Simple one-dimensional potentials

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Quantum Mechanics 1
Ninth lecture

Outline

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Bloch's theorem for periodic potentials

For a periodic potential, $V(x) = V(x + x_0)$, the Hamiltonian commutes with the translation, $T(x_0)$. If $\psi(x)$ is one of the simultaneous eigenfunctions, then $T(x_0)\psi(x) = \lambda\psi(x)$, where $\lambda = \exp(iKx_0)$, since $T(x_0)$ is unitary. Trivially, one gets Bloch's theorem, which states that an eigenfunction in a period potential has the form $\psi(x + nx_0) = T^n(x_0)\psi(x) = \exp(iKnx_0)\psi(x)$. The value of K depends on the boundary conditions one chooses.

The generalization to arbitrary dimensions is straightforward. Since the translation group is Abelian, translations in all directions commute. As a result, all these translations can be diagonalized together with a periodic Hamiltonian. So the eigenfunctions of the periodic Hamiltonian must satisfy $\psi(\mathbf{r} + \mathbf{R}) = \exp(i\mathbf{K} \cdot \mathbf{R})\psi(\mathbf{r})$, for any lattice vector $\mathbf{R}$.

Problem 8.1: the scattering matrix

A potential $V(x)$ has a finite range, if $V(x) = 0$ for $|x| > a$. A stationary solution far from the potential is the superposition

$$\psi(y;\rho) = \begin{cases} A_1 \mathrm{e}^{i\rho y} + B_1 \mathrm{e}^{-i\rho y} & (y < -1) \\ A_2 \mathrm{e}^{i\rho y} + B_2 \mathrm{e}^{-i\rho y}. & (y > 1) \end{cases}$$

The incoming waves are $\exp(i\rho y)$ for $y < -1$ and its complex conjugate on the right. The outgoing waves are the remainder. The scattering matrix relates the incoming waves to the outgoing waves,

$$\begin{pmatrix} B_1 \\ A_2 \end{pmatrix} = S \begin{pmatrix} A_1 \\ B_2 \end{pmatrix}.$$

Since the states are stationary, $|\psi|^2$ is time independent. Show that the probability current, $J = (\psi^* \hat{p} \psi + \psi \hat{p}^\dagger \psi^*)/(2m)$ is constant. Prove that, as a result, $SS^\dagger = 1$.

Problem 8.2: a transmission matrix

Define the transmission matrix, T, across the potential

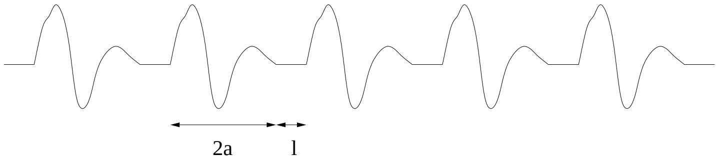
$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = T \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}.$$

The parametrization of an unitary matrix (problem 4.1)

$$S = \begin{pmatrix} z_1 & -wz_2^* \\ z_2 & wz_1^* \end{pmatrix}, \quad \text{gives} \quad T = \frac{1}{z_2} \begin{pmatrix} 1 & -wz_1^* \\ z_1 & -w \end{pmatrix},$$

where $|z_1|^2 + |z_2|^2 = 1$ and w is a pure phase, *i.e.*, $w = \exp(i\phi)$. Show that the transmission coefficient, $\mathcal{T} = |z_2|^2$ and the reflection coefficient $\mathcal{R} = |z_1|^2$. Unitarity of the S-matrix forces $\mathcal{T} + \mathcal{R} = 1$. Resonances occur when $\mathcal{T} = 1$, *i.e.*, $z_1 = 0$.

Problem 8.3: band formation



Consider a periodically repeating short ranged potential with range of $2a$ and distance l over which $V(x) = 0$ (hence $x_0 = l + 2a$). The transmission matrix from one force-free region to another is

$$Q = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda^* \end{pmatrix} T = \frac{1}{z_2} \begin{pmatrix} \lambda & -wz_1^*\lambda \\ z_1\lambda^* & -w\lambda^* \end{pmatrix}, \quad \text{where} \quad \lambda = \exp(iKl).$$

Show that the N-step transmission matrix, in the limit $N \to \infty$ has zeroes on the diagonal (no transmission) except exactly at resonance. Show that energy bands arise as a result.

Outline

The Hamiltonian for a harmonic oscillator

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

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

This describes ellipses in phase space: this is the classical motion of harmonic oscillators.

In the quantum Hamiltonian p and x become operators. In terms of the dimensionless quantities

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

Note that $[\hat{X}, \hat{P}] = i$.

Examples

1. Near the minimum of any smooth potential, its Taylor expansion is: $V(x) = V(x_0) + V''(x_0)(x - x_0)^2/2 + \cdots$, where x_0 is position of the minimum. Small amplitude motion is always harmonic.
2. Low-lying vibrational modes of molecules show almost harmonic spectrum as a result of this general fact. 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.
3. The motion of a charged particle in a magnetic field is a helix. The momentum components transverse to the field lines play the roles of X and P.

