Problems Chapter 12

[Quantum Mechanics](#)
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problemSolenoid

Problem 1

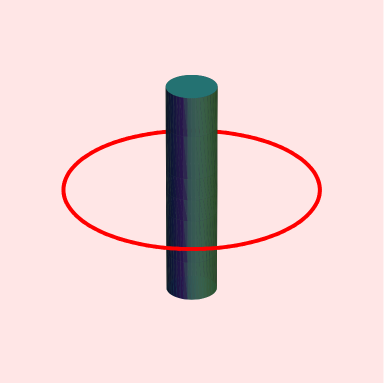
A charged particle is constrained to move along a circle of radius R, in x y plane. The circle encloses a perfectly isolated cylindrical solenoid with axis along z, radius a < R, and carrying a magnetic flux F.

1. *Find the energy eigenstates.*
2. *Describe the time evolution for the flux varying with time.*

Solution

Static field

The kinematic is shown here:



Let φ be the azimuth angle along the circle. Without external fields the Hamiltonian is

$$H = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{1}{R}\frac{\partial}{\partial\varphi}\right)^2 \tag{1.1}$$

A magnetic flux F implies a non zero vector electromagnetic potential, which can be assumed directed along the circle, A_φ. The invariance for rotations around z axis implies that A_φ is independent from φ and finally Maxwell equations give, integrating along the circle:

$$\oint A_\varphi R\, d\varphi = F, \quad \Rightarrow A_\varphi = \frac{F}{2\pi R}.$$

The coupling with electromagnetic field comes from the substitution $\mathbf{p} \to \mathbf{p} - e\,\mathbf{A}/c$, in our case

$$\frac{\hbar}{i}\frac{1}{R}\frac{\partial}{\partial\varphi} \to \frac{\hbar}{i}\frac{1}{R}\frac{\partial}{\partial\varphi} - \frac{e}{c}\frac{F}{2\pi R}.$$

Introducing the parameter

alphaparameterring

$$\alpha = \frac{eF}{2\pi\hbar c}, \tag{1.2}$$

the Hamiltonian can be written as

$$H = \frac{\hbar^2}{2mR^2}\left(\frac{1}{i}\frac{\partial}{\partial\varphi} - \alpha\right)^2. \tag{1.3}$$

If we ***require*** one-valued functions on the circle the normalized eigenfunctions and the corresponding eigenvalues are statesRing1

$$\psi_n[\varphi] = \frac{1}{\sqrt{2\pi R}} \mathrm{Exp}[i\, n\, \varphi]; \qquad E_n = \frac{\hbar^2}{2\, m\, R^2} (n - \alpha)^2; \qquad \int_0^{2\pi} \psi_k^* \psi_n R\, d\varphi = \delta_{kn}. \tag{1.4}$$

The normalization and the measure have been chosen in such a way that $|\psi|^2$ has the dimension of a probability per unit length. Let us note that for α = k+1/2 with k$\in\mathbb{Z}$, the ground state is degenerate, both states k and k+1 have the same energy. The meaning of systems with different α will be discussed in the next section.

We note that outside the solenoid there is no magnetic field, but energy spectrum, which is surely observable, has changed with respect to the free particle case.

Other interesting quantities are the charge density $\rho = e\, |\psi|^2$ and the density current $\mathbf{j} = \rho\, \mathbf{v}$. In presence of an electromagnetic field $\mathbf{v}$ = 1/m ($\mathbf{p}$ - e $\mathbf{A}$/c) and we have

$$\rho = e\,|\psi|^2; \quad \mathbf{j} = i\, e \frac{\hbar}{2\, m} ((\nabla \psi^*)\, \psi - \psi^* \nabla \psi) - \frac{e^2}{m\, c} \mathbf{A}\, |\psi|^2$$

In our case the current has only a tangential component j and:

$$\rho = e\,|\psi|^2; \quad j = i\, e \frac{\hbar}{2\, m\, R} \left(\frac{\partial \psi^*}{\partial \varphi} \psi - \psi^* \frac{\partial \psi}{\partial \varphi} \right) - \frac{e^2}{m\, c} A_\varphi\, |\psi|^2. \tag{1.5}$$

It is easy to verify that the current conservation equation holds:

$$\frac{\partial \rho}{\partial t} + \frac{1}{R} \frac{\partial j}{\partial \varphi} = 0 \tag{1.6}$$

In particular for stationary states (4)

ringcurrent

$$j_n = \left(\frac{e\, \hbar}{m\, R} n - \frac{e^2}{m\, c} A_\varphi \right) |\psi_n|^2 = \frac{1}{2\pi} \frac{e\, \hbar}{m\, R^2} (n - \alpha). \tag{1.7}$$

Let us note that for $\alpha \notin \mathbb{Z}$ the ground state has a non zero mean current.

■ Gauge invariance

Formally the vector field is a gauge transformation,

$$A_\varphi = \frac{F}{2\pi R} \frac{\partial}{\partial \varphi} \varphi; \qquad \mathbf{A} = \frac{F}{2\pi} \nabla \varphi.$$

We have stressed that this is not true as $\Lambda = \varphi$ is not a single valued function.

The situation is nevertheless more subtle than that. In the text has been pointed out that the real significance of vector field is to allow a parallel transport of the phase of the wave function, i.e. to construct phase factor of the form

$$U[A, B] = \mathrm{Exp}\left[i \frac{e}{\hbar\, c} \int_A^B A_\mu\, dx^\mu \right] \tag{1.8}$$

The physical non trivial effects come from close integrals, which locally, via Stokes theorem, are related to electromagnetic fields: taking a small contour, boundary of a space-time small surface $\sigma^{\mu\nu}$

$$\oint A_\mu\, dx^\mu \simeq F_{\mu\nu}\, \sigma^{\mu\nu}$$

Globally, as in the present case, the closed integral can be non trivial and produce physical effects even if the particle never "see" a field, in our case the particle is always outside the solenoid. **The crucial point** is that these closed integrals always appears as exponential (phase factors) and the physical effects are measured by

$$\mathrm{Exp}\left[i \frac{e}{\hbar\, c} \oint A_\mu\, dx^\mu \right]$$

In our case then the point is **not** the single valuedness of Λ but that of

$$\mathrm{Exp}\left[i \frac{e}{\hbar\, c} \oint \partial_\mu \Lambda\, dx^\mu \right] = \mathrm{Exp}\left[i \frac{e\, F}{2\pi\hbar\, c} \oint d\varphi \right] = \mathrm{Exp}[i\, 2\pi\alpha] \tag{1.9}$$

This phase is indeed trivial if α is integer, *then only fractional part of α must be physically observable*.

This is indeed the case and can be seen in two different ways.

Method 1

Consider the two Hamiltoniana for α differing by 1

$$H = \frac{\hbar^2}{2\,m\,R^2}\left(\frac{1}{i}\frac{\partial}{\partial\varphi} - \alpha\right)^2 ; \quad H' = \frac{\hbar^2}{2\,m\,R^2}\left(\frac{1}{i}\frac{\partial}{\partial\varphi} - (\alpha + 1)\right)^2 .$$

The transformation

$$\psi \to \mathrm{Exp}[i\,\varphi]\,\psi \equiv U\psi .$$

Is a unitary transformation from the space of periodic functions into itself. It is trivial to verify that indeed all scalar products are preserved. For operators

$$\left(\frac{1}{i}\frac{\partial}{\partial\varphi} - \alpha\right) \to U\left(\frac{1}{i}\frac{\partial}{\partial\varphi} - \alpha\right)U^{-1} = e^{i\varphi}\left(\frac{1}{i}\frac{\partial}{\partial\varphi} - \alpha\right)e^{-i\varphi} = \left(\frac{1}{i}\frac{\partial}{\partial\varphi} - \alpha - 1\right).$$

For the Hamiltonian follows:

$$U\,H\,U^{-1} = H' .$$

Then systems with α differing by 1 (and hence by an arbitrary integer by induction) are unitary equivalent, i,e, it is always the same system seen with different coordinates.

Method 2

Here we put our attention on physical observables. Consider two different experiment, on with α and another one with $\alpha' = \alpha+1$. Given a state described by ψ in the first experiment there exist a state $\psi' = \mathrm{Exp}[i\,\varphi]\psi$ in the second experiment which satisfy the same equation as ψ (this is in fact what gauge invariance means).

For ψ and ψ' we have

$$i\,\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2\,m\,R^2}\left(\frac{1}{i}\frac{\partial}{\partial\varphi} - \alpha\right)^2\psi; \qquad i\,\hbar\frac{\partial\psi'}{\partial t} = \frac{\hbar^2}{2\,m\,R^2}\left(\frac{1}{i}\frac{\partial}{\partial\varphi} - (\alpha + 1)\right)^2\psi';$$

If we put $\psi' = \mathrm{Exp}[i\,\varphi]\,\psi$ the second equation transforms in the first one. Note that the transformation is well defined,i.e. single valued.

Now consider a matrix element of an arbitrary operator. If the operator does not contain derivatives trivially the phase cancel between initial and final state. If it contains derivatives, gauge invariance imposes that the only observables quantities are those which depend on the combination p - e A/c, i.e. the mechanical velocity of the particle, and we have to compute, for the new experiment (it is enough to consider mean values on arbitrary functions):

$$\int d\varphi\ \psi^*\, e^{-i\varphi}\, F\left[\frac{1}{i}\frac{\partial}{\partial\varphi} - (\alpha + 1)\right] e^{i\varphi}\,\psi = \int d\varphi\ \psi^*\ F\left[\frac{1}{i}\frac{\partial}{\partial\varphi} - \alpha\right]\psi \tag{1.10}$$

Then the second experiment *measures exactly the same things* as the first one, eventually changing the name to the states.

The simplest example is the current (7). The second experiment would measure in his n-th state with energy C $(n - \alpha - 1)^2$ a current $j_n \propto$ (n-α-1).

The same result with same energy and current would be interpreted in the first experiment as a measure on the state n-1, it is just a question of labels for states!

The argument sketched above roots on the deep paper of Wu and Yang [*]. This somewhat simplified version is inspired to a similar simplification due to Berry et al. [*].

Time dependent magnetic flux

Let us consider now a time dependent magnetic flux, i.e. $\alpha = \alpha(t)$. A general approach to study time evolution in the presence of a time dependent field is to expand $\psi(t)$ in eigenfunctions parameter dependent (i.e. defined for each value of the parameter)

Ringadiabaticexpansion1

$$\Psi(\varphi, t) = \sum_n b_n(t)\,\psi_n[\varphi;\alpha]\,\mathrm{Exp}\left[-\frac{i}{\hbar}\int_0^t E_n[\alpha]\,dt\right] \tag{1.11}$$

The time dependence is both explicit and implicit, through α. The explicit energy dependent phase is usually called dynamic phase and it is the only surviving in adiabatic changes (usually). A possible additional phase generated in cyclic transformations by coefficient b_n would be the Berry phase of the system. The coefficient b_n satisfy a differential equation obtained substituting (11) in time dependent Schrödinger equation.

Our present problem is simple in that adiabatic states already contain the whole time dependence. In fact, the functions (4) *do not depend* on α, then

$$i\,\hbar\frac{\partial}{\partial t}\left(\psi_n[\varphi]\,\mathrm{Exp}\left[-\frac{i}{\hbar}\int_0^t E_n[\alpha]\,dt\right]\right) = E_n[\alpha(t)]\,\psi_n[\varphi]\,\mathrm{Exp}\left[-\frac{i}{\hbar}\int_0^t E_n[\alpha]\,dt\right],$$

and by construction for each α:

$$H[\alpha]\,\psi_n[\varphi]\,\mathrm{Exp}\left[-\frac{i}{\hbar}\int_0^t E_n[\alpha]\,dt\right] = E_n[\alpha(t)]\,\psi_n[\varphi]\,\mathrm{Exp}\left[-\frac{i}{\hbar}\int_0^t E_n[\alpha]\,dt\right].$$

This means that combinations with b_n constant satisfy Schrödinger equation, i.e. the evolution is always adiabatic, independently on the way magnetic flux varies.

Let us now compute the variation of mean energy for the would be stationary states (with α constant).

$$\frac{dE_n}{dt} = -\frac{\hbar^2}{2\,m\,R^2}(n-\alpha)\frac{d\alpha}{dt} = -\frac{2\,\pi\,\hbar}{e}\,j_n\frac{d\alpha}{dt} = -\frac{1}{c}\,j_n\frac{dF}{dt}.$$

Equations (2) and (7) have been used. The current is constant, but confined to the ring. Expressing the flux as an integral trough a disk having the circle as boundary

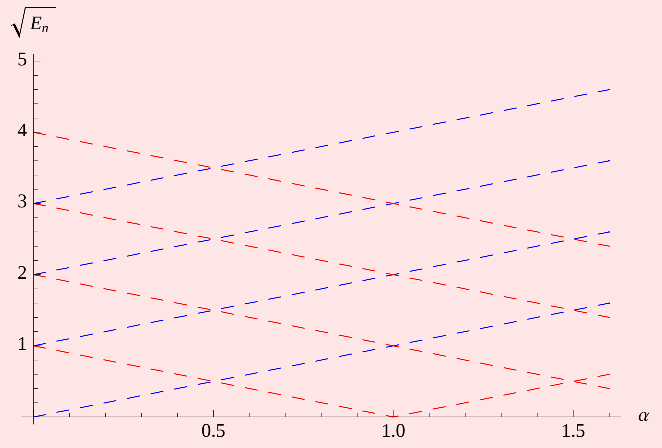
$$\frac{dE_n}{dt} = -\frac{1}{c}\int_{Disk} j_n\frac{\partial B}{\partial t}\,dS.$$

Using Maxwell equation rot E = - 1/c ∂ **B**/∂t and Stokes theorem to transform the integral in a line integral along the ring:

$$\frac{dE_n}{dt} = \oint j_n\,\mathcal{E}\,ds.$$

We see that the variation of mean energy is due to work performed by the electric field induced by magnetic flux variation.

Varying α the spectrum changes and we can obtain dynamically an "adiabatic flow". Energies are proportional to $(n-\alpha)^2$then a level degenerate for α=0 splits as α increases, its energy lower if n > 0 while rises if n < 0. the two fluxes crosses at $\alpha \in \mathbb{Z}$ + 1/2. This is clearly shown in figure below:



- **A subtle point**

Suppose that we have a particle in the ground state and the magnetic field switched off, i.e. α = 0. Now we increase α and end at time T with α=1. The final system is gauge equivalent to the original one, i.e. we have performed a *cyclic transformation*, this does *not* means that nothing happened. From (11) we see that at time T the system is in the state n=0 of the α=1 system.

$$\psi_0 = \frac{1}{\sqrt{2\,\pi\,R}}; \qquad E_n = \frac{\hbar^2}{2\,m\,R^2}(1)^2;$$

This is the gauge transformed state of the *excited* state n=1 in the α=0 system, end in fact the energy, which is gauge invariant, has changed in the transformation. In the *intermediate* states α was time dependent and from Maxwell equations an electric field

$$\mathcal{E} = -\frac{1}{c}\frac{\partial}{\partial t}A_\varphi = -\frac{1}{c}\frac{\partial}{\partial t}\frac{F}{2\,\pi\,R} = -\frac{\hbar}{e}\frac{d\alpha}{dt};$$

was acting on the particle, so the intermediate stages were not simple gauge transformations. There is no reason that for cyclic transformation a state of the system remains unchanged.

