Some aspects of the quantum-classical correspondence

Trends in Quantum Physics: Past, Present and Future
Workshop at NIT Calicut, Kozhikode 18-20 Sep, 2025

Govind S. Krishnaswami, Chennai Mathematical Institute
Email: govind@cmi.ac.in, updated: October 20, 2025

Contents

1 Abstract

We relate the formulation of classical mechanics in the Hamilton-Poisson and Hamilton-Jacobi approaches to that of quantum mechanics in the Heisenberg and Schrodinger approaches. The quantum-classical correspondence is illustrated using Ehrenfest's theorem, Bohr-Sommerfeld quantization conditions, the WKB approximation and semiclassical expansion. Finally, we use an example to motivate a trace formula connecting the quantum energy spectrum to a sum over classical periodic orbits.

2 From Hamiltonian mechanics to Heisenberg and Schrödinger's QM

Quantum mechanics was developed in the first half of the 20^{th} century to understand the properties of (especially microscopic) systems like atoms, molecules, light from stars, radiation from black bodies, behavior of solids at low temperatures, etc. Electrons, light, atoms, etc., displayed both wave-like and particle-like behavior depending on how they were observed. Quantum mechanics involves a new parameter, Planck's constant h, whose value is 6.6×10^{-34} Joule $\cdot$ sec. The smallness of h relative to quantities with the same dimensions encountered in many macroscopic phenomena explains why quantum effects are often suppressed. Quantization is a theoretical framework to pass from a classical description of a system to a quantum description. Quantization does not necessarily imply discrete physical quantities, although the discrete line spectra of light from hot gases and stars and the packet-like behavior of light photons gave the subject the name 'quantum' theory.

2.1 From PBs to Commutators and Hamilton to Heisenberg equations

• In classical mechanics we describe the dynamics of a system in terms of 'phase space' variables like the position and momentum of a particle. Classical dynamical variables or observables like position, momentum, angular momentum and energy are functions of the (generalized) positions and momenta, which furnish coordinates on the state space (phase space).

• Poisson brackets plays a key role in the formulation of classical Hamiltonian mechanics and in the passage to the quantum theory. For instance, they help in writing the equations of motion and in identifying conserved quantities. Recall the Poisson bracket between two classical observables that depend on the generalized positions and momenta, $f(x,p)$ and $g(x,p)$:

$$\{f, g\} = \sum\nolimits_{i=1}^{n} \left(\frac{\partial f}{\partial x^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x^i} \right). \tag{1}$$

• The classical phase space variables, position and momentum satisfy canonical[1] Poisson brackets. For 1 degree of freedom, they are

$$\{x, p\} = 1, \quad \{x, x\} = 0, \quad \{p, p\} = 0. \tag{2}$$

x and p are said to be canonically conjugate observables. For a particle in 3d space, we have $\{x^i, p_j\} = \delta^i_j$.

• The process of quantization involves replacing classical observables like position, momentum, angular momentum and the Hamiltonian with corresponding hermitian (more precisely self-adjoint) operators on the quantum Hilbert space. Let us call the quantum position and momentum operators $\hat{x}$ and $\hat{p}$.

• In the process of quantization, the Poisson bracket of classical Hamiltonian mechanics is replaced with (a multiple of) the commutator of operators. Multiplication of matrices/operators is in general not commutative $AB \neq BA$ (in general). The amount by which they fail to commute is called the commutator $[A, B] = AB - BA$. Any operator commutes with itself or any power of itself $[A, A^n] = A^{n+1} - A^{n+1} = 0$.

---

[1] The word canonical refers to something that is standard. Here the Cartesian position and momenta are the standard coordinates on phase space. The word canon comes from a Greek word for a rod/reed used for measuring lengths. Its use in mechanics dates back to the work of Jacobi and Gauss.

• We will postulate the quantization rule

$$\{A, B\} = C \quad \longrightarrow \quad \frac{1}{i\hbar}[\hat{A}, \hat{B}] = \hat{C}, \tag{3}$$

where $\hat{A}, \hat{B}, \hat{C}$ are the hermitian operators associated to the classical observables A, B, C.

• In particular, upon quantization, the canonical PB relations $\{x^i, p_j\} = \delta^i_j$ are replaced with Heisenberg's canonical commutation relations $[\hat{x}^i, \hat{p}_j] = i\hbar\delta^i_j$.

• Let us explain the factor $i\hbar$. Now, due to the differentiation with respect to x and p, $\{A, B\}$ has dimensions of the product of A and B divided by action (or angular momentum). On the other hand, the commutator $[\hat{A}, \hat{B}]$ has dimensions of the product of A and B. So we will need to divide the commutator by a quantity with dimensions of angular momentum in passing to the quantum theory. Up to a factor of i, this quantity is the 'reduced' Planck's constant $\hbar$. Furthermore, we check that the commutator of hermitian operators A and B is antihermitian:

$$([A, B])^\dagger = (AB - BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = BA - AB = -[A, B]. \tag{4}$$

Thus, to get a hermitian operator, we divide by i.

• An important property of the commutator is the product or Leibniz rule, check that

$$[A, BC] = [A, B]C + B[A, C]. \tag{5}$$

• Recall that Hamilton's canonical equations of motion for positions and momenta: $\dot{x}^j = \frac{\partial H}{\partial p_j}$ and $\dot{p}_j = -\frac{\partial H}{\partial x^j}$ may be written in terms of Poisson brackets

$$\dot{x}^j = \{x^j, H\} \quad \text{and} \quad \dot{p}_j = \{p_j, H\}. \tag{6}$$

In fact, we may use these to deduce that the equation of motion for any observable $f = f(x, p)$ may be expressed in terms of PBs:

$$\begin{aligned} \frac{df}{dt} &= \sum\nolimits_{i=1}^{n} \left(\frac{\partial f}{\partial x^i(t)} \frac{dx^i}{dt} + \frac{\partial f}{\partial p_i(t)} \frac{dp_i}{dt} \right) \\ &= \sum\nolimits_{i=1}^{n} \left(\frac{\partial f}{\partial x^i(t)} \frac{\partial H}{\partial p_i(t)} - \frac{\partial f}{\partial p_i(t)} \frac{\partial H}{\partial x^i(t)} \right) = \{f, H\}. \end{aligned} \tag{7}$$

• The quantum version of Hamilton's equations are got by replacing classical observables by quantum operators and the PB by the commutator divided by $i\hbar$:

$$\frac{d\hat{f}}{dt} = \frac{1}{i\hbar}[\hat{f}, \hat{H}]. \tag{8}$$

This is the Heisenberg equation of motion for the observable $\hat{f}$. We say that the Hamiltonian $\hat{H}$ generates infinitesimal time evolution via the commutator.

2.2 Schrodinger representation and Schrodinger equation

- Schrödinger proposed an alternative approach to quantum mechanical evolution by focusing on states rather than observables.

Schrodinger representation. To quantize x and p we seek hermitian operators $\hat{x}$ and $\hat{p}$ on the quantum state space that satisfy the Heisenberg commutator relation $[\hat{x},\hat{p}] = i\hbar I$. Schrödinger found a solution to this problem. Working in the position basis, our states are wave functions of position $\psi(x)$. We will represent $\hat{x}$ by multiplication by x and $\hat{p}$ by $-i\hbar\frac{\partial}{\partial x}$. In other words:

$$(\hat{x}\psi)(x) = x\psi(x) \quad \text{and} \quad (\hat{p}\psi)(x) = -i\hbar\frac{\partial\psi}{\partial x}. \tag{9}$$

- Let us check that $\hat{x}\hat{p} - \hat{p}\hat{x} = [\hat{x},\hat{p}] = i\hbar I$ by acting on a state $\psi(x)$. We will mostly omit the hats on quantum operators henceforth:

$$xp\psi = -i\hbar x\psi'(x), \quad \text{while} \quad px\psi = -i\hbar\frac{\partial}{\partial x}(x\psi) = -i\hbar x\psi'(x) - i\hbar\psi(x) \quad \Rightarrow \quad [x,p]\psi = i\hbar\psi. \tag{10}$$

- In three dimensions, we have three coordinate and momentum operators x, y, z and $p_x = -i\hbar\frac{\partial}{\partial x}, p_y = -i\hbar\frac{\partial}{\partial y}, p_z = -i\hbar\frac{\partial}{\partial z}$. It is easily seen that the momenta commute with each other and the coordinates commute among themselves, more over $[x, p_x] = i\hbar$ while $[x, p_y] = 0$, etc. Thus, the Schrodinger representation gives us a way of representing positions and momenta in the quantum theory as operators satisfying Heisenberg's canonical commutation relations: $[x_i, p_j] = i\hbar\,\delta_{ij}$.
- It may be shown that $\hat{x}$ and $\hat{p}$ are hermitian.

Time evolution: Schrödinger's equation. When left to itself, the state of the system evolves according to the Schrödinger equation (SE) $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$. H is the hermitian hamiltonian. Given the initial state $|\psi(0)\rangle$, the SE determines the state at subsequent times, just as Hamilton's equations $\dot{x} = \frac{\partial H}{\partial p}, \dot{p} = -\frac{\partial H}{\partial x}$ do in classical mechanics.
- In the position basis, the SE is

$$i\hbar\frac{\partial}{\partial t}\langle x|\psi(t)\rangle = \langle x|H\psi(t)\rangle \quad \text{or} \quad i\hbar\frac{\partial\psi(x,t)}{\partial t} = (H\psi)(x,t) \tag{11}$$

For a particle in a potential $(H\psi)(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t)$, and we get

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x). \tag{12}$$

The SE is a linear PDE, first order in time and second order in space derivatives of the unknown ψ. Contrast this with Newton's or Hamilton's equations which in general are a system of nonlinear ODEs for the classical state.

