \quad P_1 = 0.3033, \quad P_2 = 0.0758, \quad P_3 = 0.0126.$$

The variance $(\Delta n)^2$ of the Poisson distribution is equal to the mean value,

$$(\Delta n)^2 = \langle n^2 \rangle - \langle n \rangle^2 = \langle n \rangle, \quad (18)$$

and grows with $\langle n \rangle$. For large values of $\langle n \rangle$, the Poisson distribution is close to Gaussian with the width (18). For example, for $b = 4$, $\langle n \rangle = 8$,

$$\begin{aligned} P_0 &= 0.0003, & P_1 &= 0.0027, & P_2 &= 0.0107, & P_3 &= 0.0286, \\ P_4 &= 0.0572, & P_5 &= 0.0916, & P_6 &= 0.1221, & P_7 &= 0.1396, \\ P_8 &= 0.1396, & P_9 &= 0.1241, & P_{10} &= 0.0993, & P_{11} &= 0.0722, \\ P_{12} &= 0.0481, & P_{13} &= 0.0296, & P_{14} &= 0.0169, & P_{15} &= 0.0090, \\ P_{16} &= 0.0045, & P_{17} &= 0.0021, & P_{18} &= 0.0009, & P_{19} &= 0.0004. \end{aligned}$$

c. Every stationary component $|n\rangle$ of the initial wave packet (6) evolves in time with its own frequency

$$\frac{E_n}{\hbar} = \omega \left(n + \frac{1}{2} \right). \quad (19)$$

At an arbitrary time moment t ,

$$\Psi(x, t) = \sum_{n=0}^{\infty} C_n e^{-i(\hbar)E_n t} \psi_n(x), \quad (20)$$

where the amplitudes C_n are already determined, eq. (13), by the initial wave function. The addition of the time-dependent factor in (20) is equivalent to changing the real amplitudes C_n by the new complex amplitudes

$$C_n(t) = C_n e^{-i\omega(n+1/2)t}. \quad (21)$$

The factor $\exp(-i\omega nt)$ can be combined with b^n to form the time dependent displacement parameter

$$b(t) = b e^{-i\omega t}. \quad (22)$$

Extracting the factor in front, the new amplitudes can be rewritten as

$$C_n(t) = f(t) C_n(b(t)), \quad f(t) = e^{-i(b^2/2) \sin(\omega t) \exp(-i\omega t)}, \quad (23)$$

where $C_n(b(t))$ is the old amplitude $C_n(b)$, eq. (13), with the time-dependent argument (22). Now it is clear that the time-dependent wave function is again the Gaussian packet centered around the complex point $a(t) = \sqrt{\hbar/m\omega} b(t)$,

$$\Psi(x, t) = f(t) \psi_0(x - a(t)). \quad (24)$$

This means that the center of the packet is rotating in the complex plane with the oscillator frequency.

d. Now it is a straightforward exercise to calculate

$$|f(t)|^2 = e^{-(m\omega/\hbar)a^2 \sin^2(\omega t)}, \quad (25)$$

and

$$|\Psi(x, t)|^2 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-(m\omega/\hbar)[x-a \cos(\omega t)]^2}. \quad (26)$$

This can be written in a more clear way,

$$|\Psi(x, t)|^2 = |\Psi_0(x - a \cos(\omega t))|^2. \quad (27)$$

The center of the probability cloud is performing the harmonic oscillation on the real axis. This is one of the examples of the *coherent state*.

3. a. The Hamiltonian of the particle is

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 - e\mathcal{E}\hat{x}. \quad (28)$$

By constructing the complete square we rewrite this as

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \left(\hat{x} - \frac{e\mathcal{E}}{m\omega^2}\right)^2 - \frac{e^2\mathcal{E}^2}{2m\omega^2}. \quad (29)$$

With a new variable

$$y = x - a, \quad a = \frac{e\mathcal{E}}{m\omega^2}, \quad (30)$$

we obtain a standard harmonic oscillator problem, with the overall shift of energies by the last term in (29). Thus, the eigenfunctions of the problem with the field \mathcal{E} are *shifted* usual functions,

$$\psi_n(x; \mathcal{E}) = \hat{D}(a)\psi_n(x; 0) = \psi_n(x - a; 0). \quad (31)$$

This shift of the equilibrium position of a charged pendulum along the field has an obvious classical meaning. The energy spectrum is given by

$$E_n(\mathcal{E}) = \hbar\omega \left(n + \frac{1}{2}\right) - \frac{e^2\mathcal{E}^2}{2m\omega^2} \equiv E_n(0) - \Delta E. \quad (32)$$

