Chapter 23

Quantum mechanics, briefly

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

$$i\hbar\frac{\partial}{\partial t}\psi(q,t) = \hat{H}(q,\frac{\hbar}{i}\frac{\partial}{\partial q})\psi(q,t), \tag{23.1}$$

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

$$H(q,p) = T(p) + V(q)\,, \qquad T(p) = p^2/2m\,, \tag{23.2}$$

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

$$\psi_n(q,t) = e^{-iE_n t/\hbar}\phi_n(q), \tag{23.3}$$

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

$$\hat{H}\phi(q) = E\phi(q)\,. \tag{23.4}$$

If the kinetic term can be separated out as in (23.2), the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\partial^2\phi(q) + V(q)\phi(q) = E\phi(q) \tag{23.5}$$

can be rewritten in terms of a local wavenumber

$$(\partial^2 + k^2(q))\phi = 0\,, \qquad \hbar^2 k(q) = \sqrt{2m(E - V(q))}\,. \tag{23.6}$$

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

$$\int d^dq\,\phi_n(q)\phi_m^*(q) = \delta_{nm} \tag{23.7}$$

and complete

$$\sum_n \phi_n(q)\phi_n^*(q') = \delta(q - q')\,. \tag{23.8}$$

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set of functions in a Hilbert space. 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.

A given wave function can be expanded in the energy eigenbasis

$$\psi(q,t) = \sum_n c_n e^{-iE_n t/\hbar}\phi_n(q)\,, \tag{23.9}$$

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

$$c_n = \int d^dq\,\phi_n^*(q)\psi(q,0). \tag{23.10}$$

By substituting (23.10) into (23.9), we can cast the evolution of a wave function into a multiplicative form

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

with the kernel

$$K(q,q',t) = \sum_n \phi_n(q)\, e^{-iE_n t/\hbar}\phi_n^*(q') \tag{23.11}$$

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

$$K(q,q',t_1+t_2) = \int dq''\, K(q,q'',t_2)K(q'',q',t_1) \tag{23.12}$$

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

Since the propagator is a linear combination of the eigenfunctions of the Schrödinger equation, it also satisfies the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}K(q,q',t) = \hat{H}(q,\frac{i}{\hbar}\frac{\partial}{\partial q})K(q,q',t)\,, \tag{23.13}$$

and is thus a wave function defined for $t \geq 0$; from the completeness relation (23.8) we obtain the boundary condition at $t=0$:

$$\lim_{t\to 0_+} K(q,q',t) = \delta(q-q')\,. \tag{23.14}$$

The propagator thus represents the time evolution of a wave packet which starts out as a configuration space delta-function localized in the point q' at the 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 rendered "trivial", it makes sense to focus on the *Green's function*, the Laplace transformation of the propagator

$$G(q,q',E+i\epsilon) = \frac{1}{i\hbar}\int_0^\infty dt\, e^{\frac{i}{\hbar}Et-\frac{\epsilon}{\hbar}t}K(q,q',t) = \sum_n \frac{\phi_n(q)\phi_n^*(q')}{E-E_n+i\epsilon}\,. \tag{23.15}$$

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 the spectrum, one may restrict the considerations to the (formal) trace of the Green's function,

$$\mathrm{tr}\, G(q,q',E) = \int d^dq\, G(q,q,E) = \sum_n \frac{1}{E-E_n}\,, \tag{23.16}$$

where E is complex, with a positive imaginary part, and we have used the eigenfunction orthonormality (23.7). This trace is formal, since as it stands, the sum in (23.16) is often divergent. We shall return to this point in sects. 27.1.1 and 27.1.2.

A 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, fig. 23.1(a),

$$d(E) = \sum_n \delta(E-E_n). \tag{23.17}$$

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Using the identity

$$\delta(E-E_n) = -\lim_{\epsilon\to+0}\frac{1}{\pi}\mathrm{Im}\,\frac{1}{E-E_n+i\epsilon} \tag{23.18}$$

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

$$d(E) = \sum_n \delta(E-E_n) = -\lim_{\epsilon\to 0}\frac{1}{\pi}\mathrm{Im}\,\mathrm{tr}\, G(q,q',E+i\epsilon). \tag{23.19}$$

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This relation is the reason why we chose to describe the quantum spectrum in terms of the density of states. As we shall see, a semiclassical formula for right hand side of this relation will yield the quantum spectrum in terms of periodic orbits.

The density of states can be written as the derivative $d(E) = \mathrm{d}N(E)/\mathrm{d}E$ of another useful quantity, the *spectral staircase* function

$$N(E) = \sum_n \Theta(E-E_n) \tag{23.20}$$

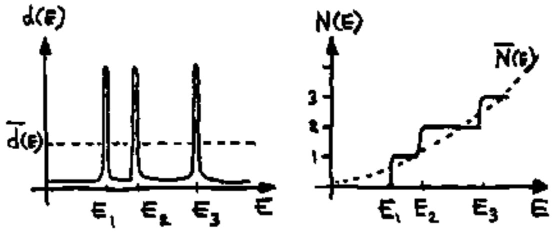

Figure 23.1: Schematic picture of **a)** the density of states $d(E)$, and **b)** the spectral staircase function $N(E)$. The dashed lines denote the mean density of states $\bar{d}(E)$ and the average number of states $\bar{N}(E)$ discussed in more detail in sect. 17.1.

which counts the number of eigenenergies below E, fig. 23.1(b). Here Θ is the Heaviside function

$$\Theta(x) = 1 \quad \text{if } x > 0; \quad \Theta(x) = 0 \quad \text{if } x < 0\,. \tag{23.21}$$

This completes our lightning review of quantum mechanics.