Time evolution operator. The Schrödinger equation $i\hbar\partial_t\psi = H\psi$ tells us how a state evolves infinitesimally in time. This time evolution can be shown to be unitary: it preserves the inner product between any pair of states $\langle\phi(t)|\psi(t)\rangle = \langle\phi(0)|\psi(0)\rangle$ and in particular the squared norm of a state. For a Hamiltonian that is not explicitly time dependent, the state at time t may be expressed in terms of the state at $t = 0$ in a simple way via a matrix eponential:

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle. \tag{13}$$

The operator $U(t) = e^{-iHt/\hbar}$ is unitary $U^\dagger U = UU^\dagger = I$ and is called the time-evolution operator.

2.3 Hamilton-Jacobi equation as a semiclassical limit of Schrödinger's equation

The Schrödinger equation for time evolution of the quantum wave function of a nonrelativistic particle of mass m in a potential V is

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\Psi + V\Psi. \tag{14}$$

For a free particle ($V = 0$), the stationary state wave function corresponding to energy E and momentum $\boldsymbol{p}$ is $\Psi(\boldsymbol{r},t) \propto e^{i(\boldsymbol{p}\cdot\boldsymbol{r}-Et)/\hbar}$. For fixed E and $\boldsymbol{p}$, we see that Ψ has an essential singularity at $\hbar = 0$. Thus, the wave function itself does not have a good (classical) limit as $\hbar \to 0$. On the other hand, the quantity S defined by $\Psi = e^{iS/\hbar}$ is better placed to have a finite $\hbar \to 0$ limit. In fact, we have

$$\partial_t\Psi = \frac{i\Psi}{\hbar}\partial_t S, \quad \boldsymbol{\nabla}\Psi = \frac{i}{\hbar}\Psi\boldsymbol{\nabla}S \quad \text{and} \quad \boldsymbol{\nabla}^2\Psi = \left[-\frac{1}{\hbar^2}|\boldsymbol{\nabla}S|^2 + \frac{i}{\hbar}\boldsymbol{\nabla}^2 S\right]\Psi, \tag{15}$$

so the Schrödinger equation becomes, upon cancelling $e^{iS/\hbar} \neq 0$,

$$-\frac{\partial S}{\partial t} = \frac{1}{2m}|\boldsymbol{\nabla}S|^2 + V - \frac{i\hbar}{2m}\boldsymbol{\nabla}^2 S. \tag{16}$$

No approximation has been made, although we assumed that Ψ is expressible[2] as $e^{iS/\hbar}$ for some S. Now, assuming S has a finite limit as $\hbar \to 0$, we ignore the last term in the limit $\hbar \to 0$ and notice that we get the Hamilton-Jacobi evolution equation of classical mechanics:

$$\frac{\partial S}{\partial t} + \frac{|\boldsymbol{\nabla}S|^2}{2m} + V = 0 \quad \text{or} \quad \frac{\partial S}{\partial t} + H(\boldsymbol{r}, \boldsymbol{\nabla}S) = 0. \tag{17}$$

Thus, we may view the Schrödinger equation as a 'quantization' of the classical HJ equation. We also say that the HJ equation arises in the semiclassical limit of the Schrödinger equation. We will say more about the HJ equation and the interpretation of S as a generator of canonical transformations in §5.2.

---

[2] S would have to diverge at points where Ψ vanishes.

2.4 Heisenberg equation from Schrödinger equation

• Here, we will show that the Schrödinger equation for states implies the Heisenberg equation for observables. This will establish the compatibility of the Heisenberg and Schrödinger approaches to quantum mechanics.
• In the Schrödinger 'picture', states $|\psi_s(t)\rangle = U(t)|\psi_s(0)\rangle$ evolve in time (via the unitary time evolution operator $U(t)$) while observables A_s like the position operator $\hat{x}$ do not depend on time. In the Heisenberg picture, the states are the initial ones $|\psi_h\rangle = |\psi_s(0)\rangle$, but the observables evolve in time. Their evolution is governed by the Heisenberg equation of motion. Let us define the Heisenberg operator $A_h(t) = U^\dagger(t) A_s U(t)$. Then

$$i\hbar \dot{U} = HU \quad \text{and} \quad -i\hbar \dot{U}^\dagger = U^\dagger H. \tag{18}$$

So

$$\begin{aligned} i\hbar\partial_t A_h &= -U^\dagger H A_s U + U^\dagger A_s H U \\ \Rightarrow i\hbar\partial_t A_h &= U^\dagger A_s U U^\dagger H U - U^\dagger H U U^\dagger A_s U = A_h H - H A_h = [A_h, H] \end{aligned} \tag{19}$$

Thus, the Heisenberg equation of motion

$$i\hbar \frac{\partial A_h}{\partial t} = [A_h, H] \tag{20}$$

follows from the Schrödinger equation for states and vice versa.
• As noted earlier, the Heisenberg equation of motion is a quantum analogue of Hamilton's equation of motion $\frac{\partial A}{\partial t} = \{A, H\}$ if we replace a classical observable A by A_h and the PB $\{\cdot,\cdot\}$ by $[\cdot,\cdot]/i\hbar$. The Hamiltonian is the same in both pictures (assuming it is time independent in the Schrödinger picture). We note that the expectation value of an observable in a normalized state may be computed in either picture

$$\langle A\rangle_\psi = \langle\psi_s(t)|A_s|\psi_s(t)\rangle = \langle\psi(0)|U^\dagger A_s U|\psi(0)\rangle = \langle\psi_h|A_h|\psi_h\rangle. \tag{21}$$

2.5 Brief comparison of classical and quantum mechanical formalisms

We will compare features of the Hamiltonian formalism of classical mechanics (CM) with the corresponding notions of quantum mechanics (QM). Like CM, QM too has concepts of states and observables as well as time evolution. A key difference is that on account of the linear superposition principle (necessitated by observations of interference and diffraction of electron and atom 'matter waves') the quantum state space is a linear vector space unlike the classical phase space which is a manifold without any linear structure.

1. In CM, the space of (pure) states is the phase space, the space of positions and momenta. It is often the cotangent bundle[3] of the configuration space $\mathcal{Q}$. In

---

[3] Velocity vectors at a point of $\mathcal{Q}$ span the tangent space to $\mathcal{Q}$ at that point. The vector space dual to the tangent space is the cotangent space and is spanned by momentum covectors. The union of all the cotangent spaces over each point of the configuration space is called the cotangent bundle.

QM, it is a vector space, the quantum mechanical Hilbert space[4] $\mathcal{H}$. Vectors in this space (up to scalar multiplication) are the possible states of the system, so linear combinations of states are also allowed states. $\mathcal{H}$ can typically be taken to be the space of square-integrable complex-valued functions on the classical configuration space: $L^2(\mathcal{Q}, \mathbb{C})$. In the so-called position representation or basis, the states of a single particle moving in $\mathcal{Q} = \mathbb{R}^3$ are complex 'wave functions' $\psi(\boldsymbol{r})$ with $|\psi(\boldsymbol{r})|^2 d\boldsymbol{r}$ interpreted as the probability to find the particle in the infinitesimal volume $d\boldsymbol{r}$ around $\boldsymbol{r}$. The squared-norm $\int |\psi|^2 d\boldsymbol{r}$ must equal one, since this is the total probability to find the particle somewhere. This is why we insist on square-integrable functions on the classical configuration space, $L^2(\mathbb{R}^3, \mathbb{C})$ in this case. It turns out that we need to allow for complex vectors to accommodate the sort of wave phenomena observed in the quantum realm, which is somewhat different from that in classical sound or electromagnetic waves. Moreover, time evolution in QM is such that even if the initial state is real, it will in general become complex at the next instant. Probabilities, being proportional to the absolute square, remain real. Evidently, we use an infinite-dimensional vector space to model the translational states of motion of a particle (the need for an infinite-dimensional space will be clarified below). On the other hand, to model the spin states of a particle, a finite-dimensional complex vector space suffices: $\mathbb{C}^2$ for spin-$\frac{1}{2}$, $\mathbb{C}^3$ for spin 1 and so forth.

2. In CM, observables $f, g, \ldots$ are smooth real-valued functions on phase space. In QM, observables $(A, B, \ldots)$ are self-adjoint (Hermitian operators whose domain coincides with that of their Hermitian adjoints) linear operators on the quantum Hilbert space. Once a basis is chosen, we may represent quantum observables as (finite or infinite) matrices. Self-adjointness is the analog of real-valuedness of classical observables, both of which ensure that results of measurements are real numbers. While each value of a classical dynamical variable f is a possible result of its measurement, the eigenvalues of A are the possible results when a quantum observable A is measured.

3. Classical observables form a commutative algebra under pointwise[5] multiplication. Thus $\alpha f + \beta g$ and $(fg)(\xi) = (gf)(\xi) = f(\xi)g(\xi)$ are observables for any $\alpha, \beta \in \mathbb{R}$ if f and g are. Linear operators on a quantum Hilbert space do not commute ($AB \neq BA$ for square matrices) in general: they form a noncommutative but associative $[(AB)C = A(BC)]$ algebra. What is more, the product of two Hermitian operators fails to be Hermitian if they do not commute. Nevertheless, it is possible to combine two observables to get a third in a different manner, as we discuss below.

4. The Poisson bracket of observables f and g in CM is another observable $\{f, g\}$.

---

[4] A Hilbert space is a complex vector space $\mathcal{H}$ with Hermitian positive-definite inner product $\langle \phi, \psi \rangle$. This means $\langle \phi, \psi \rangle = \langle \psi, \phi \rangle^*$, $\langle \psi, \psi \rangle \geq 0$ (with equality only if $\psi = 0$), linearity in ψ and consequently antilinearity in ϕ: $\langle a\phi, b\psi \rangle = a^* b \langle \phi, \psi \rangle$ and $\langle \phi_1 + \phi_2, \psi_1 + \psi_2 \rangle = \langle \phi_1, \psi_1 \rangle + \langle \phi_1, \psi_2 \rangle + \langle \phi_2, \psi_1 \rangle + \langle \phi_2, \psi_2 \rangle$ for all vectors $\psi, \phi, \ldots$ and complex numbers a, b.

