

CHAPTER 1.
ENERGY SPECTRUM AND WAVE FUNCTIONS

In this chapter, we survey the general aspects of quantum mechanics for time-independent problems that we will encounter repeatedly in later chapters of this book. We begin with a brief introduction of the concept and usage of energy spectrum and wave functions, as well as a short account of how they are probed in experiments. We then describe the general results for one dimensional systems, introducing the method of transfer matrix, and discussing the role and physical meaning of boundary conditions. This is followed by a brief account of general properties of higher dimensional systems, and some demonstration of how one builds models in the three dimensional physical space from one dimensional solutions. Here, we will discuss how effective lower-dimensional systems, such as the two dimensional electron gas, quantum wires and quantum dots, may arise as a result of geometrical confinement and low temperature. Finally, we consider extended systems, describing the concept of density of states, density matrix and Green functions, and also briefly introducing the locality principle.

I. THE HAMILTONIANS IN THIS BOOK

We will follow an approach from a general setting of quantum mechanics, examining the properties of a variety of models of Hamiltonian systems. The prototype system is a spinless particle of mass m living in a three dimensional world, whose Hamiltonian is a simple sum of kinetic and potential energies:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}). \quad (1)$$

We have learned in quantum mechanical courses how to solve the problems of the harmonic oscillator and the Hydrogen atom, and have learned how to reduce three dimensional problems into one dimensional problems by employing the rotational symmetry and the method of separation of variables. We have also learned some general knowledge of when and how bound states and scattering states may arise. Much more complicated potentials appear in condensed matter problems: $V(\mathbf{r})$ may be periodic, quasiperiodic or random functions of position; bound states in one place may be coupled to those in another place by quantum tunneling through the energy barriers; scattering states from one scatterer may be further scattered by other scatterers.

More complicated systems can be described by generalizing the above Hamiltonian in various ways. For a charged particle like an electron moving in a magnetic field $\mathbf{B}(\mathbf{r}, t)$, we must add to the momentum operator $-i\hbar\nabla$ the term $e\mathbf{A}(\mathbf{r}, t)$, where \mathbf{A} is the vector potential satisfying $\nabla \times \mathbf{A} = \mathbf{B}$. [1] The effect of an electric field $\mathbf{E}(\mathbf{r}, t)$ can be represented by either or both of the vector potential and a scalar potential $\phi(\mathbf{r}, t)$ which enters into the potential energy in the form of $-e\phi$, we have the gauge relation $\mathbf{E} = -\frac{\partial}{\partial t}\mathbf{A} - \frac{\partial}{\partial \mathbf{r}}\phi$. Therefore, one must directly deal with the gauge potentials in the Schrödinger equation, which makes this set of systems a fascinating subject of study. The

Aharonov-Bohm effect, the quantum Hall effect, and the Wannier-Stark ladders are some of the most remarkable phenomena associated with the gauge aspect of quantum mechanics. The effects of both weak (chapter 3) and strong (chapter 5,6, 8) electromagnetic fields will be studied in this book.

For many problems, the role of spins is rather passive, they just increase the degeneracy of states by a factor of two, or give two sets of states with mutually shifted energy spectrum due to the spin magnetization in a magnetic field. In some other problems, the situation is quite the opposite: the spatial motion is frozen, but the spin dynamics becomes the center of attention. The model of $\frac{1}{2}$ -spin in a magnetic field has been a paradigm system in physics, and its various properties will be studied later. Spin-orbit interaction is important in heavy atoms either in gas and condensed phase, and plays an important role in magnetism.

The ultimate complication (and richness) on the study of electronic properties is the many-body effect due to inter-particle interactions. Sometimes, one can partially deal away this complication by invoking the Fermi-liquid theory; it is still a very difficult task to determine the quantitative change of the results predicted in the independent particle picture by the interactions. The topological invariants of the integer quantum Hall effect and related phenomena are rare examples of physical quantities which are not changed by many-body interactions. In some cases, qualitatively new effects arise, such as superfluidity, superconductivity, and the fractional quantum Hall effect. No attempt will be made in this book to address systematically the effects of interactions between particles and with lattice vibrations.

Technological advancement in materials has led to the creation of lower dimensional electronic systems, such as the two dimensional electron gas, quantum wires and quantum dots, which used to exist only in pedagogical examples. Also, samples have been made clean enough that ballistic or wave-guide transport of electrons can be observed. For disordered samples, quantum coherence can be manifested in various dramatic ways when inelastic scattering is made weak enough. The physics of such nanostructures and mesoscopic systems will be emphasized in this book. Further, in response to the demand of quantum engineering, considerable attention will be given to systems with time-dependent driving.

II. GENERAL CONCEPTS

A. The eigenvalue problem

When we know the system Hamiltonian H , a great deal of information may be obtained by studying its energy spectrum and eigenstates. When H is time independent, they give complete description of the dynamical and statistical properties of the system. They also serve as a convenient basis in the description of system properties when H varies slowly in time or is weakly perturbed by time-dependent or constant terms. We therefore consider the eigenvalue problem of the Schrödinger equation

$$\epsilon|\psi\rangle = H|\psi\rangle, \quad (2)$$

where we have used the Dirac ket notation for generality and simplicity.

The simplest example is a one dimensional free particle for which $H = -i\hbar\frac{d^2}{dx^2}$. The solution of the Schrödinger equation for this example is $\psi = e^{ikx}$, or e^{-ikx} , or their linear combinations. The energy E is given by $\frac{\hbar^2k^2}{2m}$. Here, k is a complex number, whose allowed values is yet to be determined. In general, in the presence of a scalar potential in one dimension, there are two

independent solutions for any given (including complex) value of E . In higher dimensions, the number of such independent solutions become infinite.

For a physical problem, we must supply appropriate boundary conditions, which select a subset of such solutions. The boundary conditions are as important as the Schrödinger equation in determining the characteristics of the physical system. As a general quantum mechanical principle, a physical boundary condition must make the Hamiltonian a Hermitian operator, so that the energy eigenvalue E takes real values. This will constraint the form of possible solutions. For the above example, we must require k to be purely real or purely imaginary. However, a concrete set of boundary conditions is still needed to make the problem completely defined.