WuYang
1) T.T. Wu and C.N. Yang, Phys. Rev. D 12, 3845, (1975).

Berry1
2) M.V. Berry, R.G. Chambers, M.D. Large, C. Upstill and J.C. Walmsley: Eur. J. Phys. 1, 154, (1980).

problemDefect2

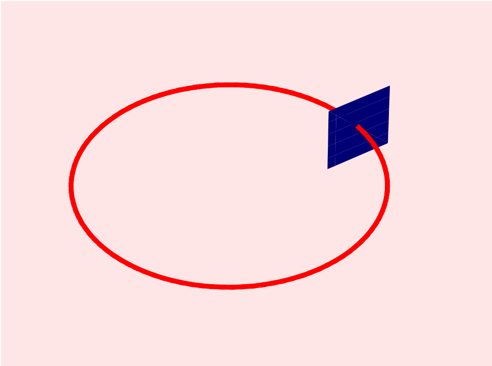
Problem 2

A particle moves on a circle of radius R. *A device on the circle adds a phase* $2\pi\,\alpha$ *when it is crossed. Study stationary state solutions and let* $\alpha = \alpha(t)$.

Solution

Static case

The kinematic is shown here :



Let φ the angle along the circle. The system can be described by:

ringDefect1

$$H = \frac{\hbar^2}{2\,m\,R^2}\left(\frac{1}{i}\,\frac{\partial}{\partial\varphi}\right)^2; \qquad \psi[2\,\pi] = e^{-i\,2\,\pi\,\alpha}\,\psi[0]. \tag{2.1}$$

The Hamiltonian is the one of a free particle but boundary conditions are different. Momentum and Hamiltonian are self-adjoint operators in the space of periodic functions up to the phase $2\pi\,\alpha$. For the momentum:

$$\langle f \mid p_\varphi \mid g\rangle = \int_0^{2\pi} f^*[\varphi]\,\frac{1}{i}\,\frac{\partial}{\partial\varphi}\,g[\varphi] = -\frac{1}{i}\int_0^{2\pi}\left(\frac{\partial}{\partial\varphi}\,f^*[\varphi]\right)g[\varphi] + \frac{1}{i}\left(f^*[2\,\pi]\,g[2\,\pi] - f^*[0]\,g[0]\right) =$$
$$-\frac{1}{i}\int_0^{2\pi}\left(\frac{\partial}{\partial\varphi}\,f^*[\varphi]\right)g[\varphi] = \left(\langle g \mid p \mid f\rangle\right)^*$$

The eigenfunctions are easy to find: they are just usual periodic eigenfunctions with an additional ($\alpha\,\varphi$) phase shifting:

defecteigenstates

$$\psi_n[\varphi] = \frac{1}{\sqrt{2\,\pi\,R}}\,\mathrm{Exp}[i\,n\,\varphi - i\,\alpha\,\varphi]; \qquad E_n = \frac{\hbar^2}{2\,m\,R^2}\,(n-\alpha)^2; \qquad \int_0^{2\pi}\psi_k^*\,\psi_n\,R\,d\varphi = \delta_{kn}. \tag{2.2}$$

The normalization and the measure have been chosen in such a way that $|\psi|^2$ has the dimension of a probability per unit length.

The reader will notice the similarity between this result and the one obtained in problem (1). Let C[α] the space of continuous periodic functions up to a phase $2\pi\alpha$. In problem (1) the set of functions was defined C[0] and the Hamiltonian was

$$H_{Sol} = \frac{\hbar^2}{2\,m\,R^2}\left(\frac{1}{i}\,\frac{\partial}{\partial\varphi} - \alpha\right)^2.$$

Let U the unitary operator from C[0] to C[α] such that

unitaryTrasfgeneral

$$U : C[0] \to C[\alpha]; \qquad \psi \to \mathrm{Exp}[-i\,\alpha\,\varphi]\,\psi. \tag{2.3}$$

We have

unitarytrasfH

$$U\left(\frac{1}{i}\,\frac{\partial}{\partial\varphi} - \alpha\right)U^{-1} = \mathrm{Exp}[-i\,\alpha\,\varphi]\left(\frac{1}{i}\,\frac{\partial}{\partial\varphi} - \alpha\right)\mathrm{Exp}[i\,\alpha\,\varphi] = \frac{1}{i}\,\frac{\partial}{\partial\varphi}; \quad U\,H_{Sol}\,U^{-1} = H. \tag{2.4}$$

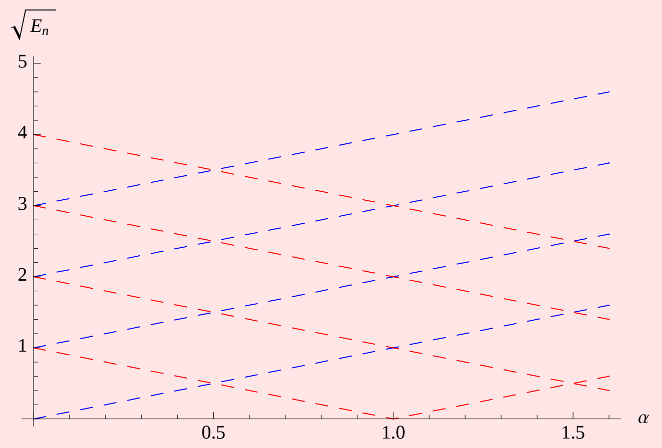
The two system are in fact connected by a unitary transformation. For completeness we notice that in (4) the derivative operator on the right hand side acts on C[α] while that on the left hand side on C[0].

Periodic systems and spectral flow

Our Hamiltonian **and** the boundary conditions (1) are explicitly periodic in α. Let us now change adiabatically α, $\alpha \to \alpha+1$. This is manifestly a cyclic transformation, we have not even to perform gauge transformations as in problem (1). The adiabatic eigenfunctions for the system are defectadiabaticSates

$$\Phi_n[\varphi, t] = \frac{1}{\sqrt{2\pi R}} \text{Exp}[i\, n\, \varphi - i\, \alpha[t]\, \varphi]\, \text{Exp}\left[-\frac{i}{\hbar}\int_0^t E_n[\alpha]\, dt\right] \tag{2.5}$$

For adiabatic transformations these states describe the evolution of the system and we see that while $\alpha \to \alpha + 1$, the eigenstate of the Hamiltonian evolve from n to n-1, apart from a trivial dynamic phase. Remember that the final system, α=1, is *identical* to the original one. Eigenvalues change, and double degenerate states present at $\alpha = 0$ split as $(n - \alpha)^2$, energy rising or lowering depending on the sign of n. We have again degeneracy when $\alpha \in \mathbb{Z} + 1/2$, or $\alpha \in \mathbb{Z}$.



This kind of behavior is characteristic of periodic systems with periodic boundary conditions.

General time evolution

Time evolution of a state wave function Ψ is described by

defectevolution1

$$i\,\hbar \frac{\partial}{\partial t}\Psi = H[\alpha]\,\Psi; \tag{2.6}$$

Remember that H depends on α through the boundary conditions. Let us consider the general expansion in terms of adiabatic states (5)

$$\Psi = \sum_n c_n[t]\; \psi_n[\varphi;\, \alpha]\; \text{Exp}\left[-\frac{i}{\hbar}\int_0^t E_n[\alpha]\, dt\right] \equiv \sum_n c_n[t]\; \psi_n[\varphi;\, \alpha]\; e^{-i\,\delta_n[t]};$$

$$H\,\psi_n[\varphi;\, \alpha] = E_n[\alpha]\; \psi_n[\varphi;\, \alpha]$$

Substituting in eq.(6) and projecting we obtain the general equation for c_n's coefficients:

defectckequation

$$\frac{d}{dt} c_k[t] = -\sum_s c_s[t]\; \text{Exp}[i\,(\delta_k[t] - \delta_s[t])]\, \left\langle k[\alpha] \left| \frac{\partial}{\partial t} \right| s[\alpha] \right\rangle \tag{2.7}$$

As in this problem the adiabatic eigenstates depend explicitly on α, the coefficients c in general vary with time and adiabatic evolution is not exact. From eq(2) it follows

defectMatrixFks

$$\left\langle k[\alpha] \left| \frac{\partial}{\partial t} \right| s[\alpha] \right\rangle \equiv F_{ks} = \frac{1}{k-s}\frac{d\alpha}{dt}(1-\delta_{ks}) + \delta_{ks}\left(-i\,\pi\frac{d\alpha}{dt}\right). \qquad \langle k \mid \varphi \mid s \rangle = \frac{i}{k-s}(1-\delta_{ks}) + \pi\,\delta_{ks} \tag{2.8}$$

As follows from general arguments, see text, the diagonal contribution in eq.(7) amount to a phase factor and adiabatic theorem asserts that this contribution is the only surviving in the adiabatic limit (the evolution follows the adiabatic state). In this limit

defectckequationadiabaticlimit

$$\frac{d}{dt} c_k[t] \simeq i\,\pi\frac{d\alpha}{dt} c_k, \quad \Rightarrow c_k[t] = \text{Exp}[i\,\pi\,\alpha]\, c_k[0]. \tag{2.9}$$

This phase cannot be reabsorbed in a redefinition of base state, we should need to put

$$\psi_n' = e^{i\,\pi\,\alpha}\frac{1}{\sqrt{2\pi R}}\text{Exp}[i\, n\,\varphi - i\,\alpha\,\varphi];$$

but this is inconsistent with the periodicity $\alpha \to \alpha+1$ of both Hamiltonian and periodic conditions.

Let us in particular consider an adiabatic cyclic evolution, i.e. $\alpha \to \alpha + 1$, in a time T. A state evolve as

$$c_n \, \mathrm{Exp}[i\, n\, \varphi - i\, \alpha\, \varphi] \to c_n \, \mathrm{Exp}[i\, n\, \varphi - i\, (\alpha + 1)\, \varphi]\, e^{-i\,\delta_n[T]}\, e^{i\,\pi} = e^{i\,\pi}\, \psi_{n-1}\, e^{-i\,\delta_n[T]}.$$

Apart from the dynamical phase and the usual spectral flow a new phase has appeared, π. This is the Berry phase for this transformation, i.e. the additional phase acquired by the system under a cyclic transformation. We see that it does not depend on the details of the transformation, only on initial and final values of the parameter α. The change in sign of ψ is reminiscent of the change in sign for spinor after a rotation of 2π.

- **N.B.**

We said above that for each α the system is unitarily equivalent to the system of problem (1). In that case the evolution was always adiabatic, why here things are different? The unitary transformation which connects the two system is S= Exp[$-i\, \alpha\, \varphi$], which is time dependent for tim varying α. Under a time dependent unitary transformation $\psi \to$ S(t) ψ we know, see text, that the Hamiltonian change as

$$H \to S\, H\, S^{-1} + i\, \hbar\, \frac{\partial S}{\partial t}\, S^{-1}$$

For the Hamiltonian H_0 of problem (1) we have

$$H_0 \to S\, H\, S^{-1} + \hbar\, \frac{d\alpha}{dt}\, \varphi$$

The first term is the Hamiltonian of this problem, the second one is new, then the two Hamiltonian do not give rise to the same time evolution. At the end of the problem the connection between the models will be used to derive in a simple way the equation of motion for operators.

Time evolution for operators

The question we want to clarify is the following: formally the Hamiltonian (1) is time independent and commutes with the momentum. On the other hand it is clear, for example via spectral flow, that momentum and energy change as α vary, how is it this compatible with the equation of motion for the operators?

To handle the problem let us consider two arbitrary states Φ[t] and Ψ[t] and compute matrix elements of momentum P, this is in fact how the evolution of this operator is defined. Using the base of states (2), denoted here with |n>, we have

$$|\Psi[t]\rangle = \sum_k a_k[t]\, |k\rangle\, ; \qquad |\Phi[t]\rangle = \sum_k b_k[t]\, |k\rangle\, .$$

In the following we put for shortness $\hbar$ = m = R = 1. It is immediate to verify that

$$\langle \Phi[t]\, |\, P\, |\Psi[t]\rangle = \sum_k b_k^*\, a_k\, (k - \alpha)\, .$$

Evolutions of coefficients a_k and b_k are obtained substituting the expansions in the Schrödinger equation (6) (no summation on repeated indexes)

$$\frac{da_k}{dt} + \sum_s F_{ks}\, a_s = -i\, E_k\, a_k\, ; \qquad \frac{db_k^*}{dt} - \sum_s F_{sk}\, b_s^* = i\, E_k\, b_k^*\, .$$

The anti-hermitian matrix (F_{ks}) is the one computed in (8), the difference with equation (7) is due to the fact that we included dynamic phase phactors in the coefficients. It follows

defectdpdt

$$\frac{d}{dt}\langle \Phi[t]\, |\, P\, |\, \Psi[t]\rangle = -\frac{d\alpha}{dt}\sum_k b_k^*\, a_k + \sum_{ks}(k - \alpha)\left(b_s^*\, F_{sk}\, a_k - F_{ks}\, b_k^*\, a_s\right). \qquad (2.10)$$

The second factor in the sum is antisymmetric in s and k so we can write the sum as

$$\frac{1}{2}\sum_{ks}((k - \alpha) - (s - \alpha))\left(b_s^*\, F_{sk}\, a_k - F_{ks}\, b_k^*\, a_s\right) = -\sum_{ks}(k - s)\, F_{ks}\, b_k^*\, a_s =$$

$$-\sum_{k\neq s}(k - s)\, F_{ks}\, b_k^*\, a_s = -\sum_{k\neq s}(k - s)\, \frac{1}{k - s}\, \frac{d\alpha}{dt}\, b_k^*\, a_s = -\frac{d\alpha}{dt}\left(\sum_{ks} b_k^*\, a_s - \sum_k b_k^*\, a_k\right);$$

The second term exactly cancels the first one in (18) and finally:

dpdtdefect1

$$\frac{d}{dt}\langle \Phi[t]\, |\, P\, |\, \Psi[t]\rangle = -\frac{d\alpha}{dt}\sum_{ks} b_k^*\, a_s = -\frac{d\alpha}{dt}\, 2\,\pi\, \Phi^*[t, \varphi = 0]\, \Psi[t, \varphi = 0]\, . \qquad (2.11)$$

We used, with basis (2), the identity:

$$\psi[0] = \sum_k a_k\, u_k[0] = \frac{1}{\sqrt{2\,\pi}}\sum_k a_k\, .$$

As an operator equation (a bit formally) dpdtdefect2

$$\frac{dP}{dt} = -\frac{d\alpha}{dt} 2\pi\,\delta\,(\varphi)\,. \tag{2.12}$$

The effect of phase variations on boundary conditions is translated as a localized force proportional to the variation rate. More correctly P has in fact an explicit time dependence on t, through α, and this is the term we have just compute. The commutation with H is obviously zero and we have

$$\frac{dP}{dt} = \frac{\partial P}{\partial t} + i\,[H,\,P] = \frac{\partial P}{\partial t} = -\frac{d\alpha}{dt} 2\pi\,\delta\,(\varphi)\,. \tag{2.13}$$

Let us consider in particular the evolution with time of expectation values of P. For long times, if we take the mean over times longer than characteristic frequencies, we expect rapid oscillating phases with zero mean , i.e.