[5] *Pointwise* means f and g are multiplied at the same point ξ to get the value of fg at ξ.

In QM, the role of the Poisson bracket is played by the commutator of operators (up to a factor of $i\hbar$). The commutator is defined as $[A, B] = AB - BA$ and one checks that $\frac{1}{i\hbar}[A, B]$ is Hermitian if A and B are. For e.g., the role of the canonical PB relation $\{x, p\} = 1$ for a particle in CM is played by the Heisenberg canonical commutation relation $\frac{1}{i\hbar}[\hat{x}, \hat{p}] = I$ where $\hat{x}$ and $\hat{p}$ are the position and momentum operators and I the identity operator. From this, we may deduce why we need an infinite-dimensional vector space to model the quantum states of a particle. For finite-dimensional ($n \times n$) matrices, the trace of the commutator $\operatorname{tr}[A, B]$ vanishes since $\operatorname{tr} AB = \operatorname{tr} BA = \sum_{1 \leq i,j \leq n} A_{ij} B_{ji}$. On the other hand, $\operatorname{tr} I = n$. So if $[\hat{x}, \hat{p}] = i\hbar I$ must hold, $\hat{x}$ and $\hat{p}$ cannot be finite-dimensional matrices. On the other hand, the trace of the commutator of a pair or infinite matrices can diverge, just like the trace of an infinite-dimensional identity matrix.

5. Classical time evolution of any observable f is governed by Hamilton's equation $\dot{f} = \{f, H\}$. In the quantum theory, an observable A evolves according to the Heisenberg equation of motion $i\hbar \partial_t \hat{A} = [\hat{A}, \hat{H}]$. Henceforth, we will often omit the hats on quantum observables.

6. A unitary transformation is a linear transformation U satisfying $U^\dagger U = U U^\dagger = I$. Unitary transformations, which act on states and observables via $|\psi\rangle \to |\psi'\rangle = U|\psi\rangle$ and $A \to A' = U A U^\dagger$, are quantum analogs of canonical transformations. Both preserve the structure of the formalism and the equations of motion. CTs preserve the basic PB relations while unitary transformations preserve the Heisenberg canonical commutation relations, since $[A', B'] = U[A, B]U^\dagger$ and in particular $[x', p'] = U[x, p]U^\dagger = U(i\hbar I)U^\dagger = i\hbar I$. For the same reason, unitary transformations leave the Heisenberg equations of motion invariant. Unitary transformations also preserve inner products (and consequently, the squared-norm $\langle\psi|\psi\rangle$) of a state:
$$\langle\phi'|\psi'\rangle = \langle U\phi|U\psi\rangle = \langle\phi|U^\dagger U\psi\rangle = \langle\phi|\psi\rangle. \tag{22}$$
Now, the norm of a state may be interpreted as the total probability of finding the system in some configuration. This makes unitary transformations appropriate for physical changes/processes in which probability is conserved.

7. In CM, time evolution is a 1-parameter family of canonical transformations (**??**) on phase space. In QM, time evolution (which conserves probabilities) is represented by a 1-parameter family of unitary transformations on the quantum Hilbert space: $U(t, 0) = e^{-iHt/\hbar}$ acts on the initial state $|\psi(0)\rangle$ to produce the state $|\psi(t)\rangle$.

3 Ehrenfest's theorem

• The expectation values $\langle x\rangle$, $\langle p\rangle$, $\langle E\rangle$ etc are functions of time (space has been integrated over). The average position and momentum of an electron will depend on time in a way governed by the Schrödinger equation. According to Ehrenfest's theorem, these expectation values evolve as do the corresponding classical variables, whose evolution is given by Newton's/Hamilton's equations! E.g. $\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}$, so the average position evolves in the same way as given by the first of Hamilton's equations. To see this and related results, we first derive a general equation for the time evolution of the expectation value of an observable A in a unit-norm state that evolves via the SE

$$i\hbar\frac{\partial}{\partial t}\langle\psi|A|\psi\rangle = -\langle\psi|HA|\psi\rangle + \langle\psi|AH|\psi\rangle = \langle\psi|[A,H]|\psi\rangle. \tag{23}$$

• Putting $A = H$ and using $[H, H] = 0$ shows that the average energy (expectation value of hamiltonian) is constant $\frac{\partial\langle\hat{H}\rangle}{\partial t} = 0$. This is the analogue of the classical constancy of energy along a trajectory.
• Taking $A = p$ we find the time evolution of mean momentum for a particle subject to the hamiltonian $H = \frac{p^2}{2m} + V$. Show that

$$[p, H] = [p, V] = -i\hbar V' \tag{24}$$

Thus we have

$$\frac{\partial\langle p\rangle}{\partial t} = \langle -V'\rangle. \tag{25}$$

Thus Newton's second law (or the second of Hamilton's equations) $\dot{p} = -V'(x)$ continues to hold in quantum mechanics, but in the sense of expectation values. The average momentum evolves as though it is a classical variable subject to an 'average force'!
• If $A = x$, then $[x, H] = [x, \frac{p^2}{2m}] = \frac{i\hbar p}{m}$. So

$$\frac{\partial\langle x\rangle}{\partial t} = \left\langle\frac{p}{m}\right\rangle. \tag{26}$$

This is the first of Hamilton's equations $\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}$, but now in the sense of expectation values.
• So if the electron is in the initial state $\psi(x, t = 0)$, Schrödinger's equation tells us how the state evolves in time. We have used this to determine the time derivatives of the average position and average momentum of the electron and found that they are related to the average momentum and average force in the same way as the evolution of the actual position and momentum of a particle are related by Hamilton's equation of classical mechanics to the momentum and force. To the extent that the expectation value of x provides an approximate position for a localized electron wave packet, we see that the quantum mechanical motion of the wave-packet mimics the classical motion of a particle. However, the wave packet typically spreads out in time, and ceases to be well-described by merely its mean position. This reduces the utility of the Ehrenfest result in determining where a quantum particle may be found at later times, based on its classical motion.

- If we model a quantum particle by a wave packet, then in general the wave packet will broaden out due to the dispersive nature of Schrödinger time evolution. However, in the classical limit, there is no dispersive broadening and the wave packet follows the classical trajectory. In particular, if the wave packet had zero width initially, then the wave packet will always have zero width. This feature can be exploited to distinguish identical particles in the classical limit using their trajectories.

4 Bohr-Sommerfeld quantization rule for classically integrable systems

Integrable system and angle-action variables. A classically integrable system is one that admits a canonical transformation from original phase space variables q^j, p_j to canonically conjugate angle-action variables θ^j, I_j with the property that the Hamiltonian depends only on the actions $H(q,p) = K(I)$. It follows that all the angle variables are cyclic coordinates so that the actions are conserved quantities. Hamilton's equations $\dot{\theta}^j = \frac{\partial K}{\partial I_j} = \omega^j(I)$ then imply that the angle variables evolve linearly in time. If we restrict to bounded motion, then the angle variables are in fact angular variables and can be taken to be defined modulo 2π, i.e., (θ, I) and $(\theta + 2\pi, I)$ represent the same physical state.

Quantization: Action and adiabatic invariants. Experimental measurements of emission and absorption frequencies of light from gases indicated the presence of discrete or line spectra. Understanding this 'quantization' of variables that were classically allowed to take a continuous range of values was one of the early challenges in the development of the quantum theory (well before the formulation of Heisenberg's matrix mechanics or Schrödinger's wave equation). Consider the simple harmonic oscillator with Hamiltonian $H = p^2/2m + \frac{1}{2}m\omega^2 x^2$. The action variable is defined as $I = \frac{1}{2\pi}\oint p\,dq$ where the integral is around a closed orbit. The formula $E = I\omega$ for the energy of the orbit is a classical precursor of the quantum mechanical formula for its energy levels $E = \hbar(n + \frac{1}{2})\omega$ where $h = 2\pi\hbar$ is Planck's unit of action and $n = 0, 1, 2, \ldots$. Indeed, Ehrenfest proposed that it is the action variables of classical systems that may take discrete values (especially for bound states) in the quantum theory. A quantity that takes discrete values in the quantum theory (such as the number of nodes of a bound state wave function), cannot change under small slow perturbations[6] or continuous time evolution. He asserted that classical quantities that were 'ripe' for quantization should not only be conserved under Hamiltonian time evolution, but also be unchanged under some slow (i.e., adiabatic) perturbations of the system. It was found that the action variable $(1/2\pi)\oint p\,dq$ is an *adiabatic invariant* of the classical system. If the spring constant is increased slowly, the energy of oscillations increases as does their frequency, but the action ratio $I = E/\omega$ remains unchanged. These ideas are implemented in the semiclassical Bohr-Sommerfeld quantization rule $\oint p\,dq = nh$ for large integers $n \gg 1$.

