

Simple one-dimensional potentials

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Quantum Mechanics 1

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The Hamiltonian for a harmonic oscillator

The harmonic oscillator is a system which obeys, Hooke's law, *i.e.*, the force on the oscillator is proportional to the displacement from its equilibrium position and points towards that position. Hence the potential is $V(x) = m\omega^2 x^2/2$. The harmonic oscillator Hamiltonian is

$$H = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}x^2.$$

The Hamiltonian above describes ellipses in phase space: this is the classical motion of harmonic oscillators. Both the position and the momentum vary with time harmonically, hence the name.

The quantum Hamiltonian is obtained as usual by using the operator forms for p and x . In terms of the dimensionless quantities

$$X = \sqrt{\frac{m\omega}{\hbar}}x \quad \text{and} \quad P = \frac{1}{\sqrt{m\omega\hbar}}p, \quad \text{one has} \quad H = \frac{\hbar\omega}{2} (P^2 + X^2).$$

Note that $[X, P] = i$; a result which follows from the canonical commutator.

Examples

- ❶ Near the minimum of any smooth potential, one can approximate the potential by its Taylor expansion:

$$V(x) = V(x_0) + V''(x_0)(x - x_0)^2/2 + \dots$$
 where x_0 is position of the minimum, *i.e.*, the point where the first derivative vanishes. Low-lying vibrational modes of molecules show almost harmonic spectrum as a result of this general fact.
- ❷ Complicated many-body interactions in a nucleus can be expanded in a similar Taylor series to give a central potential which is approximately harmonic. The addition of simple extra terms in the Hamiltonian then explain the spectra of many complex nuclei.
- ❸ The motion of a charged particle in a magnetic field is a disguised version of a harmonic oscillator. Since the particle travels in a helical path around the field lines, the momentum components transverse to the field lines play the roles of X and P .

Example: normal modes and field theories

The vibrations of rigid solids gives a theory of many independent harmonic oscillator. A linear chain of N atoms bound to each other has the lowest order potential

$$V = -\frac{1}{2} \sum_{i=1}^N (x_i - x_{i+1})^2 + \dots$$

Assume that the chain closes on itself, so that $x_{N+1} = x_1$. Fourier transforming the coordinates x_i then decomposes the coupled Hamiltonian into a sum proportional to $\sum_k x_k^2$. Thus, the coupled problem decomposes into a sum of N independent harmonically oscillating Fourier models. This is an example of a classical field theory.

Quantizing the Fourier modes gives a simple first quantized field theory. If one wants to take into account the cubic, quartic *etc.*, terms in the potential then these higher order terms can be treated as couplings between the oscillator modes.

Raising and lowering operators

Construct the operators

$$a = \frac{1}{\sqrt{2}}(X + iP), \quad \text{and} \quad a^\dagger = \frac{1}{\sqrt{2}}(X - iP).$$

Both a and a^\dagger are non-Hermitean, and are conjugates of each other. The commutator, $[a, a^\dagger] = 1$, follows using that for X and P . Now consider the Hermitean operator $\hat{N} = a^\dagger a$. One sees that $[\hat{N}, a] = -a$ and $[\hat{N}, a^\dagger] = a^\dagger$. If $|z\rangle$ is an eigenvector of \hat{N} with eigenvalue z , then $[\hat{N}, a]|z\rangle = -a|z\rangle$, and hence $\hat{N}a|z\rangle = (z - 1)a|z\rangle$, i.e., a lowers the eigenvalue of \hat{N} by one unit. Using the other commutator, one can show that a^\dagger raises the eigenvalue of \hat{N} by one unit.

For any $|\psi\rangle$, let $|\phi\rangle = a|\psi\rangle$. Since $\langle\phi|\phi\rangle \geq 0$ and $\langle\phi|\phi\rangle = \langle\psi|\hat{N}|\psi\rangle$, one finds that every eigenvalue of \hat{N} must be greater than or equal to zero. If the eigenvalues of \hat{N} are not integers, then there cannot be a lower bound to the eigenvalues, since a will always lower the eigenvalue by one unit.

So, there is a vector $|0\rangle$ such that $a|0\rangle = 0$, and $\hat{N}|0\rangle = 0$.

