

Chapter 31

Quantum mechanics the short short version

WE START WITH A REVIEW of standard quantum mechanical concepts prerequisite to the derivation of the semiclassical trace formula.

In coordinate representation, the time evolution of a quantum mechanical wave function is governed by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(q, t) = \hat{H} \left(q, \frac{\hbar}{i} \frac{\partial}{\partial q} \right) \psi(q, t), \quad (31.1)$$

where the Hamilton operator $\hat{H}(q, -i\hbar\partial_q)$ is obtained from the classical Hamiltonian by substituting $p \rightarrow -i\hbar\partial_q$. Most of the Hamiltonians we shall consider here are of the separable form

$$H(q, p) = T(p) + V(q), \quad T(p) = p^2/2m, \quad (31.2)$$

describing dynamics of a particle in a D -dimensional potential $V(q)$. For time-independent Hamiltonians we are interested in finding stationary solutions of the Schrödinger equation of the form

$$\psi_n(q, t) = e^{-iE_n t/\hbar} \phi_n(q), \quad (31.3)$$

where E_n are the eigenenergies of the time-independent Schrödinger equation

$$\hat{H}\phi(q) = E\phi(q). \quad (31.4)$$

For bound systems, the spectrum is discrete and the eigenfunctions form an orthonormal,

$$\int dq \phi_n(q) \phi_m^*(q) = \delta_{nm}, \quad (31.5)$$

and complete,

$$\sum_n \phi_n(q) \phi_n^*(q') = \delta(q - q'), \quad (31.6)$$

set of functions in a Hilbert space. Here and throughout the text,

$$\int dq = \int dq_1 dq_2 \dots dq_D. \quad (31.7)$$

For simplicity, we will assume that the system is bound, although most of the results will be applicable to open systems, where one has complex resonances instead of real energies, and the spectrum has continuous components. chapter 35

A given wave function can be expanded in the energy eigenbasis

$$\psi(q, t) = \sum_n c_n e^{-iE_n t/\hbar} \phi_n(q), \quad (31.8)$$

where the expansion coefficient c_n is given by the projection of the initial wave function $\psi(q, 0)$ onto the n th eigenstate

$$c_n = \int dq \phi_n^*(q) \psi(q, 0). \quad (31.9)$$

By substituting (31.9) into (31.8), we can cast the evolution of a wave function into a multiplicative form

$$\psi(q, t) = \int dq' K(q, q', t) \psi(q', 0),$$

with the kernel

$$K(q, q', t) = \sum_n \phi_n(q) e^{-iE_n t/\hbar} \phi_n^*(q') \quad (31.10)$$

called the *quantum evolution operator*, or the *propagator*. Applied twice, first for time t_1 and then for time t_2 , it propagates the initial wave function from q' to q'' , and then from q'' to q

$$K(q, q', t_1 + t_2) = \int dq'' K(q, q'', t_2) K(q'', q', t_1) \quad (31.11)$$

forward in time (hence the name ‘propagator’). In non-relativistic quantum mechanics, the range of q'' is infinite, so that the wave can propagate at any speed; in relativistic quantum mechanics, this is rectified by restricting the propagation to the forward light cone.

Because the propagator is a linear combination of the eigenfunctions of the Schrödinger equation, it too satisfies this equation

$$i\hbar \frac{\partial}{\partial t} K(q, q', t) = \hat{H} \left(q, \frac{i}{\hbar} \frac{\partial}{\partial q} \right) K(q, q', t), \quad (31.12)$$

and is thus a wave function defined for $t \geq 0$; from the completeness relation (31.6), we obtain the boundary condition at $t = 0$:

$$\lim_{t \rightarrow 0^+} K(q, q', t) = \delta(q - q'). \quad (31.13)$$

The propagator thus represents the time-evolution of a wave packet starting out as a configuration space delta-function localized at the point q' at initial time $t = 0$.