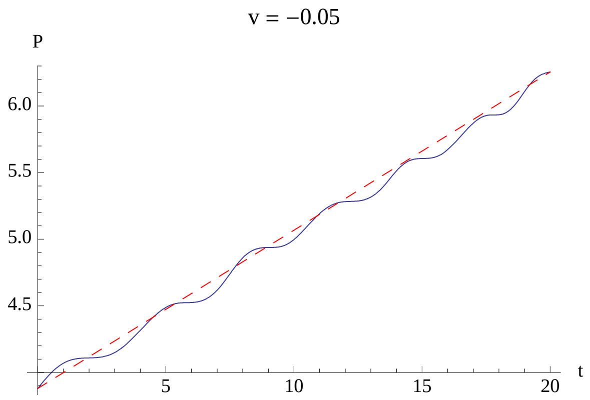
$$\overline{\sum\nolimits_{ks} a_k^* a_s} = \sum\nolimits_k a_k^* a_k = 1.$$

From (11):

$$\overline{\frac{d}{dt} < \Phi[t] \;\Big|\; P \;\Big|\; \Psi[t] >} = -\frac{d\alpha}{dt} 2\pi.$$

This is exactly the first term in (10) and would be the only one present for adiabatic evolution: we expect then that non adiabatic contributions are rapidly oscillating and typically non analytic as a function of α. This will be verified in a separate notebook devoted to the numerical analysis of this problem.

Here we give an example. The dashed line is the adiabatic (phase averaged) evolution, the wavy line represent the true evolution.



From (12) evolution of the Hamiltonian follows

$$\frac{dH}{dt} = -\frac{1}{2} 2\pi \frac{d\alpha}{dt} (\delta\,(\varphi)\,P + P\,\delta\,(\varphi))\,. \tag{2.14}$$

For the mean value on a state E[Ψ] = <Ψ|H|Ψ> we have

defectenergyvariation

$$\frac{dE[\Psi]}{dt} = -\frac{1}{2} 2\pi \frac{d\alpha}{dt} \frac{1}{i} \left(\Psi^*[0]\,\Psi'[0] - \Psi'^*[0]\,\Psi[0]\right) = -\frac{d\alpha}{dt} 2\pi\,\mathrm{Im}\left[\Psi^*[0]\,\Psi'[0]\right]. \tag{2.15}$$

This equation has a simple semiclassical interpretation. For semiclassical waves $\Psi \sim \mathrm{Exp}[i\,S]$ and $\mathrm{Im}\left[\Psi^*[\varphi]\,\Psi'[\varphi]\right] \sim i\,\partial S/\partial\varphi$. The classical momentum is given by $\partial S/\partial\varphi$ so equation (15) reads

$$\frac{dE[\Psi]}{dt} = -\frac{d\alpha}{dt} 2\pi \int \delta\,(\varphi)\,\frac{\partial S}{\partial\varphi} = < P_{cl}\,\frac{dP_{cl}}{dt} >$$

as expected (the variation of momentum, i.e. the force, has been taken from(12)).

■ Commutation relations

The last point we want to study is the following: this quite peculiar dynamics preserve commutation relations? What are the equation of motion for φ?

First of all we remember the correct form of commutation relations for compact variables is Weyl form:

weyldefect1

$$P\,W - W\,P = W; \quad W = \mathrm{Exp}[i\,\varphi]\,. \tag{2.16}$$

φ is not a good quantum variable, it is not self adjoint even in the periodic case. By inspection is evident that using base (2)

$$< \Phi[t] \mid W \mid \Psi[t] > = \sum\nolimits_{ks} b_k^* a_s \delta_{k,s+1} = \sum\nolimits_k b_{k+1}^* a_k\,.$$

Inserting a complete set of |k> for the left hand side of (16) we obtain, after a short calculation:

defectshort

$$<\Phi[t]\ |\ [P, W]\ |\Psi[t]> = \sum_{kls} b_k^* a_s\,((k-\alpha)\,\delta_{kl}\,\delta_{l,s+1} - \delta_{k,l+1}\,\delta_{ls}\,(s-\alpha)) = \sum_s b_{s+1}^* a_s. \tag{2.17}$$

The Weyl commutation relations are satisfied at all times, as it must be for a true quantum system.

The evolution equation for W are deduced as before. Using the known expressions for da_k/dt and db_k/dt we have

provvdefect1

$$\frac{d}{dt} <\Phi[t]\,\Big|\,W\,\Big|\,\Psi[t]> = \sum_{ks}\left(F_{s,k+1}\,b_s^*\,a_k - b_{k+1}^*\,F_{ks}\,a_s\right) + i\sum_k b_{k+1}^*\,a_k\,(E_{k+1} - E_k). \tag{2.18}$$

The first term vanishes, see below, the second is just the commutator with the Hamiltonian, then, using the Weyl relations, we have the equation of motion for W:

$$\frac{dW}{dt} = i\,[H, W] = \frac{i}{2}\,(W P + P W). \tag{2.19}$$

As usual these can be considered as the equation of motion in Heisenberg picture.

To show that the first term in (17) on can substitute directly the values for F_{ks} or proceed in the following way. The matrix elements of W are $W_{ks} = \delta_{k,s+1}$so the two term of the sum can be written as

$$\sum_{ks} b_s^*\,F_{s,k+1}\,a_k = \sum_{kls} b_s^*\,F_{s,m}\,\delta_{m,k+1}\,a_k = \sum_{sk} b_s^*\,(FW)_{sk}\,a_k;$$
$$\sum_{ks} b_{k+1}^*\,F_{ks}\,a_s = \sum_{kls} b_m^*\,\delta_{m,k+1}\,F_{ks}\,a_s = \sum_{mk} b_m^*\,(WF)_{mk}\,a_k$$

So in fact we have the commutator of F and W. The coefficients F_{ks} are just matrix elements of φ, which commutes with W, then the result follows.

- **Evolution from equivalence of models**

We have already stated that this model is, at each time, unitary equivalent to the model studied in problem [1]. Denoting with p and P the momentum in solenoid problem and in present problem we have shown that, see eq.(3),(4)

$$U : C[0] \to C[\alpha];\ U\psi = e^{-i\alpha\varphi}\,\psi;\quad U\,(p-\alpha)\,U^{-1} = P.$$

Consider now the time derivative of previous equation for P (always understood as matrix elements, the time dependence is in wave function of the states, as usual in Schrödinger representation). To the derivative there is a contribution coming from U

$$\frac{dP}{dt} = -i\,\frac{d\alpha}{dt}\,\varphi\,P + P\,i\,\frac{d\alpha}{dt}\,\varphi + U\left(\frac{dp}{dt} - \frac{d\alpha}{dt}\right)U^{-1} = -i\,\frac{d\alpha}{dt}[\varphi, P] - \frac{d\alpha}{dt}.$$

We used the fact that in the solenoid model p was a constant of motion. If naive commutation relaations would hold, $[\varphi,P] = i$ and P would be a constant. In fact, some care must be taken, as φ is not a well behaved operator on periodic or periodic up to a phase functions. It is essentially the same computation given above with matrices F_{ks}we repeat here for completeness.

We can use matrix elements (8) to compute carefully the commutator. Inserting a complete set of states:

$$<k\,|\,\varphi\,|\,m><m\,|\,P\,|\,s> - <k\,|\,P\,|\,m><m\,|\,\varphi\,|\,s> =$$
$$\pi\,\delta_{km} <m\,\Big|\,P\,\Big|\,s> + i\sum_{m\neq k}\frac{1}{k-m}\,\delta_{ms}\,(s-\alpha) - \pi\,\delta_{ms} <k\,\Big|\,P\,\Big|\,m> - i\sum_{m\neq s}\frac{1}{m-s}\,\delta_{km}\,(m-\alpha).$$

The terms proportional to π cancel. For the rest let us distinguish diagonal case from non diagonal case. For k=s both summation are void, so the term vanish, for k≠s the Kronecker δ canbe satisfied, because for example in the first sum if m=s, surely it will different from k. Then for off diagonal terms

$$i\,\frac{s-\alpha}{k-s} - i\,\frac{k-\alpha}{k-s} = -i$$

For a generic matrix element

$$\sum_{ks} a_k^*\,b_s <k\,\Big|\,[\varphi, P]\,\Big|\,s> = -i\sum_{k\neq s} a_k^*\,b_s = -i\sum_{ks} a_k^*\,b_s + i\sum_k a_k^*\,b_k.$$

Last term is simply the matrix element of identity operator. For a wave function with coefficient a_k in the expansion with basis (2)

$$\psi[0] = \sum_k a_k\,u_k[0] = \frac{1}{\sqrt{2\pi}}\sum_k a_k\,,\quad \int_0^{2\pi} d\varphi\,A^*[\varphi]\,B[\varphi]\,\delta(\varphi) = \frac{1}{2\pi}\sum_{ks} a_k^*\,b_s,$$

and finally we obtain the result

commutatotphiP

$$[\varphi, P] = i - i\,2\,\pi\,\delta(\varphi) \tag{2.20}$$

and for the evolution equation for P

$$\frac{dP}{dt} = -\frac{d\alpha}{dt}\, 2\pi\,\delta\,(\varphi)$$

which reproduces result (12).

problemWell1

Problem 3

A free particle moves in a box, $[x_L, x_R]$. *The boundary conditions are* $\psi[x_L] = \psi[x_R] = 0$. *The boundaries can move.*

1. Make a change of variables which brings the problem to a fixed boundary value problem.
2. Study as a particular case a rigid motion and explore the connection to Galilei transformations
3. Show that for an accelerate rigid motion the solution is unitarily equivalent to a motion in a gravitational field (Equivalence Principle).
4. For $x_L = 0$ fixed, reformulate the change of variables as a unitary scale transformation.

Solution

A change of variables

Schrödinger equation with mouving boundaries in one dimension can be easily transformed in an equation with fixed boundaries using a trasformation of variables. Consider a particle in a well with left and right boundaries $x_L[t]$ and $x_R[t]$, mouving with velocities v_L and v_R. $L = x_R - x_L$ is the instataneous with of the well. The change of variables

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$$(t, x) \to (\tau, \xi)\,; \quad x = x_L + \xi L\,; \quad t = \tau;\quad 0 \le \xi \le 1. \tag{3.1}$$

is what we need. In the new variable ξ the boundaries are fixed. First of all from the inverse of (1)

$$\xi = \frac{1}{L}(x - x_L)\,; \quad \tau = t; \tag{3.2}$$

follow

welltrasfcoord

$$\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi} + \frac{\partial \tau}{\partial x}\frac{\partial}{\partial \tau} = \frac{1}{L}\frac{\partial}{\partial \xi};$$

$$\begin{aligned}\frac{\partial}{\partial t} &= \frac{\partial \tau}{\partial t}\frac{\partial}{\partial \tau} + \frac{\partial \xi}{\partial t}\frac{\partial}{\partial \xi} = \frac{\partial}{\partial \tau} + \left(-\frac{\dot{L}}{L^2}(x - x_L) - \frac{v_L}{L}\right)\frac{\partial}{\partial \xi} = \\ &= \frac{\partial}{\partial \tau} - \left(\frac{\dot{L}}{L}\xi + \frac{v_L}{L}\right)\frac{\partial}{\partial \xi}\,.\end{aligned} \tag{3.3}$$

From now on, having explicitely exposed the role of time variable, we call again t the time.

Before to write down the Schrödinger equation we have to consider the normalization: the Jacobian for the transformation $\xi \to x$ is time dependent. If we have a solution $\psi[t, \xi]$ normalized in the transformed interval the solution in the original variables is

welltrasfpsipsi

$$\Psi[t, x] = \frac{1}{\sqrt{L}}\,\psi[t, \xi[t, x]]\,. \tag{3.4}$$

We have added a prefactor (time dependent) at the obvious change of variables. In a sense this is a definition of ψ but is useful because in this way we assure the correct normalization for each time if ψ is normalized:

$$\int_{-L}^{L} dx\, |\Psi[t, x]|^2 = \int_{-1}^{1} L\, d\xi\, \frac{1}{L}\, |\psi[t, \xi]|^2 = 1.$$

There is also a group - theoretic reason for the prefactor, as we shall see later.

The Schrödinger equation for Ψ is

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi\,; \qquad \Psi[x_L] = \Psi[x_R] = 0.$$

Inserting the definition (4) and using (3) we have welleqforpsitrasf

$$i\hbar\left(\frac{\partial\psi}{\partial t}-\left(\frac{\dot L}{L}\xi+\frac{v_L}{L}\right)\frac{\partial\psi}{\partial\xi}-\frac{1}{2}\frac{\dot L}{L}\psi\right)=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial\xi^2}. \tag{3.5}$$

The effect of the prefactor has been the non derivative term. The reader can recast (5) in a more usual shape:

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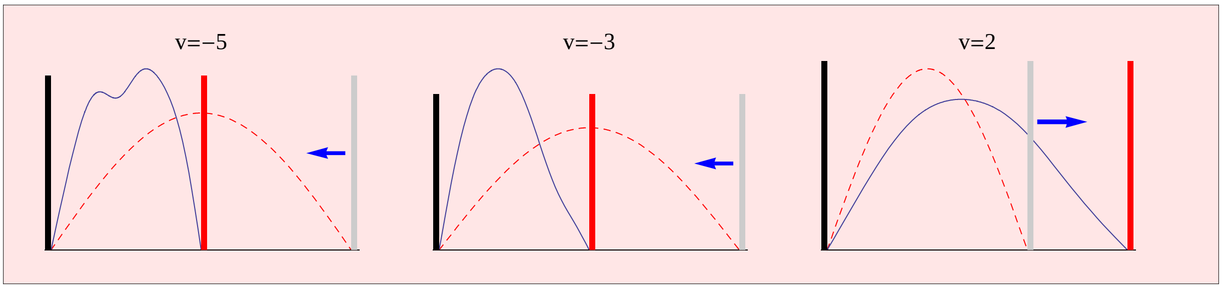
$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2mL^2}\frac{\partial^2\psi}{\partial\xi^2}+i\hbar\left(\left(\frac{\dot L}{L}\xi+\frac{v_L}{L}\right)\frac{\partial\psi}{\partial\xi}+\frac{1}{2}\frac{\dot L}{L}\psi\right). \tag{3.6}$$

The operator in the r.h.s. of (6) is a kind of effective Hamiltonian, and bare some similarity with a coupling to a vector field in more dimensions.

Here we give an example of time evolution computed using equation (6). Dashed line is the initial state.



A warning on notations for derivatives!