The eigenvalues of the Hamiltonian

One finds that

$$\hat{N} = \frac{1}{2}(X - iP)(X + iP) = \frac{1}{2}(X^2 + P^2 - 1), \quad \text{hence} \quad H = \hbar\omega \left(\hat{N} + \frac{1}{2} \right).$$

Thus, the eigenvalues of H are $E = \hbar\omega(n + 1/2)$, for integer $n \geq 0$. The lowest state satisfies

$$\left(\frac{m\omega}{\hbar}x + \frac{d}{dx} \right) \psi_0(x) = 0, \quad \text{i.e.,} \quad \psi_0(x) \propto \exp\left(-\frac{m\omega x^2}{2\hbar}\right).$$

Since this is a first order differential equation, there is a unique solution. Thus, the lowest eigenvalue of \hat{N} (and hence, of H) is unique. Then, by induction with a^\dagger we can show that none of the states are degenerate. If $|n-1\rangle = c_n a|n\rangle$, then $\langle n-1|n-1\rangle = |c_n|^2 n \langle n|n\rangle$. If $|n-1\rangle$ is normalized, then normalization of $|n\rangle$ requires $c_n = 1/\sqrt{n}$. Then $|n\rangle = a^\dagger|n-1\rangle/\sqrt{n} = (a^\dagger)^n|0\rangle/\sqrt{n!}$.

All wavefunctions at one go

The **generating function** for the wavefunctions is—

$$G(z; x) = \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \psi_n(x) = \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \langle x | \frac{(a^\dagger)^n}{\sqrt{n!}} | \psi_0 \rangle = \langle x | e^{za^\dagger} | \psi_0 \rangle.$$

Now, from the Baker-Campbell-Hausdorff formula, we find that $\exp(za^\dagger) = \exp(zX/\sqrt{2}) \exp(-izP/\sqrt{2}) \exp(-z^2/4)$. Hence

$$G(z; x) = \exp\left(-\frac{z^2}{4} + zx\sqrt{\frac{m\omega}{2\hbar}}\right) \langle x | e^{-izP/\sqrt{2}} | \psi_0 \rangle.$$

Then using the action of the exponential on the bra, and the normalized ground state wavefunction

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

we find that

$$G(z; x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar} + \sqrt{\frac{2m\omega}{\hbar}}zx - \frac{z^2}{2}\right).$$

The Hermite polynomials

Define the function $f(x) = \exp(-x^2)$ and its n -th derivative, $f^{(n)}(x) = (-1)^n H_n(x) \exp(-x^2)$. The $H_n(x)$ are called **Hermite polynomials** (**prove that they are polynomials**). By direct differentiation one can obtain the **recurrence relation**

$$H_n(x) = \left[2x - \frac{d}{dx} \right] H_{n-1}(x).$$

From the definition of the Hermite polynomials it is clear that

$$e^{-z^2+2zx} = e^{x^2} f(x-z)^2 = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(x).$$

From the recurrence relation we can write down the explicit forms—

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$H_2(x) = 4x^2 - 2.$$

Note that the even numbered polynomials have even parity.

The harmonic oscillator wave functions

Comparing the recurrence relation for harmonic oscillator wave functions

$$G(z; x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar} + \sqrt{\frac{2m\omega}{\hbar}}zx - \frac{z^2}{2}\right)$$

with that for Hermite polynomials,

$$e^{-z^2+2zx} = e^{x^2} f(x-z)^2 = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(x),$$

we find that

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

Note that the parity flips for every successive n . The wavefunction ψ_n (and hence the Hermite polynomial, H_n) has exactly n zeroes. The zeroes of successive polynomials are interleaved. The Hermite polynomials are orthogonal under the measure $dx \exp(-x^2)$.

Classical-quantum correspondence

Since $X = (a + a^\dagger)/\sqrt{2}$ and $P = -i(a - a^\dagger)/\sqrt{2}$, and the operators a and a^\dagger have vanishing diagonal elements in the eigenbasis of \hat{N} , it is clear that $\langle n|X|n\rangle = \langle n|P|n\rangle = 0$. Squaring each of these operators, we find that $\langle n|X^2|n\rangle = \langle n|P^2|n\rangle = n + 1/2$. Clearly, then one has $\langle V \rangle = \langle T \rangle = E/2$. These relations are the same as for a classical harmonic oscillator. The commutators $[H, X] = -iP$ and $[H, P] = iX$ follow from the commutators of \hat{N} with a and a^\dagger . Then

$$\begin{aligned}\frac{d\langle X \rangle}{dt} &= \frac{d}{dt} \langle \psi | e^{iHt/\hbar} X e^{-iHt/\hbar} | \psi \rangle = i \langle [H, X] \rangle \\ &= \hbar\omega \langle P \rangle \\ \frac{d\langle P \rangle}{dt} &= -\hbar\omega \langle X \rangle.\end{aligned}$$

These equations are the same as the classical Hamilton's equations.

Schrödinger and Heisenberg pictures

We have chosen a representation of quantum evolution in which the operators corresponding to time-independent classical variables remain time independent, and the states evolve by the action of the unitary evolution operator. This is called **the Schrödinger picture** of quantum dynamics.