For time-independent Hamiltonians, the time dependence of the wave functions is known as soon as the eigenenergies E_n and eigenfunctions ϕ_n have been determined. With time dependence taken care of, it makes sense to focus on the *Green's function*, which is the Laplace transform of the propagator

$$G(q, q', E + i\epsilon) = \frac{1}{i\hbar} \int_0^\infty dt e^{i(Et - \frac{i}{\hbar}t)} K(q, q', t) = \sum_n \frac{\phi_n(q)\phi_n^*(q')}{E - E_n + i\epsilon}. \quad (31.14)$$

Here, ϵ is a small positive number, ensuring the existence of the integral. The eigenenergies show up as poles in the Green's function with residues corresponding to the wave function amplitudes. If one is only interested in spectra, one may restrict oneself to the (formal) trace of the Green's function,

$$\text{tr} G(q, q', E) = \int dq G(q, q, E) = \sum_n \frac{1}{E - E_n}, \quad (31.15)$$

where E is complex, with a positive imaginary part, and we have used the eigenfunction orthonormality (31.5). This trace is formal, because the sum in (31.15) is often divergent. We shall return to this point in sects. 34.1.1 and 34.1.2.

A useful characterization of the set of eigenvalues is given in terms of the *density of states*, with a delta function peak at each eigenenergy, figure 31.1 (a),

$$d(E) = \sum_n \delta(E - E_n). \quad (31.16)$$

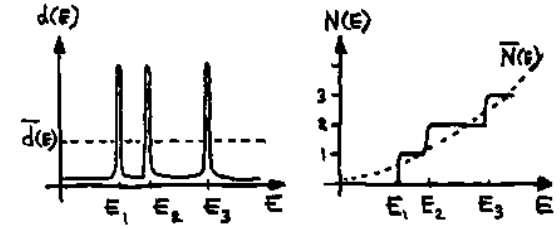


Figure 31.1: Schematic picture of a) the density of states $d(E)$, and b) the spectral staircase function $N(E)$. The dashed lines denote the mean density of states $\bar{d}(E)$ and the average number of states $\bar{N}(E)$ discussed in more detail in sect. 34.1.1.

Using the identity

$$\delta(E - E_n) = - \lim_{\epsilon \rightarrow +0} \frac{1}{\pi} \text{Im} \frac{1}{E - E_n + i\epsilon} \quad (31.17)$$

we can express the density of states in terms of the trace of the Green's function. That is,

$$d(E) = \sum_n \delta(E - E_n) = - \lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \text{Im} \text{tr} G(q, q', E + i\epsilon). \quad (31.18)$$

exercise 31.1

section 34.1.1

As we shall see (after ‘‘some’’ work), a semiclassical formula for the right-hand-side of this relation yields the quantum spectrum in terms of periodic orbits.

The density of states can be written as the derivative $d(E) = dN(E)/dE$ of the *spectral staircase* function

$$N(E) = \sum_n \Theta(E - E_n) \quad (31.19)$$

which counts the number of eigenenergies below E , figure 31.1 (b). Here Θ is the Heaviside function

$$\Theta(x) = 1 \quad \text{if } x > 0; \quad \Theta(x) = 0 \quad \text{if } x < 0. \quad (31.20)$$

The spectral staircase is a useful quantity in many contexts, both experimental and theoretical. This completes our lightning review of quantum mechanics.

Exercises

- 31.1. **Dirac delta function, Lorentzian representation.**
Derive the representation (31.17)

$$\delta(E - E_n) = - \lim_{\epsilon \rightarrow +0} \frac{1}{\pi} \text{Im} \frac{1}{E - E_n + i\epsilon}$$

of a delta function as imaginary part of $1/x$.

(Hint: read up on principal parts, positive and negative frequency part of the delta function, the Cauchy theorem in a good quantum mechanics textbook).

- 31.2. **Green's function.** Verify Green's function Laplace transform (31.14),

$$\begin{aligned} G(q, q', E + i\epsilon) &= \frac{1}{i\hbar} \int_0^{\infty} dt e^{\frac{i}{\hbar}Et - \frac{\epsilon}{\hbar}t} K(q, q', t) \\ &= \sum \frac{\phi_n(q)\phi_n^*(q')}{E - E_n + i\epsilon} \end{aligned}$$

argue that positive ϵ is needed (hint: read a good quantum mechanics textbook).