In this and in the following problem we will use frequently two space variables, x and ξ. The respective wave functions Ψ[x] and $\psi[\xi]$ are different but related via eq.(4). When we take derivation we have to specify the variable with respect to which variable. With the notation f$'$ one denotes, correctly, the differentiation with respect the argument, not a generic partial derivative. So we have:

$$\frac{\partial}{\partial x}\Psi\equiv\psi';\quad \frac{\partial}{\partial\xi}\psi\equiv\psi'[\xi].$$

Galilei transformations

The general transformation (1) is a combination of two simpler transformations: a time dependent translation and a scale transformation. In the translation L remains constant while in the scale transformation x_L is held fixed at 0 and x/L = ξ. For the particular case of v_L constant the first case is a Galilei transformation so let us begin from this simple case.

Galilei transformation

From the general theory we know that known the wave function φ in a mouving frame with velocity V the wave function in the rest frame is given by

wellGalilei1

$$\Psi[t,x]=\varphi[t,\ \xi[t,x]]\ \mathrm{Exp}[i\,m\,V\,\xi/\hbar]\ \mathrm{Exp}\left[\frac{i}{2}m\,V^2\,t/\hbar\right] \tag{3.7}$$

Here L is fixed and do not play any role, so we can put L =1 to avoid trivial rescaling. φ is not the same as ψ: the Hamiltonian for the mouving observer would be always a free Hamiltonian, not the complicated effective Hamiltonian appearing in (6):

wellgalilei2operator

$$i\hbar\frac{\partial\varphi}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial\xi^2}=0. \tag{3.8}$$

In fact ψ is the whole r.h.s. of (7), as can be verified by applying the operation (8) to the r.h.s.:

$$\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2}\right)\left(\varphi\, e^{i\,m\,V\,\xi/\hbar}\,e^{i\,m\,V^2\,t/(2\hbar)}\right)=$$

$$e^{i\,m\,V\,\xi/\hbar}\,e^{i\,m\,V^2\,t/(2\hbar)}\left(\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2}\right)\varphi+2\frac{\hbar^2}{2m}\frac{\partial\varphi}{\partial\xi}\,i\,m\frac{V}{\hbar}-\frac{\hbar^2}{2m}\left(\frac{m\,V}{\hbar}\right)^2\varphi-m\frac{V^2}{2}\varphi\right)=$$

The first termis zero due to Schrödinger equation for φ, for the second we can write

$$e^{i\,m\,V\,\xi/\hbar}\,e^{i\,m\,V^2\,t/(2\hbar)}\left(i\hbar V\frac{\partial\varphi}{\partial\xi}-m\,V^2\,\varphi\right)=i\hbar V\frac{\partial}{\partial\xi}\left(\varphi\, e^{i\,m\,V\,\xi/\hbar}\,e^{i\,m\,V^2\,t/(2\hbar)}\right).$$

Finally we have shown that if φ satisfy the usual Schrödinger equation then the r.h.s. of (7) satisfy

$$\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2}\right)\left(\varphi\, e^{i m V \xi/\hbar}\, e^{i m V^2 t/(2\hbar)}\right) = i\hbar V\frac{\partial}{\partial\xi}\left(\varphi\, e^{i m V \xi/\hbar}\, e^{i m V^2 t/(2\hbar)}\right),$$

which is exactly the equation (6) for ψ in the case dL/dt = 0, v_L= V.

Let us stress a point which can be overlooked at a first reading. *Every* change of coordinates is a unitary transformation, then do not change the physics. Expression (7) is a trivial unitary transformation (a change of phase) but its meaning his much more important because φ satisfy the same Schrödinger equation than Ψ, i.e. Galilei transformation are an invariance of the physics.

■ **Equivalence Principle**

As trivial as can appears equation (6) reserves some surprises. It is well knownthan in Classical Physics the Equivalence Principle say that we can locally get rid of a gravitational field passing to an acceleated frame. In non relativistic mechanics this amount to say that gravitational and inertial mass are the same, in this way form the Newton equations in a constant grvitational field g:

wellNewton

$$m_I\, a \equiv m_I\frac{dv}{dt} = m_g\, g \tag{3.9}$$

g can be eliminated passing to an accelerated observer with acceleration A. In the transformation a → a + A and if we choose A = g and if $m_I = m_g$, g disappears from the equation. Clearly we can always choose an appropriate A for any ratio $m_I / m_g$for one body (this is just a change of units for inertial mass an gravitational mass), the Equivalence Principle say that the ratio m_I / m_g is constant for every body, let us say 1 in usual unities, and g effectively disappears with a change of reference frame.

In Quantum Mechanics at first sight things seem different: Schrödinger equation is based on a Hamiltonian formulation (i.e. with momenta) not on a Lagrangian formulation like (9), the mass is in the denominator of kinetic term and is not clear how it is related to a gravitational term of the form U[x] = - m g x.

Let us attack the question form another point of view. Given a Hamiltonian in an inertial reference frame

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U[x] \tag{3.10}$$

we can always perform a (translational) change of frame using (1) with L =1. x_L represent the arbitrary movement of the new frame. Now we can ask for which kind of potential the wave function in the new frame is related to the original wave function by a phase transformation similar to (7)

wellGalilei2

$$\Psi[t, x] = \varphi[t, \xi[t, x]]\, \mathrm{Exp}[i S/\hbar] \tag{3.11}$$

and φ satisfies a usual Schrödinger equation, i.e. without derivative terms. We know in advance that once x has been expressedin terms of ξ, we obtain ψ[t,ξ] which satisfies (the generalization of) (5)

welleqfgeneraltrasf

$$i\hbar\left(\frac{\partial\psi}{\partial t} - V\frac{\partial\psi}{\partial\xi}\right) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial\xi^2} + U[x[\xi]]\,\psi. \tag{3.12}$$

V is the velocity of the frame. We look for solution of the form

changepsiphi1

$$\psi[t, \xi] = \varphi[t, \xi[t, x]]\, \mathrm{Exp}[i S/\hbar] \tag{3.13}$$

with S **independent** of φ, in this case we have a real phase transformation instead of a pure change of variables. The derivatives of ψ are

$$\frac{\partial\psi}{\partial t} = \left(\frac{\partial\varphi}{\partial t} + \frac{i}{\hbar}\frac{\partial S}{\partial t}\varphi\right)\mathrm{Exp}[i S/\hbar];$$

$$\frac{\partial\psi}{\partial\xi} = \left(\frac{\partial\varphi}{\partial\xi} + \frac{i}{\hbar}\frac{\partial S}{\partial\xi}\varphi\right)\mathrm{Exp}[i S/\hbar];$$

$$\frac{\partial^2\psi}{\partial\xi^2} = \left(\frac{\partial^2\varphi}{\partial\xi^2} + 2\frac{i}{\hbar}\frac{\partial S}{\partial\xi}\frac{\partial\varphi}{\partial\xi} + \frac{i}{\hbar}\frac{\partial^2 S}{\partial\xi^2}\varphi - \frac{1}{\hbar^2}\left(\frac{\partial S}{\partial\xi}\right)^2\varphi\right)\mathrm{Exp}[i S/\hbar].$$

Substitution in (12) give

welleqforphi

$$\left(i\hbar\frac{\partial\varphi}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial\xi^2}\right) = \\ -\frac{\hbar^2}{2m}\left(2\frac{i}{\hbar}\frac{\partial S}{\partial\xi}\frac{\partial\varphi}{\partial\xi} + \frac{i}{\hbar}\frac{\partial^2 S}{\partial\xi^2}\varphi - \frac{1}{\hbar^2}\left(\frac{\partial S}{\partial\xi}\right)^2\varphi\right) + i\hbar V\left(\frac{\partial\varphi}{\partial\xi} + \frac{i}{\hbar}\frac{\partial S}{\partial\xi}\varphi\right) + U\varphi + \frac{\partial S}{\partial t}\varphi. \tag{3.14}$$

The r.h.s. must be a potential term so first derivatives of φ must cancel, this poses the constraint

$$\frac{\partial S}{\partial \xi} = m V. \tag{3.15}$$

As V is a function of t only this impies that S must be *linear* in ξ, and this is what we need to cancel the imaginary term proprotional to the second derivative od S in the r.h.s. of (14). The general solution for S is then of the form

$$S = m V \xi + f[t]. \tag{3.16}$$

Substituting in the r.h.s. of (14) we have an effective potential of the form

wellUeff

$$U_{eff} = U[x[\xi]] + \frac{\partial S}{\partial t} + \frac{1}{2 m}\left(\frac{\partial S}{\partial \xi}\right)^2 - V \frac{\partial S}{\partial \xi} = U[x[\xi]] + m \frac{dV}{dt} \xi + \frac{df}{dt} - \frac{1}{2} m V^2 \tag{3.17}$$

This equation must be satisfied for any ξ and any t. In our notation $x = x_L[t] + \xi$ so we have only two possibilities

1. dv/dt = 0. Then U must be constant, let say zero, and we recover the Galilei invariance, v is any constant.
2. U **must** be linear in ξ, and as a consequence in x and we have that dv/dt is fixed. Writing for obvious reasons U = - m_g g x the r.h.s. of (17) becomes

$$- m_g g (x_L + \xi) + m \frac{dv}{dt} \xi + \frac{df}{dt} - \frac{1}{2} m V^2 \Rightarrow m \frac{dV}{dt} = m_g g.$$

For m = m we have: $V = g t + v_0$. We can neglect v , it can be reabsorbed by a Galilei transformation, and we have

$$V = g t; \quad x_L = \frac{1}{2} g t^2.$$

U_{eff} can then be taken zero by a choice of f:

$$0 = \frac{df}{dt} - \frac{1}{2} m V^2 - m g x_L ;$$

i.e.

$$f[t] = \int_0^t \left(\frac{1}{2} m V^2 + m g \frac{1}{2} g t^2\right) dt = \frac{1}{3} m g^2 t^3.$$

This is exactly the translation of Equivalence Principle: with m = m_g a particle which in a inertial frame is in a (constant) gravitational field g and satisfies a Schrödinger equation

$$i \hbar \frac{\partial \Psi}{\partial t} = \frac{\hbar^2}{2 m} \frac{\partial^2 \Psi}{\partial x^2} - m g x \Psi$$

is *unitarily equivalent* to a **free** particle solution φ[t,ξ] in an accelerated frame

$$x = \frac{1}{2} g t^2 + \xi;$$

$$\psi[t, x] = \varphi[t, \xi] \operatorname{Exp}\left[\frac{i}{\hbar}\left(m g t \xi + \frac{1}{3} m g^2 t^3\right)\right]; \tag{3.18}$$

■ General rigid motion

The arguments of previous section can be reversed to answer the following question: consider a sistem in arbitrary motion (L fixed), i.e. x_L[t] is the time dependent position of "reference frame", how looks physics of a "free" particle in that system?

We have already all the bits of information to solve the problem. In a fixed ("laboratory frame") the evolution is given by a free Hamiltonian with mouving boundary conditions. By the change of variables (1) which here can be simpified in

welltrasfvar2

$$(t, x) \to (\tau, \xi) ; \quad x = x_L + \xi ; \quad t = \tau; \quad 0 \le \xi \le L. \tag{3.19}$$

we transform the model in a "usual" fixed boundary problem and, more importantly, we pass to physical coordinates ξ which describe the motion in a reference system comouving with the well: an observer attached to the box canonly use these kind dof coordinate. In this discussion L plays no role and everithing we say is valid also for more realistic infinite systems.

Schrödinger equation in this system take the form (6) which here simplify (without L factors) in welltrasfvar3

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial\xi^2}+i\hbar V\frac{\partial\psi}{\partial\xi}. \tag{3.20}$$

Capital V, as before, denote the frame velocity. At variance with (6) ξ has dimension of a length and, if needed the Ψ function in laboratory frame is (4) without any prefactor. What we earned from previuous section is that we can get rid of the derivative term with a unitary phase transformation, i.e. a change of variable for ψ (13):

changepsiphi2

$$\psi[t,\xi]=\varphi[t,\xi]\,e^{iS/\hbar};\quad S=mV\xi+f[t]; \tag{3.21}$$

f[t] is arbitrary and we can conveniently choose (see eq.(17))

$$f[t]=\int_0^t dt\,\frac{1}{2}mV^2$$

with this choice the equation for φ becomes

equationforphi1

$$i\hbar\frac{\partial\varphi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial\xi^2}+m\frac{dV}{dt}\xi\varphi \tag{3.22}$$

The reader can verify (22) by direct substitution of (21) in (20). This is a quite interesting result by itself: every motion of the reference frame appears in the form of a linear potential dipenending from the acceleration of the frame. This is from one side in agreement with what we have seen on the equivalence principle, on the other side it is intereting as only the acceleration matters, not for example the third derivative of the position etc.

Relation (22) can be generalized in several ways.

- Motions in d = 2 and d = 3

The generalization is quite trivial, it is just necessary to write vectors :

changepsiphi3

$$\psi[t,\boldsymbol{\xi}]=\varphi[t,\boldsymbol{\xi}]\,e^{iS/\hbar};\quad S=m\mathbf{V}\cdot\boldsymbol{\xi}+f[t]; \tag{3.23}$$

$$f[t]=\int_0^t dt\,\frac{1}{2}m\mathbf{V}^2$$

The equation in the comouving frame becomes

equationforphi3

$$i\hbar\frac{\partial\varphi}{\partial t}=-\frac{\hbar^2}{2m}\nabla_\xi^{\,2}\varphi+m\frac{d\mathbf{V}}{dt}\cdot\boldsymbol{\xi}\,\varphi. \tag{3.24}$$

- Gauge transformations

From a converse point of view we can ask when vector coupling as that in eq.(20) canbe reabsorbed in a phase, i.e. with a unitary transformation. In the text and in other notebboks it is shown that this is possible only if the vector is a gradient, the related unitary transoformation is called a gauge transformation. dV/dt in equation (24) now couple to the center of mass of the system.

$$i\hbar\frac{\partial\varphi}{\partial t}=-\frac{\hbar^2}{2}\sum_i\frac{1}{m_i}\nabla_\xi^{\,2}\varphi+\sum_i m_i\frac{d\mathbf{V}}{dt}\cdot\boldsymbol{\xi}_i\,\varphi.$$

- Interacting particles

Interaction of particles is described by translation invariant potentials, of the form $U[x_i-x_j]$, these terms are unaffected by the transformation (19) so above conclusions continue to hold.

- Energy conservation

It can be interesting to observe that in the comuving frame one can speak of energy conservation, i.e. H do not depend explicitely on time, only for dV/dt = const., i.e. for uniform motions or for constant acceleration, just the two cases covered by Galilei transformations and Equivalence Principle.

Scale transformations

Let us consider the problem of the potential well for fixed x_L , the only variation is in the length L and the trasformation (1) is a (time dipendent) change of scale

wellscale1

$$x=\frac{L[t]}{L_0}\xi \tag{3.25}$$

We want to show how this scale transformation is implemented in Quantum Mechanics as a unitary operator.