Singlevaluedness of wave function and Bohr-Sommerfeld quantization condition. To see where this quantization condition comes from, we restrict to a system with

---

[6] For instance, if we increase the length l of a 1d infinite potential well slowly, the energy of the n^{th} stationary state $E_n \propto n^2/l^2$ changes, but the number of nodes of the wave function does not.

one degree of freedom for which angle-action variables θ, I are available. Suppose the original Hamiltonian $H(q,p)$ has been expressed in terms of the action variable $H = H(I)$ where $I = \frac{1}{2\pi}\oint p\,dq$. To pass to the quantum theory, we replace the time-independent HJ equation $H(I) = E$ by the time-independent Schrödinger equation $H(I)\psi = E\psi$ for the wave function $\psi(\theta)$. In the Schrödinger equation, I is 'represented' by the differential operator $-i\hbar\frac{\partial}{\partial\theta}$ leading to the eigenvalue problem

$$H\left(-i\hbar\frac{\partial}{\partial\theta}\right)\psi(\theta) = E\psi(\theta). \tag{27}$$

Here $H(I) = \omega I$ for the harmonic oscillator, but could be a nonlinear function of I for other systems which admit angle-action variables, such as the simple pendulum. Plane waves $\psi(\theta) = e^{iP\theta/\hbar}$ are solutions provided $H(P) = E$. Since classically, $H(I) = E$, we take $P = I$. What is more, if θ is an angle variable defined modulo 2π, then requiring the wave function to be singlevalued,

$$\psi(0) = \psi(2\pi) \quad \Rightarrow \quad e^{2\pi I/\hbar} = 1. \tag{28}$$

This leads to the Bohr-Sommerfeld quantization condition

$$I_n = \frac{1}{2\pi}\oint p\,dq = n\hbar, \quad \text{where } n \text{ is an integer.} \tag{29}$$

Thus, the quantum mechanical energy levels in the Bohr-Sommerfeld semiclassical treatment are given by $E_n = H(I_n) = H(n\hbar)$.

Harmonic oscillator. For the harmonic oscillator, $H(I) = \omega I$ leading to the Bohr-Sommerfeld spectrum $E_n = n\hbar\omega$, which approaches the exact spectrum $\hbar\omega(n+\frac{1}{2})$ when n is a large integer. Classically $I \geq 0$, so we restrict to $n \geq 0$.

Kepler problem and Hydrogen atom. The Kepler (or Hydrogen atom) problem for the reduced mass m has three degrees of freedom. However, the angular momentum $\boldsymbol{L}$ is conserved and the motion is on the ecliptic plane (taken to be the x-y plane) orthogonal to $\boldsymbol{L}$ (taken along z). So $z = 0$ and $p_z = 0$ at all times and we may focus on the motion on the x-y plane. In plane polar coordinates, the Hamiltonian is $H = p_r^2/2m + V_{\text{eff}}$ where $V_{\text{eff}}(r) = l^2/2mr^2 - \alpha/r$. Here the strength of the central force is $\alpha = GMm$ or $e^2/4\pi\epsilon_0$ in the Kepler and hydrogen atom contexts. The azimuthal coordinate ϕ is cyclic and its conjugate momentum $L_z = l$ is conserved. So (ϕ, l) form an angle-action pair. Although r is not an angle variable, the action variable for the radial degree of freedom is

$$I = \frac{1}{\pi}\int_{r_-}^{r_+}\sqrt{2m\left(E - l^2/2mr^2 + \alpha/r\right)}\,dr, \tag{30}$$

where $0 < r_- < r_+$ are the radial turning points for bound ($E < 0$) trajectories, determined by $E = V_{\text{eff}}(r_\pm)$. Upon evaluating the integral[7], one gets $I = -l +$

---

[7] The two terms obtained upon evaluating the integral may be partly understood using dimensional analysis. We must have $I = c_1 l + c_2\alpha/\sqrt{-E/m}$ since there are only two independent combinations of

$\alpha/\sqrt{-2E/m}$, leading to the expression for the Hamiltonian $H(l,I) = -m\alpha^2/2(I+l)^2$. If we impose the Bohr-Sommerfeld semiclassical quantization condition, then both I and l must be integer multiples of $\hbar$. Denoting $(l+I)^2 = n^2\hbar^2$ for a 'principal quantum number' n, we recover the bound state spectrum $E_n = -me^4/2(4\pi\epsilon_0\hbar n)^2$ of the Hydrogen atom upon taking $\alpha = e^2/4\pi\epsilon_0$. Max Born used angle-action variables to find the spectrum of the Hydrogen atom.

EBK quantization. The EBK (Einstein-Brillouin-Keller) quantization condition is a refinement of the Bohr-Sommerfeld quantization condition for integrable systems which can be described in terms of n action variables $I_1, \cdots, I_n$ in involution. Here the effects of turning points (where the potential is not slowly varying) are taken into account to arrive at the EBK quantization condition

$$I_j = \frac{1}{2\pi}\oint p_j dq^j = \hbar\left(n_j + \frac{\mu_j}{4} + \frac{b_j}{2}\right) \quad \text{for} \quad i = j, \cdots, n. \tag{31}$$

Here, n_j is a nonnegative integer while μ_j and b_j are so-called Maslov indices associated to the periodic orbit parametrized by θ_j. The integer μ_j is the number of classical turning points, where one imposes Dirichlet boundary conditions on the wave function. The integer b_j is the number of reflections with a hard wall, where one imposes Neumann BCs on the wave function. For example, the 1d SHO has only one degree of freedom two turning points ($\mu = 2$) and no hard wall reflections, so $b = 0$. Thus the EBK quantization condition gives

$$I_n = \frac{E_n}{\omega} = \hbar(n + \frac{1}{2}) \quad \text{or} \quad E_n = \hbar\omega(n + \frac{1}{2}). \tag{32}$$

In this instance, the EBK spectrum matches the exact quantum energy spectrum.

5 Semiclassical expansion and JWKB approximation

5.1 Semi-classical regime and slowly varying potentials

• Named after Jeffreys, Wentzel, Kramers and Brillouin. We wish to approximately solve the time-independent Schrödinger equation for stationary states that are nearly classical.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x). \tag{33}$$

To do this, we wish to exploit the knowledge of some solution of the classical (Hamilton/Newton) equations of motion. In stationary perturbation theory, the zeroth order is a solution of the unperturbed problem. In the semi-classical approximation, the zeroth order is typically a classical solution (in an appropriate form). Classically, the particle is confined to the region x where $E \geq V(x)$. So we focus on this region and postpone phenomena like tunneling through barriers, which are classically forbidden.

---

l, α, E, m that have dimensions of action (l and $\alpha/\sqrt{-E/m}$ where $E < 0$). The dimensionless coefficients c_1, c_2 are found by evaluating the integral, a priori they could be functions of the dimensionless combination $\sqrt{-2E/m}/\alpha l$.

Stationary states with semiclassical behavior. Let us recall which (stationary) states behave more classically than others. If the potential is a constant (as in an infinite square-well of length L in which $V = 0$), $\psi(x) = Ae^{ikx} + Be^{-ikx}$ where $k = \frac{\sqrt{2m(E-V)}}{\hbar}$ and the boundary conditions imply that the stationary states are $\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$. Classically, a particle with non-zero speed spends on average equal times in all subintervals of $[0, L]$ of equal length, as it bounces back and forth against the walls. This uniform distribution is approximated by the probability distribution $|\psi(x)|^2$ of highly excited states. So the classical limit here is the limit of high energies ($E_n \gg V$). This is also the limit of large wave number $k_n = \frac{n\pi}{L}$ compared to $\frac{1}{L}$. This is also the limit where the de Broglie wave length $\lambda_{dB} = \frac{h}{\sqrt{2m(E-V)}} = \frac{2\pi}{k_n} = \frac{2L}{n}$ is small compared to L.

- Notice that L here is the length scale over which the potential changes significantly. More generally, if $V = V(x)$ we say we are in the semi-classical regime if the de Broglie wave length is small compared to the length scale over which the potential varies significantly.
- This is the case, for example for a highly excited state of a particle in an SHO potential. As long as we stay away from the classical turning points, the wave function oscillates rapidly and its wavelength is small. Near the turning points, λ_{dB} diverges and the quantum effects have to be treated more carefully.

Semiclassical regime and concept of a slowly varying potential. If the potential is varying slowly with x, we may still surmise that the wave function is of the form $Ae^{\pm ipx/\hbar}$ but that $p = h/\lambda$ is no longer the constant $\hbar k$, but varies slowly with x. In other words, this suggests the ansatz $\psi \sim e^{iS(x)/\hbar}$ where for a constant potential, $S(x) = px = \pm x\sqrt{2m(E-V)}$. Before we work out the consequences of this ansatz, let us say more on what we mean by the semi-classical regime and what it means for the potential to be slowly varying.

- If $V = V(x)$, we require that the wavelength is small compared to the length scale over which the potential changes by an amount of the order of the kinetic energy of the particle[8]. Indeed, suppose the potential changes by $p^2/2m$ over a length L, then[9]

$$\frac{p^2}{2m} \approx \delta V \approx \left|\frac{dV}{dx}\right| L \quad \Rightarrow \quad L \approx \frac{p^2}{2m} \left|\frac{dV}{dx}\right|^{-1} \tag{34}$$

---

[8] We need to decide what we mean by potential 'changes appreciably'. The change in the potential has dimensions of energy and the KE of the particle is a reasonable scale of energy to compare with. Indeed, near the turning points of the SHO, the KE is small, so the length scale over which the potential changes by an amount of the order of the KE is quite small. On the other hand, far away from the turning points the KE is large (for a highly excited state), and the length scale over which the potential changes appreciably compared to the KE is large. So by this definition, the SHO potential is slowly-varying away from the turning points for a highly excited state, and not slowly-varying near the turning points. The corresponding statement about the smallness/largeness of $\lambda_{\rm dB}$ is a consequence since $\lambda = h/\sqrt{2m(E-V(x))}$ is determined by E and $V(x)$.

[9] In approximating δV by its first derivative, we assume that L is not so large that this approximation breaks down.