The Schrödinger equation and a set of boundary conditions form an eigenvalue problem. [2] A possible value of E is called an eigenenergy. A non-zero solution of the wave function is called an eigenenergy state, or simply an eigenstate. The set of eigenvalues $\{E_j\}$ is called the energy spectrum of the particle. Eigenstates belonging to different eigenenergies are automatically orthogonal to one another, and those belonging to a degenerate eigenenergy can be chosen to be mutually orthogonal. More over, they form a complete basis for the Hilbert space of states satisfying the same set of boundary conditions as the eigenvalue problem. Therefore, a wave function may be expanded in terms of the orthonormalized eigenstates as:

$$|\psi\rangle = \sum_j |\psi_j\rangle \langle \psi_j | \psi \rangle. \quad (3)$$

B. Time evolution of a wave function

Suppose we know that an electron is initially in a state of $|\psi(t=0)\rangle$; how will it evolve in time? From quantum mechanics, we know that $\psi(t)$ must satisfy the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle. \quad (4)$$

We now substitute into it the following expansion:

$$|\psi(t)\rangle = \sum_j A_j(t) |\psi_j\rangle \quad (5)$$

where $|\psi_j\rangle$ is the set of eigenstates, then

$$i\hbar \frac{\partial}{\partial t} A_j(t) = E_j A_j(t), \quad (6)$$

which is then solved by

$$A_j(t) = A_j(0) e^{\frac{1}{i\hbar} E_j t}. \quad (7)$$

The initial A_j may be determined from the initial $|\psi\rangle$ by

$$A_j(0) = \langle \psi_j | \psi(t=0) \rangle. \quad (8)$$

Therefore, once we know the initial state, its time evolution is completely specified by the eigenvalues and the eigenstates. Also, the probability on each eigenstate $|A_j|^2$ does not change in time.

Caution: The above procedure is valid only for time-independent Hamiltonians. When H depends on time, one has to solve the time-dependent Schrödinger equation in some other way.

C. Statistical physics

A collection of non-interacting identical particles is described by two parameters: the temperature T and the chemical potential μ . The average number of particles in state j is given by

$$n_j = \frac{1}{e^{(E_j - \mu)/kT} \pm 1} \quad (9)$$

where “+” is for Fermions and “-” is for bosons. The statistical average of any observable \hat{O} is given by

$$\langle \hat{O} \rangle = \sum_j O_{jj} \cdot n_j, \quad O_{jj} = \langle \psi_j | \hat{O} | \psi_j \rangle. \quad (10)$$

Fermions satisfy the Pauli exclusion principle: any one state cannot be occupied by two or more identical particles. Therefore, the average number, $n_j \leq 1$. At absolute zero temperature, n_j is either 1 or 0: for $E_j < \mu$, the exponential is 0, $n_j = 1$; for $E_j > \mu$, the exponential is ∞ , we have $n_j = 0$. In other words, all the states below μ get filled, each of them holding one particle, while those above μ are empty. In such a case, μ is also called the Fermi energy, denoted as E_F .

On the other hand, any number of bosons can occupy the same state. In particular, at low enough temperatures, some systems may have a macroscopic number of bosons occupying the lowest energy single particle state. This is the so-called Bose condensation phenomenon, responsible for superfluidity and superconductivity.

Caution: when the particles interact with one another, the above procedure fails. But, for many problems, interacting systems may be formulated in some sense as a collection of non-interacting particles to a very good approximation.

D. Probing spectral and wave function properties

Spectral information can be probed by applying sinusoidal perturbations to the system, and revealed with the help of energy conservation law shown explicitly in the Fermi golden rule for the transition rates between the initial and final states. Symmetry properties (parity, rotational, translational) of the eigenstates may also be probed with the help of selection rules for the transition matrix element in the Fermi golden rule. In a condensed matter system, bound states can be probed like those in atomic and molecular systems, while the energy dispersion of extended states can be probed by inelastic scattering of particle beams of photons, electrons, neutrons, or even positrons. Also, spectral and wave function properties can also be reflected in a collective and cruded way through susceptibility and transport measurements in the presence of static or quasi-static electromagnetic fields.

III. OPEN SYSTEMS

The concept of an open system is defined relative to a closed system. In the latter the quantum particle is confined in some finite region of the space, while in the former the particle is allowed to go to infinity. In this Section, we will limit our attention to the cases where the potential becomes zero outside a finite region, or falls off sufficiently rapidly at large distances. The spectrum consists

of the continuous line from $E = 0$ to positive infinity, where we have scattering states, and possibly a discrete set of negative energy levels, for which the states are localized about the potential region and decays to zero exponentially at large distances. The free particle model is a special case, for which the eigenstates are plane waves which form the bases of much of the discussions on scattering states.

If the potential diverges to positive infinity at large distances, such as the harmonic oscillator potential, only bound states exist which decay to zero at large distances with a rate faster than exponential. In later chapters, we will consider periodic, quasi periodic and random potentials, which do not approach a constant nor they diverge at large distances. New types of spectral and wave function properties will be found.

A. Bound states

When the potential is negative in some region (potential well), it is possible to have one or more bound states of negative energies E_j , which decay at large distances as $\sim e^{-\kappa r}$ with $\kappa = \sqrt{-E_j 2m}/\hbar$. It is instructive to consider the problem of a square well, $V(\mathbf{r}) = -V_0$ for $r < a$ and zero otherwise, where $V_0 > 0$ is the well depth. In one and two dimensions, there is always a bound ground state as long as the potential depth is nonzero. When $V_0 \ll \frac{\hbar^2}{2ma^2}$, the energy of the ground state approaches zero, and the extent of the wave function becomes very broad: $\kappa = \sqrt{2mV_0}/\hbar^2$ in one dimension, and $\kappa = \frac{1}{a} \exp(-\frac{\hbar^2}{2ma^2V_0})$ in two dimensions. In three dimensions, a minimum depth of the potential is required for the existence of a bound ground state: $V_{min} = \frac{\hbar^2}{2ma^2} (\frac{\pi}{2})^2$. Qualitatively the same results are obtained for any negative potential.