For finite volumes a scale transformation is a bi more complicated than usual. Let us call L_0 the initial length of the box. The Hilbert space in defined at t=0 is $\mathbb{L}^2[0, L_0]$, after a transformation $L_0 \to \lambda L_0$= L[t] the relevant Hilbert space is $\mathbb{L}^2[0, L]$, i.e. has changed. This changement is not there in infinite or semiinfinite domains.
We can define the unitary transformation which implement a scale transformation as

defscaletransformation

$$S_\lambda : \mathbb{L}^2[0, L_0] \to \mathbb{L}^2[0, \lambda L_0]; \qquad S_\lambda \psi = \psi_\lambda; \qquad \psi_\lambda[x] = \frac{1}{\sqrt{\lambda}} \psi\left[\frac{x}{\lambda}\right]. \tag{3.26}$$

The formulas will be simpler with L_0= 1, but we retain this parameter to show clearly the dimensions of what we write.

It is trivial to verify that S is indeed unitary (preserve scalar products). It transform functions with support in [0, L_0] in functions with support in [0, L], preserving their norm:

$$\int_0^L |\psi_\lambda[x]|^2 \, dx = \int_0^L \left|\psi\left[\frac{x}{\lambda}\right]\right|^2 \frac{1}{\lambda} dx = \int_0^{L_0} |\psi[\xi]|^2 \, d\xi.$$

Putting λ = Exp[α], and defining the infinitesimal generator D for this transformation, it follows from a Taylor xpansion of (26)

$$\lambda = e^\alpha \simeq 1 - \alpha; \quad \psi_\lambda[x] \simeq \left(1 - \frac{\alpha}{2}\right)\left(\psi[x] - \alpha x \frac{\partial}{\partial x}\psi\right) \simeq \psi[x] - \alpha\left(\frac{1}{2} + x\frac{\partial}{\partial x}\right)\psi[x].$$

defDwall

$$S_\lambda = \mathrm{Exp}\left[-\frac{i}{\hbar}\alpha D\right]; \quad D = \frac{\hbar}{2 i}\left(x\frac{\partial}{\partial x} + \frac{\partial}{\partial x}x\right) = \frac{1}{2}(x p + p x). \tag{3.27}$$

The canonical commutations relations give

commutationrelationsDxp

$$[D, x^n] = n\frac{\hbar}{i}x^n = -i n \hbar x^n; \qquad [D, p^n] = -\frac{\hbar}{i} n p = i n \hbar p. \tag{3.28}$$

D measures the dimension of operators. Some care must be taken using previous relations in finite intervals, as products of operators can bring outside Hilbert space, we always compute explicit matrix elements.
From the definition (26) we can easily compute how operators transform under S_λ:

scaletransformationxp

$$S_\lambda p S_\lambda^{-1} = \lambda p; \quad S_\lambda x S_\lambda^{-1} = \frac{1}{\lambda} x. \tag{3.29}$$

The details of the (easy) derivation are left to the reader. These relations justify the name of scale transformation at the quantum level.

Consider now a Hamiltonian defined on a box L, $H^{(L)}$. Let us denote by $H^{(0)}$ the original Hamiltonian. Applying (29) to $H^{(0)}$ we find

scaledHwall1

$$S_\lambda H^{(0)} S_\lambda^{-1} = \lambda^2 \frac{p^2}{2 m} \equiv \lambda^2 H^{(L)}. \tag{3.30}$$

The momentum p appearing on the right hand side of (30) is defined on $\mathbb{L}^2[0, L]$ so we have correctly defined $H^{(L)}$ the Hamiltonian. Let us note that both sides of (30) have the same spectrum, the one of unitary equivalent Hamiltonian $H^{(0)}$. In fact the eigenvalues of $H^{(L)}$ scale ad $1/\lambda^2$. Finally let us write

scaledHwall2

$$H^{(L)} = \frac{1}{\lambda^2} S_\lambda H^{(0)} S_\lambda^{-1} \tag{3.31}$$

We see that apart a scale factor the two Hamiltonians are equivalent, i.e. solving $H^{(0)}$ we have practically solved $H^{(L)}$. Things change for time dependent scale transformation, in fact we now (see text) that for time dependent unitry transformations the infinitesimal generator of time translations (i.e. the Hamiltonian) has a non homogenous transformation, then the evolution generated by (31) is **not** unitary equivalent to the time evolution in the box of length L_0. This is the formal reason for the different form of Schrödinger equation.

Let us take a state Φ in $\mathbb{L}^2[0, L]$, we have

$$i\hbar\frac{\partial\Phi}{\partial t} = H^{(L)}\Phi = \frac{1}{\lambda^2} S_\lambda H^{(1)} S_\lambda^{-1}\Phi.$$

The function ψ defined as $\psi = S_\lambda^{-1}\Phi$ describe the sistem in the box of length L_0. Using (27)

$$\psi = S_\lambda^{-1}\,\Phi;\quad S_\lambda^{-1} = \mathrm{Exp}\left[\frac{i}{\hbar}\,\mathrm{Log}[\lambda]\,D\right];$$

$$\frac{1}{\lambda^2}\,H^{(1)}\,S_\lambda^{-1}\,\Phi \equiv \frac{1}{\lambda^2}\,H^{(1)}\,\psi = i\,\hbar\,S_\lambda^{-1}\,\frac{\partial\Phi}{\partial t} = i\,\frac{\partial\psi}{\partial t} - i\,\hbar\left(\frac{\partial S_L^{-1}}{\partial t}\right)\Phi = i\,\frac{\partial\psi}{\partial t} + \frac{\dot\lambda}{\lambda}\,D\,S_\lambda^{-1}\,\Phi = i\,\hbar\,\frac{\partial\psi}{\partial t} + \frac{\dot\lambda}{\lambda}\,D\,\psi$$

$$i\,\hbar\,\frac{\partial\psi}{\partial t} = \frac{1}{\lambda^2}\,H^{(1)}\,\psi - \frac{\dot\lambda}{\lambda}\,D\,\psi = -\frac{\hbar^2}{2\,m\,\lambda^2}\,\frac{\partial^2\psi}{\partial x^2} - \frac{\dot\lambda}{\lambda}\,\frac{1}{i}\,\frac{1}{2}\left(x\,\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\,x\right)\psi$$

which is identical to equation (6) once made the substitutions $\lambda\to L$ and $v_L = 0$.

This derivation show that scale transformations are indeed unitary operators and that the origin of prefactor $1/\sqrt{L}$ in (4) was indeed due to unitarity.

ProblemWellModes

Problem 4

A free particle moves in a box, $[x_L, x_R]$. *The boundary conditions are* $\psi[x_L] = \psi[x_R] = 0$. *The boundaries can move.*

1. Give a formal solution as an expansion in adiabatic modes.
2. Recover the case of rigid uniform translations as a Galilei transformation.
3. Study the time dependence of the mean energy and mean momentum on a generic state.
4. Consider the case of oscillating walls and explore the possibility of resonances.

Solution

Comments and questions

Before starting the solution let us make some comments on the questions that can be posed about this problem.

1. This for novices in QuantumMechanics this problem is the source of a typical puzzle : for a sudden perturbation we expect that the wave function is practiiically unchanged, but then for a compression of the box will cut a part of ψ, in contrast with unitarity. Clearly there is no violation of unitarity, simply the sudden approximation will be valid for expansions of the box but not for compressions. In the last case higher and higher oscillations modes are excited and the function will change quite strongly. From mathematical point of view the Hilbert space is defined as $\mathbb{L}^2[0, L]$ with zero boundary conditions. When $L_1 < L_2$, $\mathbb{L}^2[0, L_1] \subset \mathbb{L}^2[0, L_2]$ so in an expansion the "new" Hilbert space can describe old functions and sudden approximation apply. On the contrary for compressions the new Hilbert space just do not have in in it all the old functions, in particular those with part of the support is outside the new interval.
2. We expect that in some way the movement of the boundaries implies an exchange of energy with the environment. How does this happen in details? In particular the exchange is confined to the boundaries? The answer to this question is yes, as we will show below, together with a simple semiclassical explanation of the phenomenon.
3. Naively the Hamiltonian of the system is always a free Hamiltonian, which commute with itself and with momentum, how these quantities can change? We have already seen this kind of questions in other problems, and we have to show that moving boundaries implies in fact a Hamiltonian explicitely time dependent, through boundaries conditions.

Formal solution

In this problem we will use the units $m = \hbar = 1$.

Let x_L and x_R the left and right bounaries of the box. At the boundaries we assume $\psi[x_L] = \psi[x_R] = 0$. The Hilbert space is $\mathbb{L}^2[x_L, x_R]$, with zero boundary conditions. A complete basis for this space is

wallbasis2

$$u_k[x; L] = \sqrt{\frac{2}{L}}\,\mathrm{Sin}\left[\frac{\pi\,k\,(x - xL)}{L}\right];\quad E_k = \frac{\hbar^2}{2\,m}\,\pi^2\,\frac{k^2}{L^2}. \tag{4.1}$$

where $L = x_R - x_L$. This has nothing to do with movements of the boundaries. The solution of Schrödinger equation can be always be expanded with respect to the basis (1)

modeexpansionWall

$$\psi[x, t] = \sum_k a_k[t]\,u_k[x; L] \tag{4.2}$$

We note that expansion (2) automatically fulfills boundary conditions eve for mouving walls.

The only difference between fixed and mouving boundaries is in the time dipendence of coefficient functions a_k. In the former case

$$a_k[t] = a_k[0]\,\mathrm{Exp}[-i\,E_k\,t/\hbar],$$

In the general case time dipendence of these functions is fixed by substituting the expansion (2) in the equation

$$i\hbar\frac{\partial}{\partial t}\psi[x,t] = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi.$$

The only non trivial point is that functions (1) depends on t through the parameters x_L and L. We have

$$\sum_s \frac{da_s}{dt}u_s + a_s\frac{du_s}{dt} = \sum_s -\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)a_s u_s = -\frac{i}{\hbar}\sum_s E_s a_s u_s.$$

Using orthonormality of the basis we can multiply by u_k and integrate, obtaining an equation of the form

wellequationsforak

$$\frac{da_k}{dt} + \sum_s F_{ks}a_s = -i E_k a_k; \tag{4.3}$$

where

wallequatonsforA2

$$F_{ks} = \int_0^L u_k\,\partial_t u_s = \frac{2ks}{k^2-s^2}\left(\frac{\dot L}{L}(-1)^{k-s} + \frac{vL}{L}\left(-1+(-1)^{k-s}\right)\right)(k\neq s);\ F_{kk}=0. \tag{4.4}$$

An easy computation show

wallequatonsforA2bis

$$F_{ks} = \frac{2ks}{k^2-s^2}\left(\frac{\dot L}{L}(-1)^{k-s} + \frac{v_L}{L}\left(-1+(-1)^{k-s}\right)\right)(k\neq s);\quad F_{kk}=0. \tag{4.5}$$

where $v_L = dx_L/dt$; $v_R = dx_R/dt$; $dL/dt = v_R - v_L$.

The matrix F being non diagonal, equation (3) imply transitions between different modes. Let us note some points:

- The basis (1) has definite parity for reflections around the mid - point:

$$x_M = \frac{(x_R + x_R)}{2};\quad x - x_M \to -(x-x_M),\ \text{i.e.}\ x \to 2x_M - x.$$

under this operation

$$u_k[x;L] \to (-1)^{k+1}u_k[x;L].$$

- For $v_R = -v_L$ (a parity preserving movement around the middle of the box) $dL/dt = -2v_L$ and

$$F_{ks} = -\frac{2ks}{k^2-s^2}\frac{v_L}{L}\left(\left(1+(-1)^{k-s}\right)\right) \tag{4.6}$$

i.e. only transitions between states with same parity are allowed.

- For vL = vR = const. we have a rigid traslation of the walls, then the solution must follows from Galilean invariance. This is indeed true, the reader can prove it by himself or read the proof below.
- The matrix F is antihermitian (see also text) and this assure conservation of the norm, as it is easily shown.

In principle solving exactly or approximatively eq.(3) is equivalent to solve Schrödinger equation.

We have to stress the following point, to avoid possible misunderstandings. The functions (1) are eigenstates of the "instantaneous" Hamiltonian defined on a box of length L and left boundary x_L, H[L], but are **not** stationary states as the time evolution in ξ coordinates is not given by H[L]. This point has been discussed in problem [3] and will be rewieved in a particular case in the next section.

Rigid translation

The coefficients a_k satisfy formally an "Hamiltonian" equation of the form

hamiltonak

$$\frac{da_k}{dt} = -\frac{i}{\hbar}\mathcal{H}_{ks}a_s;\qquad \mathcal{H}_{ks} = -i\hbar F_{ks} + E_k\delta_{ks} \equiv (\mathcal{F} + H_0)_{ks} \tag{4.7}$$

$\mathcal{H}$ is not diagonal except if we can neglect transition matrix $\mathcal{F}$, and this is the adiabatic approximation. Only in this approximation functions u_k are approximatively stationary. Schrödinger equation in ξ coordinates reads (see problem [3])

modeswelleqforpsitrasf2

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2mL^2}\frac{\partial^2\psi}{\partial\xi^2} + i\hbar\left(\left(\frac{\dot L}{L}\xi + \frac{v_L}{L}\right)\frac{\partial\psi}{\partial\xi} + \frac{1}{2}\frac{\dot L}{L}\psi\right). \tag{4.8}$$

where

modeschangexcsi

$$x = x_L + L\,\xi \tag{4.9}$$

In general the effective Hamiltonian in (8) is time dipendent and do not have stationary states at all. An exception is the rigid motion (dL/dt = 0) with constant velocity, this case must be covered by a Galilei transformation. In this case the equation simplify in

modeswelleqforpsitrasf3

$$i\,\hbar\,\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2\,m\,L^2}\,\frac{\partial^2\psi}{\partial\xi^2} + i\,\hbar\,\frac{v_L}{L}\,\frac{\partial\psi}{\partial\xi}\ . \tag{4.10}$$

Galilei invariance imply that functions u_k are stationary states, then, up to a unitary transformation, they must be the same obtained by solution of (10) or (7). We now from the general theory of Galilei transformations that given a function φ in the mouving frame the state represented by this function is described, in the rest frame, by

modesGalilei1

$$\Psi[t,\,x] = \varphi[t,\ \xi[t,\,x]]\ \mathrm{Exp}[i\,m\,V_L\,\xi/\hbar]\ \mathrm{Exp}\left[\frac{i}{2}\,m\,V_L^2\,t/\hbar\right] \tag{4.11}$$

This is in particularly true for u_k:

$$\Psi_k[t,\,x] = u_k[t,\ \xi[t,\,x]]\ \mathrm{Exp}[i\,m\,V_L\,\xi/\hbar]\ \mathrm{Exp}\left[\frac{i}{2}\,m\,V_L^2\,t/\hbar\right] \tag{4.12}$$

The stationary eigenfunctions of (10) are not u_k but their *unitary transformed* form

modesnewUbasis

$$U_k[t,\ \xi] = u_k[t,\ \xi]\ \mathrm{Exp}[i\,m\,V_L\,\xi/\hbar] \tag{4.13}$$

as it is easily verified. Had we used this set of functions as basis the matrix elements would be absent of course. With our choice the compicated equations for a_k must reconstruct the exponential missing ξ-dipendent phase. Let us show this as it is not obvious from (7).