Now

$$\lambda \ll L \quad \Rightarrow \quad \frac{2m\lambda}{p^2}\left|\frac{dV}{dx}\right| \ll 1 \quad \text{or} \quad \left|\frac{2mh}{p^3}\frac{dV}{dx}\right| \ll 1 \quad \text{or} \quad \left|\frac{dV}{dx}\right| \ll \frac{\sqrt{2m}}{h}\,|E-V(x)|^{\frac{3}{2}} \tag{35}$$

This is our condition for semi-classical behavior. It is a condition on the potential, that also involves the energy and depends on x. It is easier to satisfy this condition for a fixed potential and x, if we make E bigger: excited states behave more classically. It is easier to satisfy (for fixed E) where dV/dx is 'small'. The criterion involves x, so even for fixed $V(x)$ and E there may be some locations where the behavior *is* semi-classical ($E \gg V(x)$), and other locations where it is *not* semi-classical ($E \approx V(x)$). Also, the 'smaller' $\hbar$ is, the easier it is to satisfy this condition so in a sense $\hbar \to 0$ is the classical limit.

de Broglie wavelength and semiclassical condition. Let us re-derive this condition by thinking in terms of the de Broglie wavelength. For a non-constant $V(x)$, the de Broglie wavelength changes with x. The concept of a wavelength is useful if there are many oscillations with roughly the same wavelength. This is the case if the change in wavelength (over a length of one wavelength) is small compared to the wavelength itself. The change in wavelength over a distance δx is

$$\delta\lambda = \frac{d\lambda}{dx}\,\delta x. \tag{36}$$

So putting $\delta x = \lambda$, the change in wavelength over a wavelength is $\delta\lambda = \frac{d\lambda}{dx}\lambda$. Thus we require $\left|\frac{\delta\lambda}{\lambda}\right| = \left|\frac{d\lambda}{dx}\right| \ll 1$. We can express this as a condition on the potential using $\lambda = h/\sqrt{2m(E-V(x))}$.

$$\left|\frac{\delta\lambda}{\lambda}\right| = \left|\frac{mh}{p^3}\frac{dV}{dx}\right| \ll 1 \tag{37}$$

This is the same condition for semi-classicality as obtained earlier. So we can either say the potential is slowly varying or the de Broglie wavelength is slowly varying.

5.2 Variation of constants for slowly varying potential: HJ equation

Semiclassical energy eigenfunction from Hamilton-Jacobi equation. We motivated the ansatz $\psi = Ae^{iS(x)/\hbar}$ in seeking a solution of the time-independent Schrödinger equation in the semi-classical regime. Without further assumptions, this ansatz (for complex S and real A), does not involve any approximation, it is merely a change of dependent variable from $\psi(x)$ to $S(x)$, in terms of which the eigenvalue problem becomes

$$-\frac{\hbar^2}{2m}\psi'' = (E-V)\psi \quad \Rightarrow \quad -\frac{i\hbar}{2m}S'' + \frac{1}{2m}(S')^2 + V(x) = E. \tag{38}$$

Now we exploit the slowly varying nature of $V(x)$ to assume that $S'(x)$ is slowly varying[10] so that we may ignore $S''(x)$ and approximate the SE by

$$\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + V = E \tag{39}$$

Notice that this approximation could also be obtained by letting $\hbar \to 0$ (assuming $S(x)$ has a finite limit as $\hbar \to 0$), more on this later. Moreover, the resulting equation is the time-independent Hamilton-Jacobi equation of classical mechanics

$$H(x, \frac{\partial S}{\partial x}) = E \quad \text{where} \quad H(x,p) = \frac{p^2}{2m} + V(x) \quad \text{and} \quad p = \frac{\partial S}{\partial x}. \tag{40}$$

The time-independent HJ equation is an equation for a generating function $S(x)$ (called Hamilton's characteristic function) for a possible canonical transformation from 'old' coordinates x, p to new coordinates X, P. For n degrees of freedom, such a CT exists provided a complete solution of the HJ equation can be found, depending on n constants of integration which can be taken as the new momenta P so that we may write $S = S(x,P)$. If the time-dependent generating function (Hamilton's principal function) is defined as $\mathcal{S}(x,P,t) = S(x,P) - Et$, then the new Hamiltonian

$$K(X,P) = H(x,p) + \frac{\partial \mathcal{S}}{\partial t} \tag{41}$$

vanishes identically and $\mathcal{S}$ is said to satisfy the time-dependent HJ equation $\partial_t \mathcal{S} + H(x, \partial_x \mathcal{S}) = 0$. Note that the Hamiltonian appearing in the Schrödinger equation is the old Hamiltonian H, not K. Moreover, even though $K = 0$, this does not mean that the quantum mechanical energy levels are all zero, K is not a unitary transform of H, they do not have the same spectra. It is just that in the new coordinates ($X = \frac{\partial S}{\partial P}$ and P), the classical dynamics is as simple as it could be since X and P are both constants of motion: $\dot{X} = \frac{\partial K}{\partial P} = 0$ and $\dot{P} = -\frac{\partial K}{\partial X} = 0$. All the complications of the original Hamiltonian have been dumped in the transformation from old coordinates (x and p) to new coordinates (X and P).

- In our 1d context, we write the HJ equation in the form $S'(x)^2 = p(x)^2$ and integrate to get

$$S(x) - S(x_0) = \pm \int_{x_0}^{x} p(x')\,dx' \quad \text{where} \quad p(x) = \sqrt{2m(E - V(x))}. \tag{42}$$

Thus, our approximation for the wave function in the semi-classical regime is the exponential of ($(i/\hbar)\times$) Hamilton's characteristic function[11]

$$\psi(x) = Ae^{\frac{i}{\hbar}\int_{x_0}^{x} p(x')\,dx'} + Be^{-\frac{i}{\hbar}\int_{x_0}^{x} p(x')\,dx'}. \tag{43}$$

---

[10] For a constant potential $S'(x) = \hbar k$ is a constant, so now we imagine that this earstwhile 'constant' varies with x.

[11] By absorbing a phase and its conjugate into A and B, the limit of integration x_0 may be set equal to the left turning point of the classical trajectory.

• We will improve on this approximation shortly. But even this crude approximation leads to some interesting consequences such as a simple case of the Bohr-Sommerfeld quantization condition.

Bohr-Sommerfeld semiclassical quantization. Suppose a particle moves in the 1 dimensional potential $V(x)$ which becomes infinite for $x < 0$ and $x > L$ but is arbitrary for $0 \leq x \leq L$. Then the approximate wave function satisfying the boundary condition $\psi(0) = 0$ is

$$\psi(x) \approx A \sin\left(\frac{S(x)}{\hbar}\right) \quad \text{where} \quad S(x) = \int_0^x p(x')\, dx'. \tag{44}$$

The boundary condition $\psi(L) = 0$ then becomes $S(L) = n\pi\hbar$ which is the Bohr quantization condition

$$\oint p(x')\, dx' = 2\int_0^L p(x')\, dx' = nh. \tag{45}$$

Use this condition to find a semi-classical approximation to the square-well energy levels.

First subleading correction: slowly varyung amplitude. Let us continue with the theme of making constants vary. A simple way of improving on this approximation is to suppose that both the amplitude and phase are slowly varying functions. Let us put $\psi(x) = A(x)e^{iS(x)/\hbar}$ in the Schrödinger eigenvalue problem, and suppose that both $A(x)$ and $S(x)$ are real. We get

$$-\frac{\hbar^2}{2m}\left(A'' + \frac{i}{\hbar}\left(2A'S' + AS''\right) - \frac{AS'^2}{\hbar^2}\right) + V(x)A(x) = EA(x). \tag{46}$$

The real part gives us

$$-\frac{\hbar^2}{2m}\left(A'' - \frac{AS'^2}{\hbar^2}\right) = (E - V(x))A(x) \tag{47}$$

which reduces to the time-independent HJ equation, if we ignore the second derivative of $A(x)$. The solution is $S = \pm\int^x p(x')\, dx'$ as before. The imaginary part gives us the condition $2A'S' + AS'' = 0$ which means $(A^2 S')' = 0$ or $A(x) = \pm\frac{C}{\sqrt{S'}} = \pm\frac{C}{\sqrt{p(x)}}$ for some real constant C. The approximate wavefunction is

$$\psi(x) \approx \frac{C_1}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int^x p(x')}\, dx' + \frac{C_2}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int^x p(x')\, dx'} \tag{48}$$

where $p(x) = \sqrt{2m\,(E - V(x))}$. This is already a better approximation. The contributing amplitudes are inversely proportional to $\sqrt{p(x)}$. So aside from interference effects, the particle is less likely to be found in a place where its classical momentum is large, as we observed for a particle near the equilibrium point in an SHO potential.

• It is possible to improve on this approximation by developing a systematic semi-classical expansion that incorporates effects of more rapid variation in the potential.

5.3 Examples and features of the semi-classical limit $\hbar \to 0$

- To get the Hamilton-Jacobi equation of classical mechanics from the Schrödinger equation, we let $\hbar \to 0$ after making the ansatz $\psi = Ae^{iS/\hbar}$. So we should expect classical behaviour to emerge in the limit $\hbar \to 0$.

Gaussian wave packet as $\hbar \to 0$. To reinforce this idea, let us look at the gaussian wave packet for a free particle in this limit. The probability density of a gaussian wave packet is

$$P(x,t) = |\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi}a(t)} e^{-\frac{\left(x-\frac{p_o t}{m}\right)^2}{2a(t)^2}} \quad \text{where} \quad a(t) = a\sqrt{1+\frac{t^2}{\tau^2}} \tag{49}$$

and $\tau = \frac{2ma^2}{\hbar}$ is the characteristic time scale over which the wave packet broadens. The mean momentum of this wave packet is $\langle p \rangle = p_o = \hbar k_o$ and the mean position is $\langle x \rangle = \frac{p_o t}{m}$. We take the limit $\hbar \to 0$ holding p_o fixed (i.e., the limit of large wave number $k_o = \frac{p_o}{\hbar} \to \infty$). As $\hbar \to 0$, $\tau \to \infty$ and the wave packet does not broaden out. The dispersive effects of wave mechanics die out as $\hbar \to 0$ and the object behaves like a classical particle of fixed size a. To model a classical point-like particle, we could further let $a \to 0$ and get the probability density $P(x,t) = \delta\left(x - p_o t/m\right)$ as expected of a free point-like particle moving at velocity p_o/m.