The ground state is always nondegenerate and nodeless. In one dimension, more can be said about the excited bound states if they exist: They are nondegenerate, and the n th excited states has n nodes in the region of the potential, which is known as the node counting theorem. There is also a simple quantization formula in the WKB approximation for the levels in a classically allowed region:

$$\int dx \sqrt{2m[\epsilon_n - V(x)]}/\hbar = n + \frac{1}{2}, \quad (11)$$

if tunneling to other regions is neglected. This leads to the Thomou-Fermi formula for the number of bound states

$$n_b = \frac{1}{h} \approx \int 2p(x)dx, \quad (12)$$

for one dimension, where $p(x) = \sqrt{2m(-V(x))}$, and the integral is over the classically allowed regions at zero energy. [3] This formula just counts the classical phase space area in units of the Planck constant h .

In three dimensions, the formula becomes

$$n_b = \frac{4\pi}{3h^3} \int p^3(\mathbf{r})d^3r, \quad (13)$$

with $p(\mathbf{r})$ being the magnitude of the classical momentum at \mathbf{r} . Therefore, a given shape of the potential well, the number of bound states increases with the depth and the width of the well. The fact that the Coulomb potential can bind an infinite number of states can be seen easily from the above semiclassical formula.

For a spherically symmetric potential, the number of bound states of a given angular momentum l is related to the phase shifts (see the next subsection) at energy $E = 0^+$ through the Levinson's theorem:

$$n_l = \delta_l / \pi. \quad (14)$$

The case of $l = 0$ is exceptional, for which the left hand side of the above equation should add $\frac{1}{2}$.

B. Scattering states

In the free particle model, the energy spectrum is a continuous line from $E = 0$ to positive infinity. The wave functions are plane waves:

$$|k \rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}, \quad k^2 = 2mE/\hbar^2 \quad (15)$$

in one dimension, and

$$|\mathbf{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad \mathbf{k}^2 = 2mE/\hbar^2 \quad (16)$$

in three dimensions. The coefficients are chosen to ensure the normalizations $\langle k'|k \rangle = \delta(k - k')$, and $\langle \mathbf{k}'|\mathbf{k} \rangle = \delta(\mathbf{k} - \mathbf{k}')$. For $E > 0$, the states are two-fold degenerate in one dimension, and infinitely degenerate in two and three dimensions. Therefore, the eigenstates are equally well represented by the combinations of the degenerate plane waves. For instance, the eigenstates can be classified by the quantum numbers of the angular momentum, with the radial wave functions given by the Bessel functions of integer order in two dimensions and half-integer order in three dimensions.

In the presence of a potential confined to some region, the positive real axis still belongs to the energy spectrum. Each eigenenergy state may be written in the form of a plane wave representing an incident wave plus a wave function representing the scattered waves, which may be written as (for 3d)

$$|\psi_{\mathbf{k}} \rangle = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}, \mathbf{k}') \frac{e^{ikr}}{r} \quad (17)$$

in the region outside the potential, where $f(\mathbf{k}, \mathbf{k}')$ is a function of the angles uniquely determined by the potential and representing the scattering amplitude from \mathbf{k} to \mathbf{k}' . If the above wave function is multiplied with the coefficient $\frac{1}{(2\pi)^{3/2}}$, it will be normalized in the same way as the plane waves given in the last paragraph.

The square of the scattering amplitude is the differential cross section. The total cross section satisfies the optical theorem

$$\sigma = \frac{4\pi}{k} \text{Im} f(\mathbf{k}, \mathbf{k}), \quad (18)$$

representing the fact that the reduction of the current in the forward direction equals the total scattered current in all other directions.

Because of time reversal symmetry, the amplitude satisfies the reciprocity relation $f(\mathbf{k}', \mathbf{k}) = f(-\mathbf{k}, -\mathbf{k}')$. If the potential has spatial inversion symmetry, then $f(-\mathbf{k}, -\mathbf{k}') = f(\mathbf{k}, \mathbf{k}')$. The

combination of both symmetries yields the generalized reciprocity relation $f(\mathbf{k}', \mathbf{k}) = f(\mathbf{k}, \mathbf{k}')$. In the Born approximation which is valid for weak scatterings, we have

$$f(\mathbf{k}, \mathbf{k}') = -\frac{m}{2\pi\hbar^2} \int d^3r V(\mathbf{r}) \exp(i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}). \quad (19)$$

This obviously satisfies the reciprocity relation, and its generalized version when the potential has inversion symmetry. Even in the absence of inversion symmetry, the differential cross section satisfies $\sigma(\mathbf{k}, \mathbf{k}') = \sigma(\mathbf{k}', \mathbf{k})$ in the Born approximation.

When the potential is spherically symmetric, the scattering amplitude only depends on the angle θ between \mathbf{k}' and \mathbf{k} , and may be expanded into components of different angular momentum:

$$f(\theta) = (2ik)^{-1} \sum_0^{\infty} (2l+1)(e^{i2\delta_l} - 1)P_l(\cos\theta), \quad (20)$$

where $P_l(x)$ are the Legendre polynomials, and δ_l are the phase shifts. The phase shift δ_l for each angular momentum l is obtained by solving for the radial wave function, and comparing it with the asymptotic form $r^{-1} \sin(kr - \frac{1}{2}l\pi + \delta_l)$ in the potential free region. Literally, the phase shift is zero when there is no scattering potential. The total scattering cross-section is given by

$$\sigma = \frac{4\pi}{k^2} \sum_0^{\infty} (2l+1) \sin^2 \delta_l. \quad (21)$$

C. Transmission and reflection in one dimension

1. General properties

In one dimension, the scattering problem becomes that of transmission and reflection. Because of the topology of the one dimensional space, it is possible to formulate the scattering problem for the infinite space as a succession of scattering problems over finite intervals using the method of transfer matrix. This simplification makes it possible to deal with the more complicated and typical situation of a condensed matter system where the potential is not confined to a finite region.