A general state is written as

$$\Psi[t,\,x] = \sum_n A_n\,u_n[t,\,\xi]\ \mathrm{Exp}[i\,m\,V_L\,\xi/\hbar]\ \mathrm{Exp}\left[\frac{i}{2}\,m\,V_L^2\,t/\hbar\right].$$

ξ is expressed as a function of x with (9). By definition

$$a_k = \int d\xi\ u_k\left(\sum_n A_n\,u_n[t,\,\xi]\ \mathrm{Exp}[i\,m\,V_L\,\xi/\hbar]\ \mathrm{Exp}\left[\frac{i}{2}\,m\,V_L^2\,t/\hbar\right]\right),$$

from which follows

$$\frac{da_k}{dt} = \frac{i}{2}\,m\,\frac{V_L^2}{\hbar}\,a_k - \frac{i}{\hbar}\int d\xi\ u_k\left(\sum_n A_n\,E_n\,u_n\,e^{i\,m\,V_L\,\xi/\hbar}\,e^{\frac{i}{2}\,m\,V_L^2\,t/\hbar}\right)$$

To compute the sum we use Schrödinger equation for u and integrate by parts

$$\frac{da_k}{dt} = \frac{i}{2}\,m\,\frac{V_L^2}{\hbar}\,a_k - \frac{i}{\hbar}\,\frac{\hbar^2}{2\,m}\int d\xi\left(-u_k'' - 2\,i\,u_k'\,m\,\frac{v_L}{\hbar} + m^2\,\frac{V_L^2}{\hbar^2}\right)\left(\sum_n A_n\,u_n\,e^{i\,m\,V_L\,\xi/\hbar}\,e^{\frac{i}{2}\,m\,V_L^2\,t/\hbar}\right)$$

Last term is proportional to a and cancel exactly the first term. Using Schrödinger equation for u_k

$$\frac{da_k}{dt} = -\frac{i}{\hbar}\,E_k\,a_k - v_L\,e^{\frac{i}{2}\,m\,V_L^2\,t/\hbar}\int d\xi\ u_k'\left(\sum_n A_n\,u_n\,e^{i\,m\,V_L\,\xi/\hbar}\right)$$

The sum canbe evaluated inserting a complete set of u_s functions,which we write as scalar product:

$$\sum_s \left\langle u_k'\ \middle|\ u_s\right\rangle\left\langle u_s\ \middle|\ \sum_n A_n\,u_n\,e^{i\,m\,V_L\,\xi/\hbar}\,e^{\frac{i}{2}\,m\,V_L^2\,t/\hbar}\right\rangle = \left\langle u_k'\ \middle|\ u_s\right\rangle a_s.$$

A simple integral shows that

$$\left\langle u_k'\ \middle|\ u_s\right\rangle = \frac{1}{L}\,\frac{2\,k\,s}{k^2 - s^2}\left(-1 + (-1)^{k+s}\right)$$

and finally

$$\frac{da_k}{dt} = -\frac{i}{\hbar}\,E_k\,a_k - \frac{v_L}{L}\,\frac{2\,k\,s}{k^2 - s^2}\left(-1 + (-1)^{k+s}\right)a_s = -\frac{i}{\hbar}\,E_k\,a_k - F_{ks}\,a_s\,.$$

with reproduces the correct equation.

■ Energy variations

We want to study the variation of the mean energy on a state as wall moves. Let us take an arbitrary state Ψ and expand the wave function as a series in the basis (1)

$$\Psi = \sum_k a_k[t]\, u_k[x, L]; \qquad E[\Psi] = \frac{\hbar^2}{2\,m}\frac{\pi^2}{L^2}\sum_k a_k^* a_k\, k^2. \tag{4.14}$$

Using (3) and the antisimmetry of F:

dEdt1wall

$$\frac{dE}{dt} = -2\,\frac{\dot{L}}{L}\,E + \frac{\pi^2\,\hbar^2}{2\,L^2\,m}\sum_{ks} k^2\left(-a_k^* F_{ks}\, a_s + F_{sk}\, a_s^* a_k\right). \tag{4.15}$$

The terms in (3) proportional to E_k cancel in previous equation. Using the antisymmetry in k-s we can rewrite the sum in the r.h.s. as

$$\frac{1}{2}\sum_{ks}\left(k^2 - s^2\right)\left(-a_k^* F_{ks}\, a_s + F_{sk}\, a_s^* a_k\right) = -\sum_{ks}\left(k^2 - s^2\right) a_k^* F_{ks}\, a_s.$$

Substituting the values for F_{ks} we must remember that k=s terms are zero, then

$$-\sum_{ks}\left(k^2 - s^2\right) a_k^* F_{ks}\, a_s = -\sum_{k\neq s} 2\,k\,s\left\{\frac{\dot{L}}{L}(-1)^{k-s} + \frac{v_L}{L}\left(-1 + (-1)^{k-s}\right)\right\} a_k^* a_s =$$

$$-\sum_{k,s} 2\,k\,s\left\{\frac{\dot{L}}{L}(-1)^{k-s} + \frac{v_L}{L}\left(-1 + (-1)^{k-s}\right)\right\} a_k^* a_s + \frac{\dot{L}}{L}\sum_k 2\,k^2\, a_k^* a_k.$$

Last equality has been obtained by adding and subtracting the k=s term in the sum.

The last term inserted in (15) cancels exactly the first term in that equation and we have

$$\frac{dE}{dt} = -\frac{\pi^2\,\hbar^2}{2\,L^2\,m}\sum_{k,s} 2\,k\,s\left\{\frac{\dot{L}}{L}(-1)^{k-s} + \frac{v_L}{L}\left(-1 + (-1)^{k-s}\right)\right\} a_k^* a_s =$$

$$= -\frac{\pi^2\,\hbar^2}{2\,L^2\,m}\sum_{k,s} 2\,k\,s\left\{(-1)^{k-s}\frac{v_R}{L}\, a_k^* a_s - \frac{v_L}{L}\, a_k^* a_s\right\}$$

The relation can be a bit simplified decouping the independent sums. We note that this is possible because in the last form the sum is over unconstrained indices k and s.

modesdedtwithak

$$\frac{dE}{dt} = -\frac{\pi^2\,\hbar^2}{L^2\,m}\left\{\frac{v_R}{L}\left|\sum_k (-1)^k\, k\, a_k\right|^2 - \frac{v_L}{L}\left|\sum_k k\, a_k\right|^2\right\}. \tag{4.16}$$

From expansion (2) and from explicit form of the basis (1)

$$\partial_x\, \psi[x] = \sum_k \sqrt{\frac{2}{L}}\,\frac{\pi\, k}{L}\, a_k\, \mathrm{Cos}\left[\frac{\pi\, k\,(x - xL)}{L}\right];$$

then (remember that $x_R = x_L + L$)

psileftright

$$\psi'[x_L] = \sqrt{\frac{2}{L}}\,\frac{\pi}{L}\sum_k k\, a_k; \qquad \psi'[x_R] = \sqrt{\frac{2}{L}}\,\frac{\pi}{L}\sum_k (-1)^k\, k\, a_k. \tag{4.17}$$

and we have

$$\frac{dE}{dt} = -\frac{\pi^2\,\hbar^2}{L^2\,m}\left\{\frac{v_R}{L}\,\frac{L^3}{2\,\pi^2}\,\left|\psi'[x_R]\right|^2 - \frac{v_L}{L}\,\frac{L^3}{2\,\pi^2}\,\left|\psi'[x_L]\right|^2\right\}$$

i.e.

dedtsymm

$$\frac{dE}{dt} = \frac{\hbar^2}{2\,m}\left\{v_L\,\left|\psi'[x_L]\right|^2 - v_R\,\left|\psi'[x_R]\right|^2\right\} \tag{4.18}$$

The reader can verify that (18) has the correct dimensions ($|\psi|^2$ has dimension 1/L in one dimension). The signs are quite intuitive: if $v_L > 0$ we are compressing the system and energy grows, if $v_R > 0$ we expand the well and the energy decrease, as in a perfect gas.

More importantly (18) shows that the energy change for contact with the reservoir, we have no nonlocal properties in the game.

Semiclassical interpretation

Consider to fix the ideas a left boundary fixed and an expanding right wall, $v_R > 0$, ans consider a bound state of he system. In a de Broglie approximation for $\hbar \psi' \sim p \psi$, where p is the momentum at the boundary. As an order of magnitude $|\psi|^2 \sim 1/L$ and from eq. (18)

sclass1

$$\frac{dE}{dt} \simeq -\frac{1}{2m} v_R \frac{p^2}{L} = -m \frac{v^2}{2} \frac{v_R}{L}; \qquad (4.19)$$

v is the velocity of the particle. It is an easy kinematical exercize to show that a particle with positive velocity v which scatter against a wall mouving at velocity v_R lost in an energy 2 m v v_R. If we have N scattering for second the energy loss will be

$$\frac{dE}{dt} = -2 m v v_R N$$

In a box of length L we have N = v/(2L) scattering per second and classically

$$\frac{dE}{dt} = -2 m v v_R N = -m v^2 \frac{v_R}{L}$$

which coincides as an order of magnitude with (19). The factor of 2 is due to the fact that in a stationary state only half of the particles (in a statistical sense) are right mouving, as the classical particle considered above.

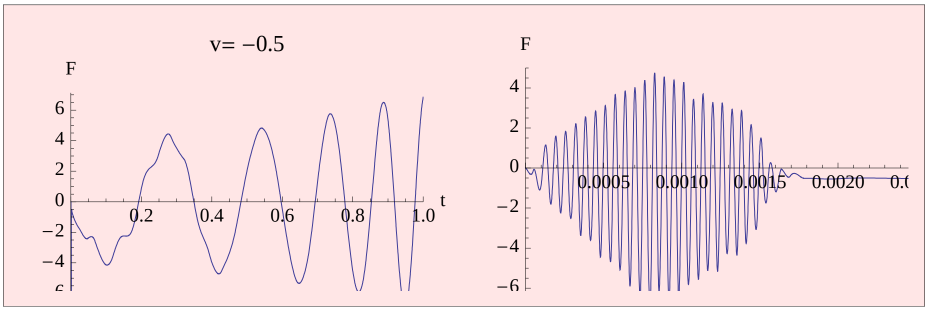
Momentum variations

We first state the result and make some comment. Let P the mean momentum on an arbitrary state Ψ, then

dpdtwell1

$$\frac{dP}{dt} = \frac{\hbar^2 \pi^2}{m L^3} \left(\left| \sum_k a_k k \right|^2 - \left| \sum_k a_k k (-1)^k \right|^2 \right) = \frac{\hbar^2}{2m} \left\{ |\psi'[x_L]|^2 - |\psi'[x_R]|^2 \right\} \qquad (4.20)$$

Last equality follows from (17). Here is an example of time variation of force F = dP/dt for fixed left boundary, the right graph show the short time regime.



A couple of coments and an unorthodox proposal :

- For $v_L = v_R = V$ we have a rigid movement and from (18) we have, as expected :

dedtdprigid

$$\frac{dE}{dt} = V \frac{dP}{dt}$$

- As definition of p we take the usual definition, i.e. $-i \hbar \partial/\partial x$, interpreting the walls as a limit case of finite barriers.

The proof of (20) can probably be done in several ways, we choose the most direct one, i.e. multiplication of matrix elements, just to avoid problems with subtle definitions of operators and so on. The derivation is quite tedious but instructive and we ask the reader to try to prove (20) before reading next paragaph.

- In one dimension energy and momentum conservation determine uniquely the final state of a scattering process. We can in this way imagine the following situation: take the barriers as real objects of mass M and suppose they have velocities $v_L$and v_R. If we apply momentum and energy conservation to the system walls + particle we have

$$M \frac{dv_L}{dt} + M \frac{dv_R}{dt} + \frac{dP}{dt} = 0; \quad M v_L \frac{dv_L}{dt} + M v_R \frac{dv_R}{dt} + \frac{dE}{dt} = 0;$$

Energy ans momentum derivatives for the particle are given by equations (18) and (20).

These two equation, plus Schrödinger equation, determine the motion of "classical" walls induced by quantum fluctuations of the particle. The equations are highly non linear, as v_L and v_R enter in the solution of Schrödinger equation.

The equations canbe reduced at one equation if one assume a rigid box. In that case the velocities are equal and the two equations coincide by virtue of (20).

Proof of eq (20)

Consider as usual a generic state with expansion's coefficients a_k in the basis (1). To compute the effect of P on a state let us start form basis functions. We can write (sum over intermidiate states)

poneigenstates

$$P\ |k\rangle = \sum_s |s\rangle\langle s|P|k\rangle \tag{4.21}$$

matrix elements are easily computed

poneigenstates2

$$\langle s|P|k\rangle = \frac{i}{L}\frac{2ks}{s^2-k^2}\left((-1)^{k-s}-1\right) \equiv \frac{i}{L}B_{sk} \tag{4.22}$$

We note the similarity of matrix B with a part of matrix F, eq.(4) this is not an accident as the derivative with respect to x is almost identical to the derivative with respect to t on the basis (1). For what follows it is convenient to keep separate the two part of matrix F, writing (always for k≠s):

defAendBforF

$$F_{ks} = \frac{\dot{L}}{L}A_{ks} + \frac{vL}{L}B_{ks}; \qquad A_{ks} = \frac{2ks}{k^2-s^2}(-1)^{k-s}; \quad B_{ks} = \left((-1)^{k-s}-1\right)\frac{2ks}{k^2-s^2}; \tag{4.23}$$

Consider now the meanvalue of p. From (21) and (22)

$$\langle\Psi|p|\Psi\rangle = P = \frac{i}{L}\sum_{sk} a_s^* B_{sk} a_k.$$

The time derivative, using equation of motion (3) is

dpdtprovv1

$$\frac{dP}{dt} = -\frac{1}{L}\frac{dL}{dt}P + \frac{i^2}{L}\sum_{sk} a_s^* B_{sk}(E_s-E_k)a_k - \frac{i}{L}\sum_{sk} a_s^*[B,F]_{sk}a_k. \tag{4.24}$$

The first sum is treated as in the case of energy

$$-\frac{1}{L}\sum_{s\neq k} a_s^* B_{sk}(E_s-E_k)a_k = -\frac{\hbar^2\pi^2}{2mL^3}\sum_{s\neq k} a_s^* B_{sk}\left(s^2-k^2\right)a_k =$$

$$-\frac{\hbar^2\pi^2}{2mL^3}\sum_{s\neq k} a_s^*\left((-1)^{k-s}-1\right)\frac{2ks}{s^2-k^2}\left(s^2-k^2\right)a_k =$$

$$-\frac{\hbar^2\pi^2}{mL^3}\left\{\left|\sum_k (-1)^k k\,a_k\right|^2 - \left|\sum_k k\,a_k\right|^2\right\}$$

We used the fact that even after simplifying $\left(s^2-k^2\right)$ the term $\left((-1)^{k-s}-1\right)$ vanishes for k=s so the sum can be extended without constraints. Using (17) equation (24) becomes

dpdtprovv2

$$\frac{dP}{dt} = -\frac{1}{L}\frac{dL}{dt}P + \frac{\hbar^2}{2m}\left\{|\psi'[x_L]|^2 - |\psi'[x_R]|^2\right\} - \frac{i}{L}\sum_{sk} a_s^*[B,F]_{sk}a_k. \tag{4.25}$$

The difficult part of the computation is the commutator [B.F]. Below we show that (A is defined in (23)):

$$[B,A]_{sk} = -B_{sk} \Rightarrow -\frac{i}{L}\sum_{sk} a_s^*[B,F]_{sk}a_k = +\frac{i}{L}\frac{1}{L}\frac{dL}{dt}\sum_{sk} a_s^* B_{sk} a_k = \frac{1}{L}\frac{dL}{dt}P;$$

i.e. the commutator cancel exactly the first term in (25) and we recover the result (20).