Raising and lowering operators

We will factorize $\hat{H}$ using the non-Hermitean operators

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{X} + i\hat{P}), \qquad \text{where} \qquad [\hat{a}, \hat{a}^\dagger] = 1.$$

Consider the Hermitean operator $\hat{N} = \hat{a}^\dagger \hat{a}$. One sees that $[\hat{N}, \hat{a}] = -\hat{a}$. If $|z\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue z, then $[\hat{N}, \hat{a}]\,|z\rangle = -\hat{a}\,|z\rangle$, and hence $\hat{N}\hat{a}\,|z\rangle = (z-1)\hat{a}\,|z\rangle$. So $|a\rangle$ lowers the eigenvalue of $\hat{N}$ by one unit.

For any $|\psi\rangle$, let $|\phi\rangle = \hat{a}\,|\psi\rangle$. 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 $\hat{a}$ will always lower the eigenvalue by one unit. On the other hand, if the eigenvalues are integers, then for $|0\rangle$ such that $\hat{N}\,|0\rangle = 0$, one also has $a\,|0\rangle = 0$. So, integer eigenvalues are allowed, and exist.

The eigenstates of the Hamiltonian

Since $\hat{N} = (\hat{X} - i\hat{P})(\hat{X} + i\hat{P})/2 = (\hat{X}^2 + \hat{P}^2 - 1)/2$, we find

$$\hat{H} = \omega \left(\hat{N} + \frac{1}{2} \right).$$

So the eigenvalues of $\hat{H}$ are $E = \omega(n + 1/2)$, for integer $n \geq 0$.
The ground state satisfies

$$\left(m\omega x + \frac{d}{dx} \right) \psi_0(x) = 0, \quad i.e., \quad \psi_0(x) = \left(\frac{m\omega}{\pi} \right)^{1/4} \mathrm{e}^{-m\omega x^2/2},$$

Since this is a first order differential equation, there is an 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!

We construct a generating function for the wavefunctions–

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

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

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

Then using the action of the exponential on the bra we find that

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

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

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

From the recurrence relation we can write down

$$H_0(x) = 1 \quad H_1(x) = 2x \quad H_2(x) = 4x^2 - 2 \quad \cdots$$

H_n has exactly n zeroes. The zeroes of successive polynomials are interleaved. Even numbered polynomials have even parity.

The harmonic oscillator wave functions

Comparing the recurrence relation for harmonic oscillator wave functions

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

with that for Hermite polynomials,

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

we find that

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

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

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

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

Schrödinger and Heisenberg pictures

We have chosen the Schrödinger representation of quantum states: the operators corresponding to time-independent classical variables remain time independent, and the states evolve by the action of the unitary time-evolution operator.

Since $\langle\psi'(t)|\hat{O}|\psi(t)\rangle = \langle\psi'(0)|U^\dagger(t)\hat{O}U(t)|\psi(0)\rangle$, physics remains unchanged if we use the Heisenberg picture. In this states are time independent and operators evolve with time through the adjoint action of the unitary evolution operator.

If $\hat{O}$ evolves, then its eigenstates evolve. Since these form a basis, the basis evolves, whereas the state remains fixed. So the difference between these pictures is the same as the active and passive views of transformations in a vector space. Show that the time evolution of wavefunctions is independent of the picture.

The thermal density matrix

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

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

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

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

Using the expression for Z above, we get

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

The Planck spectrum begins to emerge.

Outline

The classical theory

A particle of charge e and mass m moves in a magnetic field.

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

The classical equations of motion are

$$\dot{\mathbf{r}} = \mathbf{p}/m, \qquad \dot{\mathbf{p}} = e\mathbf{p} \times \mathbf{B}/m.$$

Taking the $\mathbf{B}$ in the z-direction, 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 $\omega = eB/m$. Scaling the time by a factor ω, it becomes clear that these equations of motion can be obtained from a fictitious Hamiltonian $H' = (p_x^2 + p_y^2)/2$. Writing $p_\pm = (p_x \pm ip_y)/\sqrt{2}$, 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 $\hat{\mathbf{P}} = \hat{\mathbf{p}} - e\mathbf{A}$. Then $[\hat{P}_j, \hat{P}_k] = ie\epsilon_{jkl}B_l$. With $\mathbf{B}$ in the z-direction, $[\hat{P}_j, \hat{P}_z] = 0$ for all j. Since $\hat{H} = \hat{\mathbf{P}}^2/2m$, this implies that $[\hat{H}, \hat{P}_z] = 0$.