Classical limit as a short time limit. The limit $\hbar \to 0$ is a very convenient way of approaching the classical limit. $\hbar$ is a dimensional constant, so what we mean by $\hbar \to 0$ is that certain physical quantities with dimensions of action are very large compared to $\hbar$. In the above example of a free particle gaussian wave packet, the relevant quantity with dimensions of action is $\frac{2ma^2}{t}$. So the classical limit is the one where we consider times t much shorter than the time-scale τ for quantum mechanical dispersive broadening of the wave packet.

Exited states of an oscillator. For highly excited states of the harmonic oscillator, the quantity $\frac{E_n}{\omega} = \hbar(n+\frac{1}{2})$ with dimensions of action is large compared to $\hbar$. These states behave semi-classically in many respects.

Semiclassical limit of a rigid body. E.g. L^2 eigenstates of a rigid body with very large angular momentum quantum number $l \gg 1$ behave semi-classically, the magnitude of their total angular momentum $\sqrt{\hbar^2 l(l+l)}$ is the quantity with dimensions of action, that is large compared to $\hbar$.

- **Spin is somewhat different from angular momentum.** A given rigid body or atom can be in states of very different angular momentum quantum number l. So letting $\hbar \to 0$ and simultaneously $l \to \infty$ while holding the classical quantity $|\vec{L}| = \sqrt{\hbar^2 l(l+1)}$ fixed is a classical limit. On the other hand, an electron is always a spin $s = \frac{1}{2}$ particle, so for an electron, the eigenvalue of S^2 is always $3\hbar^2/4$ which is not large compared to $\hbar^2$. So it does not make direct sense to let the spin quantum number s of an *electron* take any value other than $\frac{1}{2}$, leave alone let it go to infinity.

Essential singularity as $\hbar \to 0$. The limit $\hbar \to 0$ is not a simple one for stationary state wave functions.

- **Free particle.** The wave function of a free particle $\psi(x) = Ae^{ipx/\hbar}$ does not have a good classical limit $\hbar \to 0$, holding the classically meaningful quantities x, p fixed. Indeed, the wave function has an essential singularity as $\hbar \to 0$. However, $-i\hbar \log \psi$ does have a good limit as $\hbar \to 0$, it tends to Hamilton's characteristic function $W = px$ for a trajectory between positions 0 and x.
- **Harmonic oscillator.** In the case of the SHO, the stationary states are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{m\omega x^2}{2\hbar}} \tag{50}$$

Here too $\psi(x)$ has an essential singularity at $\hbar = 0$, but $\hbar \log \psi(x)$ has a finite limit $-\frac{m\omega x^2}{2}$ as $\hbar \to 0$.

- **The infinite square well stationary states** $\psi_n(x) = \sqrt{2/l}\sin(n\pi x/l)$ do not involve $\hbar$. So if the width of the well l and quantum number n are held fixed, these wave functions have a finite limit as $\hbar \to 0$. However, the states that behave like a classical particle bouncing between hard walls are the ones for which $n \to \infty$. In this limit, we may interpret the rapidly oscillating $|\psi_n(x)|^2$ as approximating the uniform distribution. A classical particle is equally likely to be found anywhere in the well: the distribution of times spent is uniform.

5.4 Semi-classical expansion in powers of $\hbar$

Expanding S in powers of $\hbar$. For a general potential, the above examples suggest it isn't a good idea to look for an expansion of $\psi(x)$ in powers of $\hbar$ around a 'classical wave function', since such a thing does not even exist for a free particle. It is better to make the ansatz $\psi = Ae^{iS(x)/\hbar}$ and try to expand $S(x)$ in powers of $\hbar$. Thus we will seek a solution of the time-independent SE in the form $\psi = Ae^{iS(x,\hbar)/\hbar}$ where $S(x,\hbar)$ is a (possibly complex) function of x depending on $\hbar$ and A is a constant[12]. Then

$$\psi'(x) = \frac{iS'}{\hbar}\psi(x), \quad \psi''(x) = \left(\frac{iS''}{\hbar} - \frac{S'^2}{\hbar^2}\right)\psi(x) \tag{51}$$

and the SE becomes

$$-\frac{\hbar^2}{2m}\left(\frac{iS''}{\hbar} - \frac{S'^2}{\hbar^2}\right) + V(x) = E \tag{52}$$

Now we suppose $S(x)$ is expanded in a series in $\hbar$

$$S(x) = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + \dots \tag{53}$$

In effect, we are assuming that $S(x)$ has a finite limit as $\hbar \to 0$. This is true for the free particle as well as for the highly excited states of many problems we have solved (SHO, square well, delta potential). In fact it is true even for low lying states of many of the problems we have solved (like the SHO above).

---

[12] We were in effect beginning to do this when we previously made the ansatz $\psi(x) = A(x)e^{iS(x)/\hbar} = e^{\frac{i}{\hbar}(S(x) - i\hbar\log A(x))}$.

Caution: Not all states behave semiclassically. However, it is not always the case that $S(x,\hbar)$ has a finite limit as $\hbar \to 0$. Not all states are semi-classical. This is especially true for low lying states such as the ground state of the δ potential well or the hydrogen atom, where

$$\psi_0(x) = \frac{\sqrt{mg}}{\hbar} e^{-mg|x|/\hbar^2} \quad \text{and} \quad \psi_{100}(x) = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{me^2 r}{4\pi\epsilon_o \hbar^2}} \quad \text{where} \quad a = \frac{4\pi\epsilon_o\hbar^2}{me^2}. \tag{54}$$

For both these ground states, $\hbar \log \psi$ does *not* have a finite limit as $\hbar \to 0$, though $\hbar^2 \log \psi$ has a finite limit. In both these cases, we anticipate that the above semi-classical approximation may not be accurate.

• On the other hand, the semi-classical expansion will be seen to be a good approximation in situations where our criterion for the semi-classical regime (slowly varying potential or de Broglie wavelength) is satisfied. In those situations, we may use solutions of the classical HJ equation to obtain a first approximation to semi-classical wave functions.

Caution: Semiclassical expansion may not converge. Note that we are not claiming that the expansion of $S(x,\hbar)$ in powers of $\hbar$ is convergent. This is true for the free particle where $S(x) = px$. But for other potentials, the expansion $S(x,\hbar) = S_o + S_1\hbar + S_2\hbar^2 + \cdots$ may not converge. Nevertheless, it does provide an excellent asymptotic approximation in the semi-classical regime in many cases.

Eikonal approximations. Equating coefficients of like powers of $\hbar$, we get a sequence of differential equations for S_n. At order $\hbar^0$ we recover the time-independent HJ equation, which is the nonlinear differential equation

$$\frac{S_0'(x)^2}{2m} + V(x) = E \tag{55}$$

with solution $S_0(x) = \pm\int_{x_0}^x \sqrt{2m(E - V(x'))}\; dx' = \pm\int_{x_0}^x p(x')\; dx'$. This is called the Eikonal approximation or the semiclassical WKB approximation. S_0 is called the Eikonal or Hamilton's characteristic function.

First subleading approximation. At order $\hbar$ we get a linear equation for S_1, into which we substitute the known $S_0' = p(x)$:

$$S_1'(x)S_0'(x) = \frac{i}{2}S_0'' \quad \Rightarrow \quad S_1'(x) = \frac{i}{2}\frac{S_0''}{S_0'} = \frac{i}{2}(\log S_0')' = \frac{i}{2}(\log p(x))'$$

$$\Rightarrow \quad S_1 = \frac{i}{2}\log p(x) + \text{const.} \tag{56}$$

Upon including this subleading correction, we get

$$\psi(x) \approx \frac{A_1}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int_{x_0}^x p(x')\,dx'} + \frac{A_2}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int_{x_0}^x p(x')\,dx'}. \tag{57}$$

This matches our earlier result (48). However, the present method is more systematic and allows us to find further quantum corrections around the classical limit. What is more, this method can also be applied to regions which the classical trajectory is forbidden from exploring (e.g., tunneling through a barrier).

Condition for validity of the Eikonal approximation. Let us find a condition for the validity of the eikonal approximation. Recall that we found upon substituting $S = S_0 + \hbar S_1 + \cdots$ and $\psi = e^{iS/\hbar}$ in the Schrodinger eigenvalue problem

$$(S_o')^2 + \hbar(2S_o'S_1' - iS_o'') + \mathcal{O}(\hbar^2) = 2m(E - V(x)). \tag{58}$$

Now for the Eikonal approximation to be good, the order of magnitude of the terms of order $\hbar^0$ must be large compared to that of the terms of order $\hbar$. $|(S_o)'^2|$ can be taken as the order of magnitude of the constant terms in $\hbar$ and $|i\hbar S_o''|$ the order of magnitude of the terms of linear in $\hbar$. So the condition is

$$|(S_o)'^2| \gg |\hbar S_o''| \quad \text{or} \quad \left|\frac{\hbar S_o''}{S_o'^2}\right| \ll 1 \tag{59}$$

This is the same as our earlier criterion for the semi-classical regime, that the potential or de Broglie wavelength be slowly varying $\left|\frac{d\lambda}{dx}\right| \ll 1$:

$$\lambda(x) = \frac{h}{p(x)} = \frac{h}{S_0'} \quad \Rightarrow \quad \left|\frac{d\lambda}{dx}\right| = \left|\frac{hS_0''}{S_0'^2}\right| \ll 1 \tag{60}$$

5.5 Estimation of Tunneling amplitude

• Previously, we tried to use solutions of the classical Hamilton-Jacobi equation to approximately infer the quantum mechanical wave function. This program was applicable in the classically allowed region $E > V(x)$. On the other hand, the wave function can be non-zero even in classically forbidden regions ($E < V(x)$) as in the case of tunneling through a barrier. In such classically forbidden regions, we may still obtain a semiclassical approximation to the wavefunction using the expansion in powers of $\hbar$ developed in the last section. Even if $E < V$, the condition for the semi-classical regime $|\frac{d\lambda}{dx}| \ll 1$ or $\left|\frac{dV}{dx}\right| \ll \frac{\sqrt{2m}}{h}|E - V(x)|^{\frac{3}{2}}$ can still be satisfied, especially if $E \ll V$ or if $\frac{dV}{dx}$ is small.