Consider a point x_1 in a classically allowed region, the wave function in an infinitesimal neighborhood of that point can always be written as

$$\psi(x) = \frac{A_1}{\sqrt{k_1}} e^{ik_1(x-x_1)} + \frac{B_1}{\sqrt{k_1}} e^{-ik_1(x-x_1)}, \quad (22)$$

where $k_1 = \sqrt{2m(\epsilon - V(x_1))/\hbar^2}$. The coefficients A_1 and B_1 can be thought as a linear parametrization of the wave function and its derivative at $x = x_1$. The former are used in place of the latter, because they are more readily be given a physical meaning as the amplitudes of the traveling waves to the right and to the left.

Linearity of the Schrödinger equation ensures that there is a linear relationship between the amplitudes at x_1 and those at another point x_2 (which we also assume to be classically allowable):

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} M_1 & M_2 \\ M_2^* & M_1^* \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \quad (23)$$

where the particular structure (Cayley form) of the transfer matrix follows from the time reversal symmetry of the problem: the complex conjugate of the wave function also satisfies the Schrödinger equation.

Let the coefficients be related by the transfer matrix as

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}. \quad (24)$$

In the time reversed situation, $A_{1,2}^*$ play the same role as $B_{1,2}$, and $B_{1,2}^*$ play the same role as $A_{1,2}$, we therefore have

$$\begin{pmatrix} B_2^* \\ A_2^* \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} B_1^* \\ A_1^* \end{pmatrix}. \quad (25)$$

Comparing the complex conjugate of this matrix relation with the previous one then shows that $M_{21} = M_{12}^*$ and $M_{22} = M_{11}^*$.

Problem: Show that the product of two matrices in the Cayley form is still of the Cayley form.

The two independent entries of the transfer matrix are related to the transmission and reflection amplitudes from the following considerations. Setting $A_1 = 1$, and $B_2 = 0$, we have a scattering situation of unit incident wave from the left (assuming $x_2 > x_1$). Then A_2 should be equal to the transmission amplitude t and B_1 the reflection amplitude r . Then the two equations in (23) give $M_1 = 1/t^*$ and $M_2 = -(r/t)^*$. Conservation of probability current, $|t|^2 + |r|^2 = 1$, requires that the determinant of the transfer matrix to be unity, i.e., $|M_1|^2 - |M_2|^2 = 1$.

Similar consideration shows that $M_1 = 1/t'^*$ and $M_2 = r'/t'$, where t' and r' are the transmission and reflection amplitudes from the right. We therefore have $t' = t$, and $r' = r^*(-t/t^*)$. Therefore, both the transmission and reflection coefficients, defined as the absolute-value-squared of the corresponding amplitudes, are independent of the incident direction. The direction independence of the reflection coefficient is a remarkable fact of quantum mechanics, because one would think that reflection is mostly due to scattering from the incident side of the potential, and the two sides of the potential is generally different.

If the potential is symmetrical about the middle of x_1 and x_2 , even the phase of the reflection amplitudes from the two sides are the same, which implies that r/t and M_2 are imaginary. The phase δ of the transmission amplitude plays the same role as the phase shift introduced in the last subsection.

2. Resonances and tunneling

It is again instructive to consider the square potential $V(x) = V_0$ for $|x| < a$, and zero otherwise. The transmission amplitude between $x_1 = -a$ and $x_2 = a$ for $E > V_0$ is given by

$$t = [\cos(2\alpha a) - \frac{i}{2}(\frac{k}{\alpha} + \frac{\alpha}{k})\sin(2\alpha a)]^{-1}, \quad (26)$$

where $\alpha = [2m(E - V_0)/\hbar^2]^{\frac{1}{2}}$. For a potential well $V_0 < 0$, this result is valid for all positive energies. For a potential barrier, it is valid for energies above the barrier top. In both cases, a classical particle would pass the potential without reflection, but the quantum particle can suffer some reflection except for a sequence of energies when the well width fits an integer number of wave lengths: $2\alpha a = \pi, 2\pi, 3\pi, \dots$, at which the transmission amplitude becomes unity in magnitude. Complete transparency for an infinite sequence of energies above the potential occurs generally if the potential is symmetrical.

When the energy is below the potential barrier, we need to replace α in the above formula by $i\beta$, where $\beta = [2m(V_0 - E)/\hbar^2]^{\frac{1}{2}}$, and the transmission amplitude becomes

$$t = [\cosh(2\beta a) - \frac{i}{2}(\frac{k}{\beta} - \frac{\beta}{k})\sinh(2\beta a)]^{-1}. \quad (27)$$

When $e^{-4\beta a} \ll 1$, the expression reduces to the form $Ae^{-2\beta a}$. The exponential factor is recognized as a special case of the WKB formula of barrier tunneling amplitude

$$e^{-\int dx \kappa(x)}, \quad (28)$$

where $\kappa(x) = \sqrt{2m(V(x) - E)/\hbar^2}$, and the integration is over the classically disallowed region. [4]

Transmission through a double barrier is also a very interesting problem. By multiplying three transfer matrices for the different parts of the double barrier structure, we find that the transmission coefficient T satisfies

$$\frac{1}{T} = \frac{1}{T_1 T_2} [1 + R_1 R_2 - (r'_1 r_2 e^{-i2\phi} + c.c.)], \quad (29)$$

where $T_{1,2} = |t_{1,2}|^2$ and $R_{1,2} = |r_{1,2}|^2$ are the transmission and reflection coefficients of the two barriers, and ϕ is the phase accumulation for traveling between the barriers. We have used the fact that $r' = r^*(-t/t^*)$ for reflection from the right, and have assumed that the region between the barriers is free of reflections. It is seen that the transmission coefficient T is generally on the order of $T_1 T_2$, which is extremely small if both T_1 and T_2 are small. However, for $T_1 = T_2$ the transmission coefficient becomes unity when the resonance condition is satisfied: $\phi = \phi_r + \pi j$, where ϕ_r is the phase of $r'_1 r_2$. This is also the condition for the existence of a bound state between the barriers if tunneling out of the barriers are neglected. [5]

When the barriers are different, the resonant transmission coefficient is given by $\frac{4T_1 T_2}{(T_1 + T_2)^2}$, which is still a substantial fraction when T_1 and T_2 are not too different (say, within a factor of 10).