All levels are shifted down as a whole (a result of the dipole polarization, see point c); the step of the ladder (the quantum of the oscillation frequency) is unchanged.

b. The *Problem 2* answers this question. The wave function $\psi_0(x; \mathcal{E})$ is now an initial state; the shift a is determined by (30). The probability

distribution for the stationary states $|n\rangle$ of the oscillator centered at an unperturbed position $x = 0$ is Poissonian, eq. (17), with the mean value of excited quanta

$$\langle n \rangle = \frac{m\omega a^2}{2\hbar} = \frac{e^2 \mathcal{E}^2}{2m\hbar\omega^3}. \quad (33)$$

This quantity has a simple meaning: the system now has energy higher than in the presence of the field by the amount of the shift ΔE , eq. (32). This amount is transformed in the average excitation,

$$\Delta E = \hbar\omega\langle n \rangle. \quad (34)$$

c. With no field, there is no dipole moment (stationary states have certain parity). The induced dipole moment for the ground state in the presence of the field is given by the expectation value of the dipole operator $\hat{d} = e\hat{x}$,

$$\langle \hat{d} \rangle = e \int_{-\infty}^{\infty} dx x |\psi_0(x; \mathcal{E})|^2 = e \int_{-\infty}^{\infty} dx x |\psi_0(x - a; 0)|^2 = ea = \frac{e^2}{m\omega^2} \mathcal{E}. \quad (35)$$

Thus, the static polarizability of the harmonic oscillator is equal to

$$\alpha = \frac{e^2}{m\omega^2}. \quad (36)$$

4. a. To find the corresponding integral operator we start with the definition. For the coordinate operator \hat{x} the action on a wave function is merely multiplication,

$$\hat{x}\psi(x) = x\psi(x). \quad (37)$$

On the other hand, this should be expressed in terms of the kernel $X(x, x')$,

$$\hat{x}\psi(x) = \int dx' X(x, x')\psi(x'). \quad (38)$$

The comparison of these two expressions that should be valid for an arbitrary $\psi(x)$ leads to the *local* kernel

$$X(x, x') = x\delta(x - x'). \quad (39)$$

For the momentum operator and the corresponding kernel $P(x, x')$ we have

$$\hat{p}\psi(x) = -i\hbar \frac{d\psi}{dx} = \int dx' P(x, x')\psi(x'). \quad (40)$$

From here we see that the kernel is the derivative of the δ -function,

$$P(x, x') = i\hbar \frac{d}{dx'} \delta(x - x'). \quad (41)$$

Indeed, with this kernel, the last expression in (40) becomes (with the aid of the integration by parts)

$$\begin{aligned} & i\hbar \int dx' \left[\frac{d}{dx'} \delta(x-x') \right] \psi(x') \\ &= i\hbar \int dx' \left\{ \frac{d}{dx'} [\delta(x-x')\psi(x')] - \delta(x-x') \frac{d\psi(x')}{dx'} \right\}, \end{aligned} \quad (42)$$

and the integrated term vanishes for any finite x when taken on the limits $x' \rightarrow \pm\infty$, whereas the last term provides the needed result after the integration with $\delta(x-x')$. The derivative with respect to x' can be substituted by (with the opposite sign) the derivative with respect to x , then

$$P(x, x') = -i\hbar \frac{d}{dx} \delta(x-x'). \quad (43)$$

For the inversion we have

$$\hat{\mathcal{P}}\psi(x) = \psi(-x) = \int dx' \mathcal{P}(x, x')\psi(x'), \quad (44)$$

which shows that

$$\mathcal{P}(x, x') = \delta(x+x'). \quad (45)$$

In the case of the displacement operator,

$$\hat{\mathcal{D}}(a)\psi(x) = \psi(x-a) = \int dx' \mathcal{D}(a; x, x')\psi(x'), \quad (46)$$

that shows immediately that

$$\mathcal{D}(a; x, x') = \delta(x-x'-a). \quad (47)$$

Finally, for the scaling transformation,

$$\hat{\mathcal{M}}(\alpha)\psi(x) = \sqrt{\alpha}\psi(\alpha x) = \int dx' \mathcal{M}(\alpha; x, x')\psi(x'), \quad (48)$$

$$\mathcal{M}(\alpha; x, x') = \sqrt{\alpha}\delta(x'-\alpha x). \quad (49)$$

b. An operator \hat{F} commuting with \hat{x} has to be a function of \hat{x} only,