• For simplicity let us consider scattering against a barrier in one dimension that extends between $x = -L$ and L, such as a rectangular barrier with an undulating top $V(x) > 0$ for $|x| \le L$ and $V(x) = 0$ for $|x| > L$. Classically if the energy $E > V_{\rm max}$, the particle 'rolls over' the barrier, but is reflected otherwise. Quantum mechanically, even if $E < V_{max}$ there can be a non-zero transmission probability due to tunneling. We wish to get a semi-classical estimate for the transmission coefficient in cases where it is small. (After all, it is zero classically.)

• Let us consider scattering from the left with incident energy $E = \hbar^2k^2/2m < V_{max}$. Suppose the repulsive potential is such that there are just two classical turning points ($x_L = -L$ on the left of the barrier and $x_R = L$ on the right) between which $V(x) > E$, as is the case for a rectangular barrier.

• In the classically allowed regions to the left ($\psi(x) = Ae^{ikx} + Be^{-ikx}$) and right ($\psi(x) = Fe^{ikx}$) of the barrier, the WKB approximation gives the exact free particle wave functions since the potential is a constant. The transmission coefficient we wish to find is $|F/A|^2$. Instead of trying to solve the SE in the classically disallowed region, we use the WKB approximation

$$\psi(x) \approx \frac{C'}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int_{x_L}^{x} p(x')dx'} + \frac{D'}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int_{x_L}^{x} p(x')dx'} \tag{61}$$

Here $p(x) = \sqrt{E - V(x)}$ is purely imaginary and we may absorb some phases into C' and D' and write

$$\psi(x) \approx \frac{C}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_{x_L}^{x} \sqrt{2m(V(x)-E)}dx'} + \frac{D}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar}\int_{x_L}^{x} \sqrt{2m(V(x)-E)}dx'}. \tag{62}$$

- Since we assumed the tunneling probability is small, the barrier must be high (compared to E) or wide (compared to the de Broglie wavelength of the incident wave). In this case, the coefficient D of the exponentially growing wavefunction must be very small and we ignore it ($D \to 0$ as the barrier width $L \to \infty$). This can be motivated by imposing continuity of $\psi(x)$ and its first derivative at the classical turning points x_L, x_R. The attenuation of the wavefunction is approximately

$$\frac{|F|}{|A|} \approx e^{-\frac{1}{\hbar}\int_{x_L}^{x_R} \sqrt{2m(V(x')-E)}dx'} \equiv e^{-\gamma} \tag{63}$$

So the WKB estimate for the transmission probability is

$$T \approx e^{-2\gamma} = e^{-\frac{2}{\hbar}\int_{x_L}^{x_R} \sqrt{2m(V(x')-E)}dx'} \tag{64}$$

We see that as $\hbar \to 0$, $T \to 0$ exponentially fast and classically the particle is not transmitted.

- Tunneling was used by Gamow and others to explain the decay of a nucleus to a daughter nucleus by emission of an $\alpha(nnpp)$ particle. The strong nuclear forces create something like an attractive finite spherical potential well inside the nucleus for the alpha particle. Outside the nucleus, the alpha particle is repelled by the electrostatic force with the positively charged daughter nucleus. But in order to escape, the alpha particle has to tunnel through a potential barrier.

6 Trace formula for particle on a circle: spectrum and periodic orbits

6.1 Classical free particle on a circle S^1

Consider a point particle of mass m that is free to move on a circle of radius r with θ as its angular coordinate. The Lagrangian is $L = \frac{1}{2}mr^2\dot\theta^2$. The angular momentum conjugate to θ is $p_\theta = mr^2\dot\theta$ while the Hamiltonian is $H = p_\theta^2/2mr^2$. The classical equation of motion is $mr^2\ddot\theta = 0$ with the solution $\theta(t) = \theta(0) + \omega t$ where $\omega = \dot\theta$ is the constant angular velocity. Consider a periodic trajectory that goes once round the circle counterclockwise ($\omega > 0$). Its time period is $T = 2\pi/\omega$. The action of this once winding periodic orbit is

$$S_1 = \int_0^T L\,dt = \frac{1}{2}mr^2\omega^2 T = \pi m r^2\omega = \frac{2\pi^2 m r^2}{T}. \tag{65}$$

Other periodic trajectories wind round the circle n times, where n is an integer. Negative n pertain to clockwise orbits. The energy of a trajectory with angular velocity ω is $\frac{1}{2}mr^2\omega^2$, so fixed energy corresponds to fixed ω. On the other hand, we may consider trajectories of a fixed duration T in time.

6.2 Stationary states of quantum free particle on S^1

In the quantum theory, we will suppose that the wave function $\psi(\theta)$ is a 2π periodic function of θ. This is consistent[13] with the requirement that the probability densities at the physically identical points $\theta = 0, 2\pi$ be the same: $|\psi(0)|^2 = |\psi(2\pi)|^2$. In the Schrödinger picture, we represent θ by a multiplication operator while the conjugate angular momentum us represented by $p_\theta = -i\hbar\partial_\theta$. The Hamiltonian becomes

$$H = \frac{p_\theta^2}{2mr^2} = -\frac{\hbar^2}{2mr^2}\frac{\partial^2}{\partial\theta^2}. \tag{66}$$

Where convenient, we will work in units where $r = 1$ and $\hbar^2/2m = 1$. The Schrödinger eigenvalue problem for an energy eigenstate with energy E is

$$H\psi = E\psi \quad \text{or} \quad -\frac{\partial^2}{\partial\theta^2}\psi(\theta) = E\psi(\theta). \tag{67}$$

For the ansatz $\psi(\theta) = Ae^{il\theta}$ we find $\psi''(\theta) = -Al^2e^{il\theta}$ so that $E = l^2$. Imposing 2π periodicity $\psi(0) = \psi(2\pi)$ we get the condition $e^{2\pi il} = 1$ which implies that l must be an integer, say $l = n$. Thus the energy spectrum and energy eigenfunctions are

$$E_n = \frac{n^2\hbar^2}{2mr^2} \quad \text{and} \quad \psi_n(\theta) = Ae^{in\theta} \quad \text{for} \quad n = 0, \pm1, \pm2, \cdots . \tag{68}$$

We may pick $A = 1/\sqrt{2\pi}$ to ensure that the eigenfunctions are orthonormal

$$\langle\psi_m|\psi_n\rangle = \int_0^{2\pi} |A|^2 e^{i(n-m)\theta} d\theta = \delta_{mn}. \tag{69}$$

6.3 Euclidean time evolution and heat operator

The time evolution operator is given by $U(t) = e^{-iHt/\hbar}$. We will be interested in the Euclidean time evolution operator, which is also called the heat operator. Let us continue t to a negative imaginary time so that $\beta = it/\hbar$ is a positive real number viewed as the inverse temperature $\beta = (k_bT)^{-1}$. Then we define the heat operator as

$$h_\beta = U(-i\hbar\beta) = e^{-\beta H}. \tag{70}$$

The name heat operator is given because if we view β as time, then h_β is the fundamental solution of the heat equation on the circle. In fact,

$$\frac{\partial}{\partial\beta}h_\beta = -He^{-\beta H} \quad \Rightarrow \quad \frac{\partial h_\beta}{\partial\beta} = \frac{\partial^2 h_\beta}{\partial\theta^2}, \tag{71}$$

---

[13] Mere general 'quasiperiodic' boundary conditions $\psi(2\pi) = e^{i\phi}\psi(0)$ are possible for a nontrivial phase $e^{i\phi}$, but will not be considered here.

where we have viewed h_β in the position (angle) basis in the second equation; more on this shortly. It is called the fundamental solution since it tends to the identity as time goes to zero:

$$\lim_{\beta\to 0^+} h_\beta = I. \tag{72}$$

6.4 Partition function

The partition function is defined as the trace of the heat operator:

$$Z(\beta) = \operatorname{tr} e^{-\beta H}. \tag{73}$$

Evaluating the trace in the basis of energy eigenfunctions, we get

$$Z(\beta) = \sum_{n\in\mathbb{Z}} \langle \psi_n | e^{-\beta H} | \psi_n \rangle = \sum_{n=-\infty}^{\infty} e^{-\beta n^2}. \tag{74}$$

Let us examine the convergence of this series. Now $\beta > 0$ so $0 \le e^{-\beta} < 1$. If we denote $z = e^{-\beta}$, then

$$Z(\beta) = 1 + 2(z + z^4 + z^9 + \cdots). \tag{75}$$

By comparing with the geometric series, we see that this series converges absolutely for $|z| < 1$. So the above series for $Z(\beta)$ converges for all $\beta > 0$.

There is another expression for the partition function which is obtained by evaluating the trace of the heat operator in the position basis. For this we need the matrix elements of the heat operator between position eigenstates, this is the so-called heat kernel.