The resonant width (full width at half maximum) for $T_1 = T_2$ is given by $\delta\phi = T_1$. Since $\hbar \frac{\partial\phi}{\partial\epsilon}$ is the half time cycle for traveling between the barriers, the life time of the resonant state may be taken as $\tau = \frac{T_1}{\hbar} (\frac{\partial\phi}{\partial\epsilon})^{-1}$. Therefore, the resonant width in energy is given in terms of the life time as $\delta\epsilon = \frac{\hbar}{\tau}$. Unlike the over barrier resonances which are very broad, the tunneling resonances are narrow because of the exponential smallness of the transmission through each barrier.

IV. CLOSED SYSTEMS

In a closed system, the wave functions are confined within a finite range under certain Hermitian boundary conditions. The boundary conditions may arise as limiting cases of physical situations, or may be imposed artificially for various purposes of theoretical treatment of large systems. In the latter case, one hopes and is usually warranted that the calculated bulk properties of system does not depend on the particular boundary condition that one chooses. In recent years, there is an increased awareness of the importance of boundary conditions because of the experimental and theoretical development in nanostructures and mesoscopic systems.

The energy spectrum is always a discrete and infinite set in a closed system. The eigenstates form a basis of the Hilbert space of all functions satisfying the *same* boundary conditions. As a general result of the variational principle, the eigenenergies always increase as the size is decreased under the same boundary condition.

A. Boundary conditions

One kind of Hermitian boundary condition is the Dirichlet type: $\psi|_{\mathbf{r} \in \text{boundary}} = 0$, which is also commonly called as the box boundary condition. This may be regarded as a limiting case of a

quantum well bounded by very sharp and high potential steps. The solutions for a one dimensional free particle are $\psi = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{L}$, and $\epsilon = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$, with $n = 1, 2, \dots$, where L is the size of the system.

Another kind of Hermitian boundary condition is the von Neumann type, $\mathbf{n} \cdot \psi|_{\mathbf{r} \in \text{boundary}} = 0$, where \mathbf{n} is a normal vector of the boundary. In the context of elastic wave problems, such a boundary condition arises when the media is free of constraints at the boundary, so it is also called as free or natural boundary condition. In a quantum system, if the potential is symmetric about a certain plane and if we are only interested in the symmetrical wave functions, we can limit our attention to only one side of the system by applying the von Neumann boundary condition on the plane. Otherwise, It is not clear how this kind of boundary condition can be devised in a simple quantum system as a limiting case of some potential configurations. In a complex quantum system such as a superconductor or superfluid, the von Neumann boundary condition arises in an effective theory such as the Ginsburge-Landau equations.

A very different kind of Hermitian boundary condition is the periodic boundary condition $\psi(x + L) = \psi(x)$. There is really no boundary in such a system. The allowed solutions for a one dimensional free particle are $\psi = \sqrt{\frac{1}{a}} e^{ikx}$, with $k = 2\pi n/L$, $n = \text{integers}$. A physical realization of such a boundary condition is a ring of length L , with x being the coordinate around the ring. The periodic boundary condition is physically imposed on the system, if we regard the ring as a part of a singly connected piece of a two or three dimensional region, because the wave function in a singly connected region must be single-valued. [6]

Different boundary conditions give different sets of eigenenergies and wave functions. The box boundary condition is more repulsive than the free boundary condition: in the same potential, the n th eigenvalue under the former condition is higher than the n th eigenvalue under the latter. In the same sense, the repulsiveness of the periodic boundary condition lies in between of these two conditions.

In one dimension, the eigenenergies under the box and free boundary conditions are non-degenerate. Also, the node counting theorem applies in both cases, with the nodes at the boundaries discounted. Because the number of nodes increases with energy, the n th eigenenergy under the box condition is still lower than the $(n + 1)$ th under the free boundary condition. The eigenenergies under the periodic boundary condition generally become non-degenerate [7], if the potential is non-zero (non-flat). The node counting theorem then becomes applicable.

B. Effect of magnetic fluxes

A generalized or twisted periodic boundary condition can arise effectively in the following way. In the presence of a magnetic flux ϕ passing through the ring, a vector potential enters in the Hamiltonian by adding $eA(x)$ to the momentum operator $-i\hbar \frac{d}{dx}$. One may gauge away this vector potential from the Hamiltonian by the unitary transformation $\psi = \exp[i\frac{e}{\hbar} \int_0^x A(x) dx] \tilde{\psi}$. We assume that any leakage of the wave function into the hole of the ring is negligible. However, the periodic boundary condition for ψ is transformed into the twisted periodic boundary condition for $\tilde{\psi}$ as

$$\tilde{\psi}(x + a) = e^{i2\pi\phi/\phi_0} \tilde{\psi}(x), \quad (30)$$

where $\phi_0 = \frac{h}{e}$ is the flux quantum, and we have used the fact that the integral of $A(x)$ around the ring equals the flux. In the absence of a scalar potential, the eigen solutions are still plane waves, but with $k = 2\pi(n + \phi/\phi_0)/L$, $n = \text{integers}$. Since physical properties such as the energy spectrum do depend on the boundary condition, the effect of the flux is real even if the flux does not touch the electrons on the ring. Also, the periodic flux dependence of this so-called Aharonov-Bohm effect is evident.

In the presence of a potential along the ring, the degeneracies occurring at $\phi/\phi_0 =$ integers or half-integers will be lifted in general according to the Wigner–von Neumann theorem. When the potential is weak, the gaps developed at the attempted crossings are small. For a strong potential, the gaps are large, making the energy–flux dispersion very flat. More discussions of this will be made in connection with periodic potentials, persistent currents, and localization phenomena.

V. BUILDING PHYSICAL MODELS USING 1D SOLUTIONS

3d, quantum sheet, quantum wire, quantum dot. quantum anulus, ring, disc, cylinder, quantum dash, quantum sphere, tube, stadium.