Observables $\langle \psi'(t) | O | \psi(t) \rangle$ are time dependent through unitary evolution of states $\langle \psi'(0) | U^\dagger(t) O U(t) | \psi(0) \rangle$. Therefore they remain unchanged if we use **the Heisenberg picture**, in which states are time independent and operators evolve with time through the adjoint action of the unitary evolution operator. The time evolution of expectation values can be computed exactly as for the harmonic oscillator. Since the analogous equations hold in any state, one can interpret this as the operator evolution equation in the Heisenberg picture—

$$\frac{dO}{dt} = i[H, O].$$

The thermal density matrix

For a single harmonic oscillator placed inside a heat bath, one finds the partition function

$$Z(\beta) = \text{Tr} \exp(-H\beta) = e^{-\hbar\omega\beta/2} \sum_{n=0}^{\infty} e^{-\hbar\omega\beta n} = \frac{\exp(-\hbar\omega\beta/2)}{1 - \exp(-\hbar\omega\beta)},$$

where $\beta = 1/k_B T$. Since $\rho(T) = \exp(-H\beta)/Z$, the expectation value of the energy is

$$\langle H \rangle = \frac{1}{Z} \text{Tr} H \exp(-\beta H) = -\frac{1}{Z} \frac{dZ}{d\beta} = -\frac{d \log Z}{d\beta}.$$

Using the expression for Z above, we get

$$\langle H \rangle = \frac{1}{2} \hbar\omega + \frac{\hbar\omega}{\exp(\hbar\omega\beta) - 1}.$$

The Planck spectrum begins to emerge.

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The classical theory

The Hamiltonian of a particle of charge e and mass m in a magnetic field is

$$H = \frac{1}{2m}(P - e\mathbf{A})^2, \quad \mathbf{B} = \nabla \times \mathbf{A}.$$

The classical equations of motion which follow from this are

$$\frac{d\mathbf{r}}{dt} = \frac{\mathbf{p}}{m}, \quad \frac{d\mathbf{p}}{dt} = \frac{e}{m}\mathbf{p} \times \mathbf{B}.$$

Taking the z -direction to be the direction of \mathbf{B} , we obtain, $p_z(t) = p_z(0)$, and

$$\frac{d}{dt} \begin{pmatrix} p_x \\ p_y \end{pmatrix} = i\omega\sigma_2 \begin{pmatrix} p_x \\ p_y \end{pmatrix},$$

where the **cyclotron frequency** is given by $\omega = eB/m$. On scaling the time by a factor ω , it is clear that these equations of motion can be obtained from a fictitious Hamiltonian $H' = (p_x^2 + p_y^2)/2$. The harmonic solutions are obtained from the above equations by an unitary transformation to $p_{\pm} = (p_x \pm ip_y)/\sqrt{2}$. The solutions are $p_{\pm}(t) = p_{\pm}(0)\exp(\mp i\omega t)$. Since the phase space is 6d and the motion is integrable, there are three conserved quantities: E , p_z , and $|p_{\pm}|$.

Quantization

Introduce $\mathbf{P} = \mathbf{p} - e\mathbf{A}$. Then $[P_j, P_k] = i\epsilon_{jkl}B_l$. With the choice made of the coordinate axes, one sees that $[P_j, P_z] = 0$ for all j . Since $H = \mathbf{P}^2/2m$, this implies that $[H, P_z] = 0$. The remainder of the Hamiltonian is

$$H' = (P_x^2 + P_y^2)/2m, \quad \text{where} \quad [P_x, P_y] = ieB.$$

Since $[H, H'] = 0$, N is a conserved quantum number. Therefore the Hamiltonian is exactly that of the harmonic oscillator. The eigenvalues are called **Landau levels**, and are given by

$$E(N, k_z) = \frac{\hbar^2}{2m}k_z^2 + \hbar\omega \left(N + \frac{1}{2} \right).$$

The third operator which commutes with H has a continuous spectrum, hence the Landau levels are infinitely degenerate. (**Find the third commuting operator**)

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The energy eigenvalues and eigenvectors