The commutator

As [B, B] = 0, in the commutator [B,F] only the term [B,A] is different from zero. the first term in B is identical to A, then commute, and the only contribution come from the second term, the one proportional to -1 in (23). Explicitely (we put a minus sign for convenience)

$$-[B,A]_{sk} = \sum_m{}' \frac{2sm}{s^2-m^2}\frac{2mk}{m^2-k^2}(-1)^{m-k} - \sum_m{}' \frac{2sm}{s^2-m^2}(-1)^{s-m}\frac{2mk}{m^2-k^2}$$

Here and below in the primed sum terms with m=k, or m=s are axcluded, they were zero in both A and B. Summing together the two termsand isolating the m-independent part:

$$-[B, A]_{sk} = \sum_m{}' \frac{2\,s\,k\,m^2}{s^2 - m^2} (-1)^m \left((-1)^k - (-1)^s\right) =$$

$$= 4\,s\,k \left((-1)^k - (-1)^s\right) \frac{1}{k^2 - s^2} \sum_m{}' \left(\frac{k^2\,(-1)^m}{k^2 - m^2} - \frac{s^2\,(-1)^m}{s^2 - m^2} \right).$$

We repeat : in the sum are exluded both m = s and m = k terms.

The sum canbe evaluated with he following trick. Consider a generic complex value z, instead of k or s. Each term is now well defined and we can *first* sum without constraints *then* subtract the unwanted terms and *at the end* take the limit for z to k or s. The complete sum is well known, you check it also with *Mathematica* :

$$\sum_{L=1}^{\infty} \frac{(-1)^L}{x^2 - L^2} = \frac{-1 + \pi\,x\,\mathrm{Csc}[\pi\,x]}{2\,x^2} = T[x]$$

For the limit $x \to k$ we pose x = k + z and Taylor expand:

$$T[k + z] = \frac{(-1)^k}{2\,k\,z} + \left(-\frac{1}{2\,k^2} - \frac{(-1)^k}{2\,k^2}\right) + O(z)$$

The pole term is what must be subtracted, it is in fact the limit of the series term as $x \to k$, of the series, S

$$S_{pole} = \frac{(-1)^k}{(k + z)^2 - k^2} \simeq \frac{(-1)^k}{2\,k\,z} - \frac{(-1)^k}{4\,k^2}$$

Then, after multiplication by k^2

$$\mathrm{Lim}_{z\to 0}\, k\hat{}2 \left(T[k + z] - S_{pole}\right) = k^2 \left(-\frac{1}{2\,k^2} - \frac{(-1)^k}{2\,k^2} + \frac{(-1)^k}{4\,k^2}\right) = \left(-\frac{1}{2} - \frac{1}{4} (-1)^k\right).$$

We have also to subtract the term with m = s, this is easy, and the first sum becomes

$$\sum_m{}' \frac{k^2\,(-1)^m}{k^2 - m^2} = \left(-\frac{1}{2} - \frac{1}{4} (-1)^k\right) - \frac{k^2\,(-1)^s}{k^2 - s^2}$$

The second sum is obtained interchanging the roles of s and k, then we have

$$-[B, A]_{sk} = 4\,s\,k \left((-1)^k - (-1)^s\right) \frac{1}{k^2 - s^2} \left\{ \frac{s^2\,(-1)^k}{s^2 - k^2} - \frac{k^2\,(-1)^s}{k^2 - s^2} + \frac{\left((-1)^s - (-1)^k\right)}{4} \right) \right\}$$

The first two term after multiplication by the signs in the prefactor become

$$\frac{s^2 \left(1 - (-1)^{k+s}\right)}{s^2 - k^2} - \frac{k^2 \left((-1)^{s+k} - 1\right)}{k^2 - s^2} = -(-1)^{k+s} + 1$$

while the last two terms give

$$\left((-1)^k - (-1)^s\right) \left((-1)^s - (-1)^k\right) = 2 \left((-1)^{k+s} - 1\right)$$

Summing

$$-[B, A]_{sk} = 4\,s\,k \frac{1}{k^2 - s^2} \left((-1)^{k+s} - 1\right) \left(-1 + \frac{1}{2}\right) = -2\,s\,k \frac{1}{k^2 - s^2} \left((-1)^{k+s} - 1\right) = B_{sk}.$$

This is what announced.

■ Adiabatic variations

The complicated variations in time of both E and P comes from the transition matrix F. In the adiabatic approximation these transition elements are negligible (see text) so in this limit the only variation in time come from the factors L in front of matrix elements, see eq.(15) and (22). Energy scale as $1 / L^2$ and p as 1/L, then, in this limit

adiabaticPandE

$$\frac{dE}{dt} = -2 \frac{1}{L} \frac{dL}{dt} E; \quad \frac{dP}{dt} = -\frac{1}{L} \frac{dL}{dt} P; \tag{4.26}$$

Scale transformations

In problem [3] the unitary transformation corresponding to scale variations has been introduced

modesdefscaletransformation

$$S_\lambda : \mathbb{L}^2[0, L_0] \to \mathbb{L}^2[0, \lambda L_0]; \qquad S_\lambda \psi = \psi_\lambda; \qquad \psi_\lambda[x] = \frac{1}{\sqrt{\lambda}} \psi\left[\frac{x}{\lambda}\right]. \tag{4.27}$$

Infinitesimal generator D and commutations relations are reported below, see problem [3] for more details:

$$\lambda = e^\alpha \simeq 1 - \alpha; \quad \psi_\lambda[x] \simeq \left(1 - \frac{\alpha}{2}\right)\left(\psi[x] - \alpha\, x \frac{\partial}{\partial x} \psi\right) \simeq \psi[x] - \alpha \left(\frac{1}{2} + x \frac{\partial}{\partial x}\right) \psi[x].$$

modesdefDwall

$$S_\lambda = \operatorname{Exp}\left[-\frac{i}{\hbar} \alpha D\right]; \quad D = \frac{\hbar}{2 i}\left(x \frac{\partial}{\partial x} + \frac{\partial}{\partial x} x\right) = \frac{1}{2}(x p + p x). \tag{4.28}$$

The canonical commutations relations are

modescommutationrelationsDxp

$$[D, x^n] = n \frac{\hbar}{i} x^n = -i n \hbar x^n; \qquad [D, p^n] = -\frac{\hbar}{i} n p = i n \hbar p. \tag{4.29}$$

modesscaletransformationxp

$$S_\lambda p S_\lambda^{-1} = \lambda p; \quad S_\lambda x S_\lambda^{-1} = \frac{1}{\lambda} x. \tag{4.30}$$

Consider a system with x_L=0 fixed and width L_0. An expansion (or contraction) to L[t] = λ L_0 is a scale transformation. it is easy to show, see again problem [3] that Hamiltonians in the final box, $H^{(L)}$ and that in the initial box, $H^{(1)}$ are related by a scale transformation

modesscaledHwall2

$$H^{(L)} = \frac{1}{\lambda^2} S_\lambda H^{(0)} S_\lambda^{-1} \tag{4.31}$$

Taking the time derivative of the previuos relation and using the definition of D we have

$$\frac{d}{dt} H^{(L)} = -2 \frac{\dot{\lambda}}{\lambda} H^{(L)} + \left(-i \frac{\dot{\lambda}}{\lambda}\right) \frac{1}{\hbar}\left[D, H^{(L)}\right].$$

The naive use of commutation relations (29) would give zero, but care must be taken in computing the commutator. On energy eigenstates

$$< k \left| \left[D, H^{(L)}\right] \right| s > = (E_s - E_k) < k \mid D \mid s > = (E_s - E_k) \frac{\hbar}{2 i} < k \left| x \partial_x + \partial_x x \right| s >$$

A short calculation shows that

$$< k \mid D \mid k > = 0; \quad < k \mid D \mid s > = i \hbar \frac{2 k s}{k^2 - s^2} (-1)^{k-s}; \; k \neq s.$$

We are exactly with the same kind of sums considered in previous derivations. We leave to the reader the proof that final result is again (16).

Oscillations

If movement of the walls is periodic there is a possibility to produce a resonance phenomenon between particle states. The general equations for a_k coefficients:

wallequatonsforAoscill

$$\frac{da_k}{dt} + \sum_s F_{ks} a_s = -i E_k a_k; \tag{4.32}$$

are known to produce resonance for external periodic perturbation. Let us recall briefly the theory. Extracting the "free evolution", i.e. time dependence due to E_k with the change of variables

$$a_k = c_k[t] \operatorname{Exp}\left[-i \int_0^t E_k \, dt\right] \equiv c_k[t] \operatorname{Exp}[-i \delta_k[t]], \tag{4.33}$$

equations (32) take the form

transitionc

$$\frac{dc_k}{dt} + \sum_s \operatorname{Exp}[i (\delta_k - \delta_s)] F_{ks} c_s = 0, \tag{4.34}$$

well suited for an iterative solution. If we start with a system in a state α, i.e. $c_\alpha = 1$, all other c's zero, a perturbative corrections to c_k, for k≠ α, is readily obtained

transition0order

$$\frac{dc_k}{dt} + \text{Exp}[i\,(\delta_k - \delta_\alpha)]\,F_{k\alpha}\,c_\alpha = 0;\ \Rightarrow\ c_k \simeq -\int_0^t \text{Exp}[i\,(\delta_k - \delta_\alpha)]\,F_{k\alpha} \tag{4.35}$$

At first order in the "small" perturbation due to F matrix only the term with s=α has been extracted, because at zero order only $c_\alpha$is not zero. Usually the right hand side of (35) is a rapid oscillating function, keeping small the value of the integral, This is the usual perturbation theory (see text). The exception being if in F is present a frequency which cancel the factor $\delta_k - \delta_\alpha$ in this case there is not depression and the amplitude for transition can be large. If we limit to the case of one frequency and assume that approximatively the energy are fixed this happens when the external frequency is near a difference E_β- E_α. We can approximatively restrict our attention to the two system level α-β but we can try to resolve exactly eq.(34) for this reduced system

$$\frac{dc_\beta}{dt} + \text{Exp}[i\,(\delta_\beta - \delta_\alpha)]\,F_{\beta\alpha}\,c_\alpha = 0; \qquad \frac{dc_\alpha}{dt} + \text{Exp}[i\,(\delta_\alpha - \delta_\beta)]\,F_{\alpha\beta}\,c_\beta = 0.$$

Consider for simplicity E_k constants and assume $E_\beta > E_\alpha$. The resonant term in $F_{\beta\alpha}$ is of the form

$$F_{\beta\alpha} = \mathcal{F}\,\text{Exp}[-i\,\Omega\,t]; \qquad F_{\alpha\beta} = -\mathcal{F}\,\text{Exp}[i\,\Omega\,t]; \quad \Omega \simeq E_\beta - E_\alpha.$$

The form of $F_{\alpha\beta}$ has been deduced from antihermiticity of the matrix F . The equations can be solved, and simplify greatly at exact resonance. For $c_\alpha[0] = 0,\ c_\beta[0] = 1$:

$$\frac{dc_\beta}{dt} + \mathcal{F}\,c_\alpha = 0; \quad \frac{dc_\alpha}{dt} - \mathcal{F}\,c_\beta = 0; \quad c_\beta[t] = \text{Cos}[\mathcal{F}\,t]; \quad c_\alpha[t] = \text{Sin}[\mathcal{F}\,t].$$

The system oscillated with period $2\pi/\mathcal{F}$. Populations of the levels, $|c_k|^2$ become 1 with period $\pi/\mathcal{F}$.

In the present case the matrix F has the general form (4)

fksoscill

$$F_{ks} = \int_0^L u_k\,\partial_t\,u_s = \frac{2\,k\,s}{k^2 - s^2}\left(\frac{\dot{L}}{L}\,(-1)^{k-s} + \frac{vL}{L}\left(-1 + (-1)^{k-s}\right)\right)\ (k \neq s)\ ;\ F_{kk} = 0. \tag{4.36}$$

Consider for instance an oscillating box with

$$L = L_0\,(1 + A\,\text{Cos}[\Omega\,t])$$

The system (36) allows resonance transtions. We can excite the system in two different ways: take fixed one of the walls, the left for definitess, of move both of them in opposite directions, in the last case vR = - vL, vL = - 1/2 dL/dt. In the two cases w ehave respectively

fksresonance

$$\begin{aligned} F_{ks} &= \frac{2\,k\,s}{k^2 - s^2}\,\frac{\Omega\,A\,\text{Sin}[\Omega\,t]}{L_0\,(1 + A\,\text{Cos}[\Omega\,t])}\,(-1)^{k-s}; \\ F_{ks} &= \frac{2\,k\,s}{k^2 - s^2}\,\frac{\Omega\,A\,\text{Sin}[\Omega\,t]}{L_0\,(1 + A\,\text{Cos}[\Omega\,t])}\,\frac{1}{2}\left((-1)^{k-s} + 1\right) \end{aligned} \tag{4.37}$$

In the first case all transitions are allowed, in the second case only transitions without change of parity. For small oscillations amplitudes, decomposing the trigonometric functions, we see that the "strength factor" $\mathcal{F}$ is given in the two cases by the same expression, as the sum ($1 + (-1)^{k-s}$) cancel the factor 1/2 in the second case:

$$\mathcal{F} = \frac{1}{2}\,\frac{2\,k\,s}{k^2 - s^2}\,\frac{\Omega\,A}{L_0}.$$

Matrices (37) allow resonances induced by higner harmonics, in fact expanding the denominator a whole series of frequencies appear. Another kind of nonlinear resonances can be induced if the transition k → s can be achieved by k→ i→s, this would correspond to a correction to the model of two states system, or inperturbation theory to higher orders. If corections are just induced by higher harmonics in the perturbation they are simply computed, for example in (37) we have, expanding the denominator

$$\frac{2\,k\,s}{k^2 - s^2}\,\frac{\Omega\,A\,\text{Sin}[\Omega\,t]}{L_0\,(1 + A\,\text{Cos}[\Omega\,t])} \simeq \frac{2\,k\,s}{k^2 - s^2}\,\frac{\Omega\,A}{L_0}\left(\text{Sin}[\Omega t] - A\,\frac{1}{2}\,\text{Sin}[2\,\Omega\,t] + \ldots\right)$$

Passing from trigonometric functions to exponentials this is seen to correspond to an effective strength

$$\mathcal{F}_2 = \frac{k\,s}{k^2 - s^2}\,\frac{\Omega\,A^2}{L_0}\,\frac{1}{2}$$

Problem 5

A particle moves in a box, [0,L]. Study the evolution of the states for a moving wall at x=L. Generalize the problem for the case of both walls moving. Try to construct a self-consistent equation for the walls, defining a mass for them. Study the case of wall oscillations and associated selection rules.