VI. CHARACTERIZATION OF EXTENDED SYSTEMS

In the field of condensed matter physics, one often needs to study systems whose size is large compared with the typical wave length of the occupied states. Since the energy levels are closely spaced in the large size limit, it becomes useful to consider the density distribution of such levels called the density of states. Also, for many purposes one is interested in finding the spatial distribution of the particle density, defined for fermion systems as the sum of the probability densities of the occupied states. A joint characterization of the density of states and density of particles is described by the local density of states, which is routinely measured in scanning tunneling microscope experiments. We will also discuss characterization functions depending on the phase information of the wave functions, the density matrix and the Green function. The former describes general equilibrium statistical properties, and latter is particularly useful in perturbation theory and for linear response properties. Explicit results for these functions are given for free electron gases.

We devote a section on a general discussion of the locality properties of these functions. In classical physics in the absence of long range forces, physical properties in a region does not depend on conditions at far away places from the region. We will find that this is also true for noninteracting Fermions in quantum mechanics at least for those properties describable by the density, the local density of states, or the equilibrium density matrix. At nonzero temperatures, the sensitivity to far away conditions is an exponentially decaying function of the distance. At zero temperature, the decay becomes a power law with a Friedel type oscillating amplitude. We will also discuss the off-diagonal locality for the density matrix and the Green function, i.e., the decaying properties of these quantities as a function of the distance between their spatial variables.

Thomas–Fermi method.

A. Density of states

Consider first the one-dimensional free electron problem with periodic boundary condition. Since the wave number $k = \frac{2\pi n}{L}$ is closely spaced for large size L , we have

$$\sum_k f(k) = L \int \frac{dk}{2\pi} f(k), \quad (31)$$

where $f(k)$ is any smooth function of k , and the summation is over allowed values of k . More over, if f depends on k only through the energy $\epsilon(k) = \frac{\hbar^2 k^2}{2m}$, we can write

$$\sum_k f(\epsilon(k)) = L \int dE n(E) f(E), \quad (32)$$

where $n(E) = \int \frac{dk}{2\pi} \delta(E - \epsilon(k))$ is the density of states, counting the number of energy levels per unit energy interval and per unit length. The result is $n(E) = \frac{1}{2\pi\hbar} \sqrt{\frac{2m}{E}}$. If spin degeneracy is counted, this result is increased by a factor of 2.

Does this result depend on the particular boundary condition we took? No. Consider for instance the box boundary condition for which $k = \frac{\pi n}{L}$, where the right hand side miss a factor of 2 compared with the case for the periodic boundary condition, but here n is restricted to positive integers only.

The summation formula can be easily generalized to the cases of higher dimensional electron gases: replace L by the area A or volume V , dk by the area or volume element in the \mathbf{k} space, and 2π by its power of 2 or three, respectively. The density of states can be similarly found to be $n(E) = \frac{m}{2\pi\hbar^2}$ for two dimensions, and $n(E) = \frac{(2m)^{3/2}}{4\pi^2\hbar^3} E^{1/2}$ for three dimensions. Again, these formulas need to be multiplied by a factor of 2 when spin degeneracy is counted. These results are illustrated in the figure below.

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The total density of energy levels for the whole system is proportional to the size of the system. This is a general result for any system that is homogeneous on the scale of the system size. We therefore generally define the density of states as

$$n(E) = \frac{1}{V} \sum_j \delta(E - E_j), \quad (33)$$

where V is the volume of a three dimensional system. In 1D and 2D, V should be replaced by the length L and area A , respectively.

To see how the size dependence in the density of states vanish in the thermodynamic limit, we consider an electron gas in a two dimensional billiard of area A on whose boundary the wave functions are zero. If the perimeter has length L , curvature $\kappa(s)$, and sharp corners of interior angles θ_i , then the total number of energy levels below E is [8]

$$N(E) = \frac{mE}{2\pi\hbar^2} A - \frac{(2mE)^{1/2}}{4\pi\hbar} L + \sum_{\text{corners}} \frac{\pi^2 - \theta_i^2}{2\pi\theta_i} + \frac{1}{12\pi} \oint \kappa(s) ds. \quad (34)$$

In deed, in the thermodynamic limit $A \rightarrow \infty$, the first term on the right hand side dominate over the other terms, yielding the same density of states that we obtained above for two dimensional electron gases.

Three dimensional generalization of this result may be obtained in ...

Expansion on level-spacing distributions,....

B. Spatial density distribution

In the last subsection, we considered the distribution of energy levels. In this subsection, we will consider physical quantities also depending on the spatial probability distribution of the eigenenergy states. We first introduce the local density of states defined as

$$\rho(E, \mathbf{r}) = \sum_j \delta(E - E_j) |\psi_j(\mathbf{r})|^2, \quad (35)$$

which measures the density of electrons at position \mathbf{r} when the states in a unit energy interval at E are occupied. If we average the local density of states over the system size, we obtain a general formula for the density of states $n(E)$. For systems with running plane wave eigenstates, $\rho(E, \mathbf{r})$ is independent of \mathbf{r} and is simply equal to the density of states.

The particle density at temperature T and chemical potential μ is given by

$$\rho(\mathbf{r}) = \sum_j \frac{|\psi_j(\mathbf{r})|^2}{e^{(\epsilon_j - \mu)/k_B T} \pm 1}, \quad (36)$$

which may be expressed as an energy integral of the local density of states times the thermal distribution function. For an electron gas and at zero temperature, all states below the Fermi energy E_f are occupied. The electron density $\rho(\mathbf{r})$ is obtained by integrating $\rho(E, \mathbf{r})$ up to the Fermi energy:

$$\rho(\mathbf{r}) = \sum_{E_j < E_f} |\psi_j(\mathbf{r})|^2. \quad (37)$$

For systems with running plane wave eigenstates, the square of the wave function is the inverse of the system size, yielding a density equal to the integral of the density of states $n(E)$ up to the Fermi energy. Therefore, the density per spin component is $\frac{1}{\pi\hbar} \sqrt{2mE_f} = k_f/\pi$ for 1D, $\frac{mE_f}{2\pi\hbar^2} = k_f^2/4\pi$ for 2D, and $\frac{(2mE_f)^{3/2}}{6\pi^2\hbar^3} = k_f^3/6\pi^2$ for 3D, where $k_f = \sqrt{2mE_f}/\hbar$ is the Fermi wave number.