$$\hat{F} = f(\hat{x}). \quad (50)$$

The corresponding kernel is

$$F(x, x') = f(x)\delta(x-x'). \quad (51)$$

c. An operator \hat{G} commuting with \hat{p} has to be a function of \hat{p} only,

$$\hat{G} = g(\hat{p}). \quad (52)$$

The kernel of this operator contains a corresponding function g of the differentiation operator acting onto the δ -function, compare (41),

$$G(x, x') = g(i\hbar d/dx')\delta(x - x'). \quad (53)$$

d. Only an operator \hat{C} of multiplication by a constant c commutes both with \hat{x} and \hat{p} . The corresponding kernel is

$$C(x, x') = c\delta(x - x'). \quad (54)$$

e. For the factorized kernel

$$\hat{F}\psi(x) = f(x) \int dx' g(x')\psi(x'). \quad (55)$$

An arbitrary matrix element F_{12} of this operator in the coordinate representation has a form

$$F_{12} = \int dx \psi_1^*(x) \hat{F}\psi_2(x) = \int dx dx' \psi_1^*(x) f(x) g(x') \psi_2(x'). \quad (56)$$

For a Hermitian operator, $\hat{F} = \hat{F}^\dagger$,

$$F_{12} = F_{21}^* = \int dx dx' \psi_2(x) f^*(x) g^*(x') \psi_1(x'). \quad (57)$$

Interchanging here the variables $x \leftrightarrow x'$ and comparing with (56), we find the condition of hermiticity

$$f(x)g(x') = f^*(x')g^*(x) \quad \rightsquigarrow \quad g(x) = f^*(x). \quad (58)$$

Thus, for a Hermitian factorized operator, the kernel should be unitary-symmetric,

$$\hat{F} = \hat{F}^\dagger \quad \rightsquigarrow \quad F(x, x') = f(x)f^*(x'). \quad (59)$$

The eigenvalue problem for this operator,

$$\hat{F}\psi(x) = \lambda\psi(x), \quad (60)$$

takes the form

$$\lambda\psi(x) = f(x) \int dx' f^*(x')\psi(x'). \quad (61)$$

Since the integral in the right hand side here is just a number, an inner product $\langle f|\psi\rangle$, we see that the entire x -dependence of $\psi(x)$ is given by $f(x)$ if $\langle f|\psi\rangle \neq 0$. Multiplying eq. (61) by $\langle f|$, we get

$$(\lambda - \langle f|f\rangle)\langle f|\psi\rangle = 0. \quad (62)$$

Thus, we see two possibilities. (i) If $\psi(x) = \text{const} \cdot f(x)$, then the product $\langle f|\psi\rangle \neq 0$, and

$$\lambda = \langle f|f\rangle = \int dx |f(x)|^2. \quad (63)$$

(ii) Any function $\psi(x)$, which is *orthogonal* to $f(x)$ so that $\langle f|\psi\rangle = 0$, is also, according to (61), an eigenfunction of \hat{F} with the eigenvalue $\lambda = 0$. Therefore the operator

$$\hat{\Lambda} = \frac{\hat{F}}{\langle f|f\rangle} \quad (64)$$

is a *projection* operator which projects out a component of any vector in Hilbert space along the axis corresponding to $f(x)$; for a vector along this axis the eigenvalue of $\hat{\Lambda}$ is 1. For any orthogonal vector, the eigenvalue is 0. The nonzero eigenvalue is nondegenerate while the degeneracy of the zero eigenvalue is infinite.

f. The Schrödinger equation for a particle in the potential \hat{U} is, as usual,

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, t) + \hat{U} \Psi(\mathbf{r}, t). \quad (65)$$

For a nonlocal potential with a kernel $U(\mathbf{r}, \mathbf{r}')$ this means that

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, t) + \int d^3 r' U(\mathbf{r}, \mathbf{r}') \Psi(\mathbf{r}', t). \quad (66)$$

The complex conjugate equation reads

$$-i\hbar \frac{\partial \Psi^*(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi^*(\mathbf{r}, t) + \int d^3 r' U^*(\mathbf{r}, \mathbf{r}') \Psi^*(\mathbf{r}', t). \quad (67)$$