The remainder of the Hamiltonian is like a harmonic oscillator,

$$\hat{H}' = (\hat{P}_x^2 + \hat{P}_y^2)/2m, \qquad \text{where} \qquad [\hat{P}_x, \hat{P}_y] = ieB.$$

By rescaling, $P'_{x,y} = P_{x,y}/\sqrt{eB}$, the Hamiltonain becomes the same as that of a harmonic oscillator with $\omega = eB/m$. These eigenvalues are called Landau levels. Eigenvalues of the full Hamiltonian are

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

Gauge invariance

Classically, gauge invariance means that for any function $\phi(\mathbf{r})$, $\mathbf{A}' = \mathbf{A} + \nabla\phi$ gives the same $\mathbf{B} = \nabla \times \mathbf{A}' = \nabla \times \mathbf{A}$. In the quantum theory, the algebra of $\hat{\mathbf{P}}$ depends only on B, and hence is gauge invariant. However, $\hat{a} = (\hat{P}_x + i\hat{P}_y)/\sqrt{2}$ is translated by a scalar

$$\hat{a}' = \hat{a} - \frac{e}{\sqrt{2}}(\phi_x + i\phi_y),$$

where the subscripts denote derivatives. This has no effect on the algebra of operators, but may affect states.

Problem 8.4: Gauge invariance

Find the eigenstates with any choice of gauge, then investigate what happens under gauge transformations. If $\hat{a}\left|0\right\rangle = 0$, and $\hat{a}'\left|0'\right\rangle = 0$, then what can one say about $\langle 0'|0\rangle$? Using the generating function for the other states, what can one say about the effect of gauge invariance on states?

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The energy eigenvalues and eigenvectors

The isotropic harmonic oscillator in D dimensions has the Hamiltonian

$$\hat{H} = \frac{\omega}{2}(\hat{\mathbf{P}}^2 + \hat{\mathbf{X}}^2),$$

where $\hat{\mathbf{X}} = \hat{\mathbf{x}}\sqrt{m\omega}$ and $\hat{\mathbf{P}} = \hat{\mathbf{p}}/\sqrt{m\omega}$. Introducing the ladder operators $\hat{a}_j = (\hat{X}_j + i\hat{P}_j)/\sqrt{2}$, as before, there are D number operators $\hat{N}_j = \hat{a}_j^\dagger \hat{a}_j$. One can write

$$\hat{H} = \omega \left[\frac{D}{2} + \sum_{j=1}^{D} N_j \right].$$

The energy eigenstates can be specified in the form $|n_1, \cdots, n_D\rangle$ where n_i are the eigenvalues of $\hat{N}_i$. Writing $N = n_1 + \cdots + n_D$, the energies are $E = \omega(N + D/2)$. Since the n_i do not individually enter the expression for the energy, there could be a high degree of degeneracy. So the Hamiltonian must have symmetries.

Extended symmetry for D=2

For $D = 2$, n_2 is fixed once N and n_1 are given. However, for each N, n_1 can take any value from 0 to N. Hence the level is $(N + 1)$-fold degenerate.

One can increase n_2 by 1 and decrease n_1 by 1 without changing the energy. This can be done by the operator $a_1^\dagger a_2$. In fact, the 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 $|N, n_1 + 1\rangle$.

Problem 8.5: the symmetry algebra

Evaluate $[\hat{H}, s_1]$, $[\hat{H}, s_2]$, and $[s_1, s_2]$. Complete the symmetry algebra by forming commutators of all the new operators formed. Continue the process until no new operators can be generated.

Matrix representations of algebras

Given an algebra, such as $A^2 = 1$, one can construct many different sizes of matrices which represent A. For example, $A = -I$ where I is the $n \times n$ identity matrix represents the algebra. Different representations of the symmetry algebra of the 2D harmonic oscillator can be obtained by acting on states of different N. For example, acting on the $N = 0$ space, we find the representations by integers: $\hat{H} = 1$ and $s_1 = s_2 = 0$.
The $N = 2$ space of states has $|1\rangle = |1, 0\rangle$ and $|2\rangle = |0, 1\rangle$. This gives the matrix representations

$$\hat{H} = \omega \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad s_1 = \omega \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad s_2 = \omega \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

For any N, the representation of $\hat{H}$ is the $(N + 1) \times (N + 1)$ identity matrix. And the other operators?

The symmetry group SU(2)

Any linear combination of the degenerate eigenstates of an isotropic 2-dimensional harmonic oscillator is generated by the unitary matrix $U = \exp\left(i \sum_j \theta_j s_j\right)$. Note that $\det U = 1$ (because the trace of its logarithm is zero). Since this mixes states with the same energy, all these U must commute with the Hamiltonian. In particular, this is true of the two-dimensional subspace with $N = 1$. 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 H is SU(2). The higher dimensional matrices which commute with H are not all possible larger unitary matrices, but a subgroup which is isomorphic to SU(2). These matrices of different sizes are called different representations of SU(2). The Hermitean operators s_1, s_2 and s_3 are called the generators of SU(2), or elements of the algebra 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).

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

Outline

Keywords and References

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Bloch's theorem, lattice vector, finite range potential, scattering matrix, transmission matrix, resonances, harmonic oscillator, Rayleigh coefficient, ground state, generating function, Hermite polynomials, recurrence relation, Schrödinger representation, Heisenberg picture, cyclotron frequency, Landau levels, the group SU(2), representations of SU(2), generators of SU(2).

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