We now derive an expression for the density distribution in the 1D free electron gas under the box boundary condition. Using the formula (37), and turning the summation over k into an integral in the large size limit, we obtain

$$\rho(x) = \frac{2}{\pi} \int_0^{k_f} dk \sin^2 kx = \frac{k_f}{\pi} \left[1 - \frac{\sin 2k_f x}{2k_f x} \right]. \quad (38)$$

We see that there is a density depletion near the boundary $x = 0$, and that this depletion is healed in a few Fermi wavelength $\lambda_f = 2\pi/k_f$ away from the boundary. The oscillation in the healing process is called the Friedel oscillation, which also occurs near a scatterer and in higher dimensions. The oscillation is due to the sharp Fermi surface. At finite temperatures, the oscillation is accompanied with an exponential factor, whose exponent is the imaginary part of $2\sqrt{k_f^2 + ik_T^2}$, where the Fermi wave number k_f is now defined in terms of the chemical potential, $k_T = \sqrt{2\pi mk_B T}/\hbar$ is the thermal wave number.[9]

C. Density matrix

In this and the next subsection, we consider quantities also depending on the phase information of the wave functions. The quantity which is useful in equilibrium statistical physics is the density matrix, defined by

$$\hat{\rho} = \sum_j \frac{|\psi_j\rangle \langle \psi_j|}{e^{(\epsilon_j - \mu)/k_B T} \pm 1}. \quad (39)$$

The thermal average of any operator \hat{O} is simply the trace of $\hat{O}\hat{\rho}$. In the position representation, the density matrix becomes a function of two position variables

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_j \frac{\psi_j(\mathbf{r})\psi_j^*(\mathbf{r}')}{e^{(\epsilon_j - \mu)/k_B T} \pm 1}. \quad (40)$$

The diagonal part of the density matrix $\rho(\mathbf{r}, \mathbf{r})$ gives the spatial particle density distribution.

The density matrix for the 1D free electron gas is given by

$$\rho(x, x') = \int_{-\infty}^{+\infty} dk \frac{e^{ik(x-x')}}{2\pi e^{(\frac{\hbar^2 k^2}{2m} - \mu)/k_B T} + 1}, \quad (41)$$

which is just a Fourier transform of the Fermi distribution function. At zero temperature, we have the result

$$\rho(x, x') = \frac{\sin k_f(x - x')}{\pi(x - x')}. \quad (42)$$

The oscillatory fall off with the distance $(x - x')$ is again due to the sharp Fermi surface. At finite temperatures, the density matrix falls off exponentially at large distances as the imaginary part of $\frac{4m}{\hbar^2 \sqrt{k_f^2 + ik_T^2}} \exp[i\sqrt{k_f^2 + ik_T^2}|x - x'|]$, which can be obtained from a complex pole analysis of the Fermi distribution function. If the Fermi energy lies in an energy gap, e.g., a gap between Bloch bands in a periodic potential, the density matrix also falls off exponentially with the off-diagonal distance.

The vanishing of the density matrix at large off-diagonal distances is a general property of Fermions, with or without many-body interactions. On the other hand, a boson gas can develop a long range off-diagonal order below the temperature of Bose-Einstein condensation, in the sense that

$$\rho(\mathbf{r}, \mathbf{r}') \rightarrow \rho_0 \alpha, \quad \text{as } |\mathbf{r} - \mathbf{r}'| \rightarrow \infty, \quad (43)$$

where α is the fraction of particles in the ground state. This is the bench mark of superfluidity. For Fermions, long range off-diagonal order can only develop in the two (or higher order) particle density matrix, which is the case for superconductors.[10]

It is also interesting to consider the Boltzmann density matrix,

$$\rho_B(\mathbf{r}, \mathbf{r}') = \sum_j \psi_j(\mathbf{r}) \psi_j^*(\mathbf{r}') e^{-\beta(\epsilon_j - \mu)}, \quad (44)$$

where $\beta = 1/k_B T$. For systems with time-reversal symmetry, the density matrix $\rho(\mathbf{r}, \mathbf{r}')$ is positive for all positions. There is a path-integral representation of the Boltzmann density matrix [11]

$$\rho_B(\mathbf{r}, \mathbf{r}') = \int \mathcal{D}\mathbf{r}(u) \exp\left\{-\int_0^\beta \frac{du}{\hbar} \left(\frac{m}{2} \dot{\mathbf{r}}^2(u) + V(\mathbf{r}(u))\right)\right\}, \quad (45)$$

where u is the imaginary ‘time’ and $\mathcal{D}\mathbf{r}(u)$ denotes integration over all paths starting at \mathbf{r} when $u = 0$ and ending at \mathbf{r}' when $u = \beta$. Since the measure of the path integration is positive, the above expression shows evidently that the Boltzmann density matrix is positive. In the presence of a magnetic field, an imaginary term, $i\dot{\mathbf{r}}(u) \cdot \mathbf{A}(\mathbf{r}(u))$, should be added to the potential energy in the action, making the density matrix complex in general.