Multiplying (66) by Ψ^* and (67) by Ψ , subtracting the second equation from the first and defining in a standard way the probability density $\rho(\mathbf{r}, t)$ and current $\mathbf{j}(\mathbf{r}, t)$,

$$\rho(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2, \quad \mathbf{j}(\mathbf{r}, t) = \frac{\hbar}{2mi} (\Psi^* \nabla \Psi - (\nabla \Psi^*) \Psi), \quad (68)$$

we obtain the analog of the continuity equation

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} + \text{div} \mathbf{j}(\mathbf{r}, t)$$

$$= -\frac{i}{\hbar} \left\{ \Psi^*(\mathbf{r}, t) \int d^3 r' U(\mathbf{r}, \mathbf{r}') \Psi(\mathbf{r}', t) - \Psi(\mathbf{r}, t) \int d^3 r' U^*(\mathbf{r}, \mathbf{r}') \Psi^*(\mathbf{r}', t) \right\}. \quad (69)$$

Because of the nonlocality of the potential, the conventional continuity equation is not fulfilled, the probability density can be changed not only by the current through the surface but also by an action at a distance. Integrating eq. (69) over the infinite volume and assuming that there is no current through an infinitely remote surface, we come to

$$\frac{\partial}{\partial t} \int d^3 r \rho(\mathbf{r}, t) = \int d^3 r d^3 r' [\Psi^*(\mathbf{r}, t) U(\mathbf{r}, \mathbf{r}') \Psi(\mathbf{r}', t) - \Psi(\mathbf{r}, t) U^*(\mathbf{r}, \mathbf{r}') \Psi^*(\mathbf{r}', t)]. \quad (70)$$

Interchanging in the last term of (70) $\mathbf{r} \leftrightarrow \mathbf{r}'$ and using the *Hermiticity* of the kernel,

$$U(\mathbf{r}, \mathbf{r}') = U^*(\mathbf{r}', \mathbf{r}), \quad (71)$$

we come to the conservation of the total probability (normalization)

$$\int d^3 r \rho(\mathbf{r}, t) = \text{const.} \quad (72)$$

The Hermitian (even nonlocal) potential does not create or annihilate particles and preserves the total probability.

5. Let list all N eigenvalues f_i , $i = 1, \dots, N$, of the operator \hat{F} . An operator $\hat{F} - f_1$ has eigenvalues

$$0, f_2 - f_1, \dots, f_N - f_1.$$

In the same way, the operator $(\hat{F} - f_2)(\hat{F} - f_1)$ has eigenvalues

$$0, 0, (f_3 - f_2)(f_3 - f_1), \dots, (f_N - f_2)(f_N - f_1).$$

The operator \hat{Z} constructed as a product of all binomial expressions $\hat{F} - f_i$ has N zero eigenvalues, i.e. in this N -dimensional space

$$\hat{Z} = \prod_{i=1}^N (\hat{F} - f_i) = 0. \quad (73)$$

Indeed, the set $|i\rangle$ of eigenvectors of a Hermitian operator \hat{F} is complete. Any vector can be expanded as

$$|\Psi\rangle = \sum_i C_i |i\rangle. \quad (74)$$

For any component in the expansion (74), there is a factor in the product (73) which vanishes. Thus, for any $|\Psi\rangle$,

$$\hat{Z}|\Psi\rangle = 0. \quad (75)$$

But performing explicitly the multiplication in the product (73) we get \hat{Z} as a polynomial of the N^{th} order in \hat{F} ,

$$\hat{Z} = \hat{F}^N - \hat{F}^{N-1} \sum_i f_i + \hat{F}^{N-2} \sum_{i \neq j} f_i f_j + \dots + \prod_i (-f_i). \quad (76)$$

Since $\hat{Z} \equiv 0$, this allows one to express \hat{F}^N as a linear combination of all lower powers F^n , $n = 0, 1, \dots, N - 1$.

For the inversion operator $\hat{\mathcal{P}}$ the result is especially simple. Hilbert space is effectively two-dimensional, $N = 2$, the eigenvalues are 1 and -1, for even or odd functions, respectively, so that

$$\hat{Z} = (\hat{\mathcal{P}} - 1)(\hat{\mathcal{P}} + 1) = 0 \quad \rightsquigarrow \quad \hat{\mathcal{P}}^2 = 1. \quad (77)$$

b. We need to find an operator which annihilates all components with $j \neq i$ but gives the result equal to 1 acting on the vector $|i\rangle$. Therefore we need to take

$$\hat{\Lambda}_i = \prod_{j(\neq i)} \frac{\hat{F} - f_j}{f_i - f_j}. \quad (78)$$

c. See (64).