The isotropic harmonic oscillator in two dimensions is specified by the two position variables x_1 and x_2 and the two conjugate momenta p_1 and p_2 . Isotropy implies that the angular frequency, ω is the same in all directions. Then introducing the scaled quantities $X_i = x_i \sqrt{m\omega/\hbar}$ and $P_i = p_i / \sqrt{m\omega\hbar}$, one has the Hamiltonian

$$H = \frac{\hbar\omega}{2}(P_1^2 + P_2^2 + X_1^2 + X_2^2).$$

Introducing the shift operators $a_j = (X_j + iP_j)/\sqrt{2}$ and their Hermitean conjugates, a_j^\dagger , as before, one can show that H can be written in terms of two number operators $N_j = a_j^\dagger a_j$ in the form $H = \hbar\omega[(N_1 + 1/2) + (N_2 + 1/2)]$. As a result, the energy eigenstates can be specified in the form $|n_1, n_2\rangle$ where n_i are the eigenfunctions of N_i . The energies of these states are $E = \hbar\omega(n_1 + n_2 + 1)$. Equivalently, one could write the eigenstates as $|N, n_1\rangle$ and energies as $E = \hbar\omega(N + 1)$. Since n_1 does not enter the expression for the energy, and it has the range $0 \leq n_1 \leq N$, the eigenvalue is $(N + 1)$ -fold degenerate. Therefore there is a larger symmetry in the problem.

Extended symmetry

The degeneracy of the states, $|N, n_1\rangle$ due to the multiplicity of n_1 means that if one changes n_1 and n_2 simultaneously, while keeping $N = n_1 + n_2$ fixed, then the energy does not change. An operator of the form $a_1^\dagger a_2$ does precisely this. The two Hermitean operators $s_1 = a_1^\dagger a_2 + a_2^\dagger a_1$ and $s_2 = ia_1^\dagger a_2 - ia_2^\dagger a_1$ acting on a level $|N, n_1\rangle$ produce linear combinations of $|N, n_1 - 1\rangle$ and $|N, n_1 + 1\rangle$. **Check this logic by evaluating $[H, s_1]$ and $[H, s_2]$. Construct the full algebra using $[s_1, s_2]$, and commutators with any new operators formed in this process)**

This process generates the combinations $s_0 = N_1 + N_2$, s_1 , s_2 and $s_3 = N_1 - N_2$. The commutation relations between these operators is the same as that between Pauli matrices. (**Check that in the subspace of $E = 2\hbar\omega$ these operators are exactly the Pauli matrices**). However, when acting in the eigenspace of larger values of E , the operators are represented by larger matrices. Compute the operator $S^2 = s_1^2 + s_2^2 + s_3^2$ in the degenerate subspace of any E . Also compute the matrix representation of s_3 in this subspace.

The symmetry group $SU(2)$

An arbitrary (new) linear combination of the degenerate eigenstates of the isotropic two-dimensional harmonic oscillator is generated by the unitary matrix $U = \exp\left(i \sum_j \theta_j s_j\right)$. Note that $\text{Det } U = 1$ (because the trace of its logarithm is zero). Since these linear combinations all have the same energy, all these U must commute with the Hamiltonian.

In particular, this is true of the two-dimensional subspace with $N = 1$. All 2×2 unitary matrices with unit determinant form a group. This is called **the group $SU(2)$** . Since all these matrices commute with H , the symmetry group of this problem is $SU(2)$. The higher dimensional matrices generated by the above prescription do not exhaust all possible unitary matrices of that size, but a subgroup which is isomorphic to $SU(2)$. These matrices of different sizes are called different **representations** of $SU(2)$. The trace of S^2 in each representation is characteristic of that representation. The Hermitean operators s_1 , s_2 and s_3 are called the **generators** of $SU(2)$, or elements of **the algebra $\mathfrak{su}(2)$** .

A problem

Consider the isotropic harmonic oscillator in three dimensions. In analogy with the construction we have presented here, find the complete group of symmetries of this problem: it is called $SU(3)$.

- ➊ Construct the complete algebra of operators from Hermitean combinations of the bilinears of the shift operators which leave the energy unchanged.
- ➋ Find the commutators of these operators, and construct the completion of this algebra. How many operators are there in the algebra?
- ➌ Find a complete set of commuting operators among these.
- ➍ In the degenerate space of eigenstates corresponding to the energy eigenvalue $E = 5\hbar\omega/2$, construct the representations of the elements of the algebra.
- ➎ Construct the representation of the algebra in the space of energy eigenstates with eigenvalue $E = 7\hbar\omega/2$.

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- ❶ Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz. The material in this lecture are scattered through chapters 3 and 15 of this book. The later chapter deals with the topic of Landau levels.
- ❷ Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë. Chapter 5 of this book discusses the harmonic oscillator. Read, in particular, the many applications of this model potential.
- ❸ Solid State Physics, by N. W. Ashcroft and N. D. Mermin. Chapter 14 of this book deals with the many applications of Landau levels to solid state physics phenomena.
- ❹ The article by M. Harvey in the book Advances in Nuclear Physics, vol 1 (Plenum Press, New York) discussed the Elliott Model, which is an application of the $SU(3)$ symmetry of the three dimensional harmonic oscillator to problems in nuclear physics.
- ❺ Classical groups for Physicists, by B. G. Wybourne. This book is highly recommended for a good exposition on Lie groups.