D. Green functions

Green functions were introduced in the theory of inhomogeneous linear equations. It has important applications in electromagnetism, where one can use it to find the field of a distribution of charges or currents. Green functions are also heavily used in perturbation theory in quantum mechanics, by regarding the perturbing term in the Hamiltonian as an inhomogeneous term.[12]

In operator form, the Green function is defined as:

$$\hat{G}(\lambda) = \frac{1}{\lambda - \hat{H}}, \quad (46)$$

where λ is a complex energy parameter. This may be resolved in terms of the eigenstates of the Hamiltonian as

$$\hat{G}(\lambda) = \sum_j \frac{|\psi_j\rangle\langle\psi_j|}{\lambda - E_j}. \quad (47)$$

If we integrate the above expression divided by $2\pi i$ over a contour in the complex λ plane, we obtain the projection operator onto those states whose eigenvalues lie within the contour. In the coordinate representation,

$$G(\mathbf{r}, \mathbf{r}', \lambda) = \sum_j \frac{\psi_j(\mathbf{r})\psi_j^*(\mathbf{r}')}{\lambda - E_j}. \quad (48)$$

Therefore, the density matrix for an electron gas at zero temperature can also be written as

$$\int_C \frac{d\lambda}{2\pi i} G(\mathbf{r}, \mathbf{r}', \lambda), \quad (49)$$

where C is the contour surrounding the spectrum below the Fermi energy. The Green function is also related to the local density of states by

$$\rho(\mathbf{r}, E) = \frac{1}{\pi} \text{Im} G(\mathbf{r}, \mathbf{r}, E - i\eta), \quad (50)$$

where η is a positive infinitesimal.

For free electrons, the Green function is simply the spatial Fourier transform of $1/(\lambda - \frac{\hbar^2 k^2}{2m})$, and yields

$$G = -i \frac{m}{q\hbar^2} e^{iq|x-x'|} \quad (51)$$

in one dimension, where $q = \sqrt{\frac{2m\lambda}{\hbar^2}}$ and the square root is taken in the branch of $0 < \arg(\lambda) < 2\pi$. In three dimensions, we have

$$G = -\frac{m}{2\pi\hbar^2|\mathbf{r} - \mathbf{r}'|} e^{iq|\mathbf{r} - \mathbf{r}'|}. \quad (52)$$

The 2D Green function can be expressed in terms of the Hankel function, and has the long distance behavior of

$$\frac{2m}{\hbar^2} \sqrt{\frac{2}{\pi q|\mathbf{r} - \mathbf{r}'|}} e^{iq|\mathbf{r} - \mathbf{r}'| - i\pi/4} \quad (53)$$

and the short distance behavior of

$$\frac{m}{\pi\hbar^2} \ln(q|\mathbf{r} - \mathbf{r}'|). \quad (54)$$

We now discuss off-diagonal locality property of the Green functions. There is a general theorem stating that G decays exponentially at large off-diagonal distances $|\mathbf{r} - \mathbf{r}'|$, whenever λ is away from the spectrum of H . [13] This is clearly demonstrated by the above examples of free electron Green

functions, where the rate of decay is $\text{Im } q$ per unit length, which is everywhere nonzero except when λ touches the positive real axis.

A general demonstration (not a proof) of the theorem can also be done for a one dimensional system in an arbitrary potential, where the Green function can be written as

$$G(x, x', \lambda) = \frac{1}{W(\lambda)} \{ \theta(x - x') \psi_r(x) \psi_\ell(x') + \theta(x' - x) \psi_r(x') \psi_\ell(x) \}. \quad (55)$$

In the above expression, $\theta(x) = 1$ for $x > 0$, and is zero otherwise; $\psi_r(x)$ is a solution of $(\lambda - H)\psi = 0$ satisfying the boundary condition on the right, and $\psi_\ell(x)$ on the left; $W(\lambda)$ is $\hbar^2/2m$ times the Wronskian of the two solutions $\psi_r'(x)\psi_\ell(x) - \psi_r(x)\psi_\ell'(x)$, which is independent of x . If λ is not in the energy spectrum, we generally expect that $\psi_r(x)$ grows exponentially to the left while $\psi_\ell(x)$ grows exponentially to the right.[14] This implies that G decays exponentially as x goes away from x' on either side.

The off-diagonal locality no longer holds in general if λ approaches the spectrum. For example, for the 1D free particle, the Green function behaves as $\sim e^{\pm ik|x-x'|}$ if $\lambda = \frac{\hbar^2 k^2}{2m} \pm i\eta$. However, when λ lies in a spectral range of exponentially localized states, the Green function can still be local.

E. Locality of physical properties

In 1978, Kohn and Yaniv considered the

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- [1] We use the MKS unit system, in which the speed of light does not enter here.
 - [2] See Courant and Hilbert, *Methods of Mathematical Physics*, Vol. 1
 - [3] We assume that the classically allowed regions are not pathologically irregular, e.g. consisting of many small pieces separated far from each other.
 - [4] The pre-exponential factor of the WKB formula is unity if the potential has finite slopes at the boundaries separating the classically allowed regions and the disallowed region. If the potential is discontinuous, the prefactor is more complicated as is shown by the results of the square barrier problem.
 - [5] In fact, in the WKB approximation, $\phi_r = \pi/2$ and $\phi = \int k(x)dx$. The resonance condition is the same as the WKB quantization formula.
 - [6] Single-valuedness of the wave function does not follow from single-valuedness of physical quantities such as the probability density and the current density. The wave function can still change a nontrivial phase around a mathematical line. However, such a line introduces a strong inhomogeneity to the physical space; there must be some physical entity going through the line, whose strength is finite but whose thickness is unmeasurably thin. Therefore, the wave function must be single valued if we assume that such a singular entity does not exist in our system.
 - [7] See the section on the Wigner-von Neumann theorem in Chapter 2
 - [8] See M. V. Berry, *Annals of Physics* **131**, 163–216 (1981).
 - [9] See the discussions on density matrices below
 - [10] C. N. Yang, *Rev. Mod. Phys.*, 34, 694-704 (1962).
 - [11] See R. P. Feynman, *Statistical Mechanics*, (W.A. Benjamin, Inc., London, 1972), Chapter 3, pp72-78.
 - [12] See Economou, *Green's Functions in Quantum Physics*.
 - [13] B. Simon Schrödinger Semigroup, *Bull. Am. Math. Soc. New Ser.* 7, 447-526 (1982)
 - [14] In a 1D periodic potential, the spectrum consists of Bloch bands. For any λ there are two wave functions of the form $e^{\pm ikx} u_\pm(x)$, where $u_\pm(x+a) = u_\pm(x)$. If λ is in a band, k is real; if λ is outside the bands, k is complex. Therefore one of the wave functions falls off exponentially to the left and the other falls off to the right.