6.5 Heat kernel on the circle

The matrix elements of the heat operator in the position basis $|\theta\rangle$ is called the heat kernel:

$$h_\beta(\theta, \theta') = \langle \theta | h_\beta | \theta' \rangle. \tag{76}$$

As a consequence of (71) and (72), it satisfies the heat equation on the circle

$$\frac{\partial}{\partial \beta} h_\beta(\theta, \theta') = \frac{\partial^2}{\partial \theta^2} h_\beta(\theta, \theta') \tag{77}$$

with initial condition corresponding to the kernel of the identity operator:

$$\lim_{\beta\to 0^+} h_\beta(\theta, \theta') = \delta(\theta - \theta', \operatorname{mod} 2\pi). \tag{78}$$

Since θ, θ' are defined modulo 2π, on the RHS we have the delta function on the circle, which is nonzero only when $\theta - \theta'$ is a multiple of 2π. If we think of θ, θ' as real numbers, then we may write the delta function on the circle as a sum of Dirac delta functions ('Dirac comb') on the real line supported at integer multiples of 2π:

$$\lim_{\beta\to 0^+} h_\beta(\theta,\theta') = \sum_{n=\infty}^{\infty} \delta(\theta-\theta'+2n\pi). \tag{79}$$

The heat kernel on the circle may be expressed in terms of the heat kernel $K_\beta(x,x')$ on the real line:

$$h_\beta(\theta,\theta') = \sum_{n=-\infty}^{\infty} K_\beta(\theta,\theta'+2n\pi). \tag{80}$$

6.6 Heat kernel on $\mathbb{R}$

The heat kernel on the real line gives the matrix elements of the heat operator between position eigenstates $K_\beta(x,x') = \langle x|e^{-\beta H}|x'\rangle$ where $H = -\frac{\partial^2}{\partial x^2}$ is the free particle Hamiltonian in units where $\hbar^2/2m = 1$. The heat kernel may also be viewed as the free particle propagator (position representation of the time evolution operator) in imaginary time and is the solution of the heat equation

$$\partial_\beta K_\beta(x,x') = \frac{\partial^2}{\partial x^2} K_\beta(x,x') \quad \text{with IC} \quad K_{\beta\to 0}(x,x') = \delta(x-x'). \tag{81}$$

It is a Gaussian

$$K_\beta(x,x') = \frac{1}{\sqrt{4\pi\beta}} \exp\left(-\frac{(x-x')^2}{4\beta}\right). \tag{82}$$

To obtain this formula, we first use translation invariance to observe that $K_\beta(x,x') \equiv K_\beta(x-x')$ can only depend on the separation. Expressing it in Fourier space

$$K_\beta(y) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{iky} \tilde{K}_\beta(k), \tag{83}$$

the heat equation (81) becomes an ODE for each Fourier mode:

$$\partial_\beta \tilde{K}_\beta(k) = -k^2 \tilde{K}_\beta(k). \tag{84}$$

Thus, the heat kernel in Fourier space is a Gaussian:

$$\tilde{K}_\beta(k) = N e^{-k^2\beta}, \tag{85}$$

where N is a normalization constant to be fixed by requiring that $K_\beta(y) \to \delta(y)$ as $\beta \to 0^+$. The heat kernel in position space is obtained by inverting the Fourier transform. We evaluate the Gaussian integral by completing a square:

$$\begin{aligned} K_\beta(y) &= N\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-\beta(k^2-iky/\beta)} = N\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-\beta\left[(k-iy/2\beta)^2+y^2/4\beta^2\right]} \\ &= N e^{-y^2/4\beta} \int_{-\infty}^{\infty} \frac{dk'}{2\pi} e^{-\beta k'^2} = \frac{N}{\sqrt{4\pi\beta}} e^{-y^2/4\beta}. \end{aligned} \tag{86}$$

We used $\int e^{-\beta k'^2} dk' = \sqrt{\pi/\beta}$. Thus, the heat kernel is a Gaussian in position space as well. Moreover, we find $\int_{-\infty}^{\infty} K_\beta(y) dy = N$ for any $\beta > 0$. Recall that the Dirac delta distribution is a limit of normalized Gaussians as the width tends to zero. So taking $N = 1$ ensures that $K_\beta(y) \to \delta(y)$ as $\beta \to 0$. Thus, we have established (82).

6.7 Partition function from heat kernel on S^1

We now use the heat kernel on $\mathbb{R}$ to obtain a formula for the heat kernel on the circle:

$$h_\beta(\theta, \theta') = \sum_{n=-\infty}^{\infty} K_\beta(\theta, \theta' + 2n\pi) = \frac{1}{\sqrt{4\pi\beta}} \sum_{n=-\infty}^{\infty} e^{(\theta-\theta'-2n\pi)^2/4\beta}. \tag{87}$$

The partition function is got by taking a trace of h_β, i.e., put $\theta = \theta'$ and integrate over the circle:

$$Z(\beta) = \int_0^{2\pi} h_\beta(\theta, \theta) d\theta = \frac{1}{\sqrt{4\pi\beta}} \int_0^{2\pi} \sum_n e^{-4n^2\pi^2/4\beta} d\theta = \frac{2\pi}{\sqrt{4\pi\beta}} \sum_{n=-\infty}^{\infty} e^{-n^2\pi^2/\beta}. \tag{88}$$

Notice that for any $\beta > 0$, $0 < e^{-\pi^2/\beta} < 1$. Thus, by comparison with the geometric series, this series converges absolutely for any such β.

Thus, we have found two formulae for the circle partition function by evaluating the trace in the energy and position bases. Equating (74) and (88) we get a 'trace formula' relating two infinite sums for the partition function:

$$Z(\beta) = \operatorname{tr} e^{-\beta H} = \sum_{n=-\infty}^{\infty} e^{-n^2\beta} = \frac{2\pi}{\sqrt{4\pi\beta}} \sum_{n=-\infty}^{\infty} e^{-n^2\pi^2/\beta}. \tag{89}$$

Notice the reciprocal manner in which β appears in the exponent on the left and right sides.

6.8 Relation to Poisson summation formula

The trace formula (89) is a special case of the Poisson summation formula, which states that

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{n=-\infty}^{\infty} \tilde{f}(2\pi n), \tag{90}$$

where $\tilde{f}(k) = \int e^{-ikx} f(x)\, dx$ is the Fourier transform of $f(x)$. Indeed, if we take

$$f(x) = e^{-\beta x^2} \quad \text{then} \quad \tilde{f}(k) = \sqrt{\pi/\beta} e^{-k^2/4\beta} \tag{91}$$

then we recover the trace formula.

6.9 High temperature - low temperature relation

Consider again the trace formula giving two expressions for $Z(\beta)$:

$$Z(\beta) = \sum_n e^{-n^2\beta} = \sqrt{\pi/\beta} \sum_n e^{-n^2\pi^2/\beta}. \tag{92}$$

Although valid for all $\beta > 0$, it is convenient to view the LHS as a large β (low temperature) expansion while the RHS can be viewed as a small β (high temperature) expansion. Using this language, we find the following remarkable relation between the partition function at high and low temperatures:

$$Z(\pi^2/\beta) = \sqrt{\beta/\pi} Z(\beta). \tag{93}$$

Such identities also appear in the theory of the Jacobi theta functions.

6.10 Interpretation in terms of periodic orbits

The RHS of the trace formula (89)

$$Z(\beta) = \operatorname{tr} e^{-\beta H} = \frac{2\pi}{\sqrt{4\pi\beta}} \sum_{n=-\infty}^{\infty} e^{-\pi^2 n^2/\beta} \tag{94}$$

may be interpreted in terms of classical quantities associated to a free particle on a circle.

• The prefactor 2π in the numerator may be regarded as the volume of the classical configuration space: in the case at hand it is the unit circle with circumference 2π

• The sum may be viewed as a sum over classical periodic trajectories. The trace on the LHS implies a sum over a basis of quantum states where the initial and final states are the same. The classical analogue of this is a sum over periodic classical orbits. There is one primitive periodic orbit, say the one where the free particle goes round the circle once counter clockwise. This primitive orbit may be retraced n times for any integer n leading to a closed classical trajectory that winds n times around the circle. Negative n corresponds to orbits that wind clockwise. Since $\beta = it/\hbar$ is fixed, we will suppose that the time duration of these trajectories is fixed ($t = T$), so that the angular frequency of the orbit that winds n times is $\omega_n = 2\pi n/T$. Orbits with larger $|n|$ have larger energy.

• The quantity in the exponent may be interpreted in terms of the classical action. In fact, the classical action of an orbit that winds n times in a time T is

$$S_n = \int_0^T \frac{1}{2} m r^2 \dot{\theta}^2 dt = \frac{1}{2} m r^2 \omega_n^2 T = \frac{2mr^2\pi^2 n^2}{T}. \tag{95}$$

Putting $T = -i\hbar\beta$, we get

$$\frac{iS_n}{\hbar} = -\frac{2mr^2\pi^2 n^2}{\hbar^2 \beta} = -\frac{\pi^2 n^2}{\beta}, \tag{96}$$

where in the last step we have specialized to units where $r = 1$ and $\hbar^2/2m = 1$ as before. Thus, the summand on the RHS of (94) may be interpreted as $e^{iS_n/\hbar}$, the familiar probability amplitude/weight assigned to a classical trajectory in the path integral approach to quantum mechanics.

• The prefactor $1/\sqrt{4\pi\beta} = e^{-\frac{1}{2}\log 4\pi\beta}$ in (94) may be viewed as a subleading correction for small β. It is familiar from the first subleading correction to the wavefuction we found in the semiclassical expansion (48). Thus, we may write:

$$Z(\beta) = \text{Vol(configuration space)} \sum_{\substack{\text{periodic orbit} \\ \text{winding } n \text{ times}}} e^{iS_n/\hbar - \frac{1}{2}\log(4\pi\beta)}. \qquad (97)$$

As noted, we consider here periodic orbits that wind n times around the circle in a fixed time T and then replace T by $-i\hbar\beta$.

• We have thus interpreted the partition function (or trace of the heat kernel or time evolution operator) for a free particle moving on a circle as a sum over classical periodic orbits. In this case, the partition sum could be evaluated exactly both in the energy and position bases. For more general systems, we are usually unable to evaluate the partition sum exactly. However, an analogue of the sum over periodic orbits may still provide an approximate formula for the quantum mechanical trace. An important example of such a formula is the semiclassical trace formula for the density of states developed by M C Gutzwiller in the 1970s.