Solution

Introduction and mode expansion

The Hamiltonian is the free Hamiltonian, with boundary conditions,

$$H = \frac{p^2}{2\,m};\quad \psi[0] = \psi[L] = 0. \tag{5.1}$$

From now on we use $\hbar = m = 1$.

Eigenfunctions and eigenvalues are:

wallbasis

$$u_k[x;\,L] = \sqrt{\frac{2}{L}}\,\mathrm{Sin}\left[\frac{\pi\,k\,x}{L}\right];\quad E_k = \frac{1}{2}\,\pi^2\,\frac{k^2}{L^2}. \tag{5.2}$$

As the boundary moves L depends on t. We can always expand in the previous complete base

modeexpansionWall

$$\psi[x,\,t] = \sum\nolimits_k a_k[t]\,u_k[x;\,L] \tag{5.3}$$

Introducing this expansion in the Schrödinger equation it is easily found (see also text and previous problems)

wallequatonsforA

$$\begin{aligned}&\frac{da_k}{dt} + \sum\nolimits_s F_{ks}\,a_s = -\mathrm{i}\,E_k\,a_k\,;\\ &F_{ks} = \int_0^L u_k\,\partial_t\,u_s = \frac{\dot{L}}{L}\left((-1)^{k-s}\,\frac{2\,k\,s}{k^2-s^2}\right)\ (k \neq s)\,;\ F_{kk} = 0.\end{aligned} \tag{5.4}$$

It is easily shown that from orthonormality of the basis F must be anti-hermitian.. Diagonal elements are zero for a real basis. We leave to the reader as an easy excercise to show that these properties preserve the norm for an *arbitrary* state. This for novices in QuantumMechanics is the source of a typical puzzle: for a sudden perturbation we expect that the wave function is practiically unchanged, but then for a compression of the box this will cut a part of ψ, in contrast with unitarity. Clearly there is no violation of unitarity, simply the sudden approximation will be valid for expansions of the box but not for compressions. In the last case higher and higher oscillations modes are excited and the function will change quite strongly.

From mathematical point of view the Hilbert space is defined as $\mathbb{L}^2[0,\,L]$ with zero boundary conditions. When $L_1 < L_2$, $\mathbb{L}^2[0,\,L_1] \subset \mathbb{L}^2[0,\,L_2]$ so in an expansion the "new" Hilbert space can describe old functions and sudden approximation apply. On the contrary for compressions the new Hilbert space just do not have in in it all the old functions, in particular those with part of the support outside the new interval.

Equations of motion and scale transformations

Equations (4) in principle (and also in practice as we will show in a numeric notebook) solve the problem. It is nevertheless interesting to approach the problem as a solution of a differential equation with moving boundary conditions directly, this would be imperative if, for example, we do not know the explicit form of eigenfunctions for fixed boundary or if mode expansion converge slowly.

A very simple way to circumvent the moving boundary, in this case, is to make a change of variables in the Schrödinger equation. For clarity we introduce also a temporary new name for time, τ

$$x\,/\,L = \xi;\quad t = \tau;$$

Now as ξ varies between 0 and 1 we can recover whatever box. A bit of care must be taken in changing variables and for didactic reasons we report all passages.

$$\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x}\,\frac{\partial}{\partial \xi} + \frac{\partial \tau}{\partial x}\,\frac{\partial}{\partial \tau} = \frac{1}{L}\,\frac{\partial}{\partial \xi};$$

$$\frac{\partial}{\partial t} = \frac{\partial \tau}{\partial t}\,\frac{\partial}{\partial \tau} + \frac{\partial \xi}{\partial t}\,\frac{\partial}{\partial \xi} = \frac{\partial}{\partial \tau} - \frac{\dot{L}}{L^2}\,x\,\frac{\partial}{\partial \xi} = \frac{\partial}{\partial \tau} - \frac{\dot{L}}{L}\,\xi\,\frac{\partial}{\partial \xi}.$$

In the new variables (we put again t for the time) the Schrödinger equation becomes, with $\Psi = 1/\sqrt{L}\ \psi$ for normalization conditions

$$\mathrm{i}\,\hbar\left(\frac{\partial}{\partial t} - \frac{\dot{L}}{L}\,\xi\,\frac{\partial}{\partial \xi}\right)\frac{\psi}{\sqrt{L}} = -\frac{\hbar^2}{2\,m}\,\frac{1}{L^2}\,\frac{\partial^2 \psi}{\partial \xi^2}\,\frac{1}{\sqrt{L}};$$

or

wallequationInxi

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{L^2}\left(\frac{\partial^2\psi}{\partial\xi^2} - i\,2\,m\,L\,\dot{L}\,\xi\,\frac{\partial\psi}{\partial\xi} - i\,m\,L\,\dot{L}\,\psi\right);\quad \psi[0,t] = \psi[1,t] = 0. \tag{5.5}$$

The problem has been transformed in a usual fixed boundary problem, alb6eit a kind of "external field" has now appeared. Once a solution of (5) is found, f[ξ,t], the solution in the original variables will be Ψ[x,t] = f[x/L[t],t]/$\sqrt{L}$.

Let us note that

$$\xi\frac{\partial}{\partial\xi} + \frac{1}{2} = \frac{1}{2}\left(\xi\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\xi}\xi\right)$$

and write (with $\hbar$=1= m)

wallequationinxi2

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{1}{L^2}\left(\frac{\partial^2\psi}{\partial\xi^2} - i\,L\,\dot{L}\left(\xi\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\xi}\xi\right)\right)\psi;\quad \psi[0,t] = \psi[1,t] = 0. \tag{5.6}$$

It is instructive to consider this change of variables as a scale transformation and apply all the machinery of unitary operators.

A scale transformation is defined as

p5defscaletransformation

$$S_\lambda : \mathbb{L}^2[0,1] \to \mathbb{L}^2[0,\lambda];\qquad S_\lambda\,\psi = \psi_\lambda;\qquad \psi_\lambda[x] = \frac{1}{\sqrt{\lambda}}\,\psi\left[\frac{x}{\lambda}\right]. \tag{5.7}$$

It is trivial to verify that S is indeed unitary (preserve scalar products). It transform functions with support in [0,1] in functions with support in [0,L], preserving their norm.

Putting λ = Exp[α], and defining the infinitesimal generator D for this transformation, it follows from a Taylor xpansion of (7):

p5defDwall

$$\lambda = e^\alpha;\ S_\lambda = \mathrm{Exp}\left[-\frac{i}{\hbar}\,\alpha\,D\right];\quad D = \frac{\hbar}{2\,i}\left(x\frac{\partial}{\partial x} + \frac{\partial}{\partial x}x\right) = \frac{1}{2}(x\,p + p\,x). \tag{5.8}$$

The canonical commutations relations give (exceptionally we put also the right powers of $\hbar$)

p5commutationrelationsDxp

$$[D, x^m] = \frac{\hbar}{i}x^m = -i\,m\,\hbar\,x;\qquad [D, p^m] = -\frac{\hbar}{i}\,m\,p = i\,m\,\hbar\,p. \tag{5.9}$$

D measures the dimension of operators. Some care must be taken using previous relations in finite intervals, as products of operators can bring outside Hilbert space, we always compute explicit matrix elements.

From the definition (7) we can easily compute how operators transform under S_λ:

p5scaletransformationxp

$$S_\lambda\,p\,S_\lambda^{-1} = \lambda\,p;\qquad S_\lambda\,x\,S_\lambda^{-1} = \frac{1}{\lambda}x. \tag{5.10}$$

The details of the (easy) derivation are found in the Complements of chapter 7.

Consider now a Hamiltonian defined on a box L, $H^{(L)}$. Applying (10) to $H^{(1)}$ we find

p5scaledHwall1

$$S_L\,H^{(1)}\,S_L^{-1} = L^2\frac{p^2}{2m} \equiv L^2\,H^{(L)}. \tag{5.11}$$

The momentum p appearing on the right hand side of (11) is defined on $\mathbb{L}^2[0, L]$ so we have correctly defined $H^{(L)}$ the Hamiltonian. Let us note that both sides of (11) have the same spectrum, the one of unitary equivalent Hamiltonian $H^{(1)}$. In fact the eigenvalues of $H^{(L)}$ scale ad $1/L^2$. Finally let us write

p5scaledHwall2

$$H^{(L)} = \frac{1}{L^2}\,S_L\,H^{(1)}\,S_L^{-1} \tag{5.12}$$

We see that apart a scale factor the two Hamiltonians are equivalent, i.e. solving $H^{(1)}$ we have practically solved $H^{(L)}$. Things change for time dependent scale transformation, in fact we now (see text) that for time dependent unitry transformations the infinitesimal generator of time transla-tions (i.e. the Hamiltonian) has a non homogenous transformation, then the evolution generated by (12) is **not** unitary equivalent to the time evolution in the box of length 1. This is the formal reason for the different form of Schrödinger equation.

Let us take a state Φ in $\mathbb{L}^2[0, L]$, we have (with $\hbar = 1$)

$$i \frac{\partial\Phi}{\partial t} = H^{(L)}\,\Phi = \frac{1}{L^2} S_L\, H^{(1)}\, S_L^{-1}\,\Phi.$$

The function ψ defined as $\psi = S_L^{-1}\,\Phi$ describe the sistem in the box of length 1. Using (8)

$$\psi = S_L^{-1}\,\Phi; \quad S_L^{-1} = \mathrm{Exp}[i \,\mathrm{Log}[L]\, D];$$

we have

$$\frac{1}{L^2} H^{(1)}\, S_L^{-1}\,\Phi = \frac{1}{L^2} H^{(1)}\,\psi = i\, S_L^{-1} \frac{\partial\Phi}{\partial t} = i \frac{\partial\psi}{\partial t} - i \left(\frac{\partial S_L^{-1}}{\partial t}\right) \Phi = i \frac{\partial\psi}{\partial t} + \frac{\dot{L}}{L} D\, S_L^{-1}\,\Phi = i \frac{\partial\psi}{\partial t} + \frac{\dot{L}}{L} D\,\psi$$

and finally

$$i \frac{\partial\psi}{\partial t} = \frac{1}{L^2} H^{(1)}\,\psi - \frac{\dot{L}}{L} D\,\psi = -\frac{1}{2\,L^2} \left(\frac{\partial^2\psi}{\partial x^2} + 2\,L\dot{L}\, \frac{1}{i}\,\frac{1}{2} \left(x \frac{\partial}{\partial x} + \frac{\partial}{\partial x}\, x\right) \psi\right)$$

which is identical to equation (6).

- **Energy variations**

We want to study the variation of the mean energy on a state as wall moves.Take an arbitrary state Ψ and expand the wave function as a series in the basis (2)

$$\Psi = \sum_k a_k[t]\, u_k[x, t]; \qquad E[\Psi] = \frac{1}{2}\,\frac{\pi^2}{L^2} \sum_k a_k^*\, a_k\, k^2.$$

Using (4)

wallequatonsforA2bis

$$F_{ks} = \frac{2\,k\,s}{k^2 - s^2} \left(\frac{\dot{L}}{L} (-1)^{k-s} + \frac{v_L}{L} \left(-1 + (-1)^{k-s}\right)\right) (k \neq s); \quad F_{kk} = 0. \tag{5.13}$$

p5dEdt1wall

$$\frac{dE}{dt} = -2\,\frac{\dot{L}}{L}\,E + \frac{\pi^2}{2\,L^2} \sum_k \sum_s k^2 \left(-a_k^*\, F_{ks}\, a_s + F_{sk}\, a_s^*\, a_k\right). \tag{5.14}$$

Using antisymmetry in k-s of the terms in parenthesis

$$\sum_{ks} k^2 \left(-a_k^*\, F_{ks}\, a_s + F_{sk}\, a_s^*\, a_k\right) = \frac{1}{2} \sum_{ks} \left(k^2 - s^2\right) \left(-a_k^*\, F_{ks}\, a_s + F_{sk}\, a_s^*\, a_k\right) = -\sum_{ks} \left(k^2 - s^2\right) a_k^*\, F_{ks}\, a_s.$$

Substituting the values for F_{ks} we must remember that k=s terms are zero, then

$$-\sum_{ks} \left(k^2 - s^2\right) a_k^*\, F_{ks}\, a_s = -\frac{\dot{L}}{L} \sum_{k\neq s} (-1)^{k-s}\, 2\,k\,s\; a_k^*\, a_s =$$

$$-\frac{\dot{L}}{L} \sum_{k,s} (-1)^{k-s}\, 2\,k\,s\; a_k^*\, a_s + \frac{\dot{L}}{L} \sum_k 2\,k^2\; a_k^*\, a_k.$$

The last term exactly cancel the first term in (14). Then

$$\frac{dE}{dt} = -\frac{\pi^2}{L^2}\,\frac{\dot{L}}{L} \left| \sum_k (-1)^k\, k\, a_k \right|^2$$

From mode expansion:

$$\frac{d\Psi}{dx} = \sum_k a_k \sqrt{\frac{2}{L}}\; \mathrm{Cos}\left[\frac{\pi\, k\, x}{L}\right] \frac{\pi}{L}\, k; \quad \Psi'[L] = \sum_k a_k \sqrt{\frac{2}{L}}\; (-1)^k\, \frac{\pi}{L}\, k;$$

and

energyloss

$$\frac{dE}{dt} = -\frac{\pi^2}{L^2}\frac{\dot{L}}{L}\frac{L^3}{2\pi^2}\left|\Psi'[L]\right|^2 = -\frac{1}{2}\dot{L}\left|\Psi'[L]\right|^2;$$
$$\frac{dE}{dt} = -\frac{\dot{L}}{2m}\left|\hbar\,\partial_x\Psi[L]\right|^2;\ (\text{in normal units}). \tag{5.15}$$

We see that, as intuitively expected, we have an energy loss when box grows and an energy gain for compressions. Eq.(15) has a nice semiclassical interpretation. For a de Broglie wave $\hbar\,\partial_x\Psi[L] \sim p\,\psi$, where p is the momentum at the wall.

$$\frac{dE}{dt} \sim -\frac{\dot{L}}{2m}p^2\left|\psi\right|^2.$$

$\dot{L}$ is the velocity V of the wall,let us suppose positive for example (expansion). $|\psi|^2$ is the density and for one particle $|\psi|^2 \sim 1/L$. For the energy loss we have

$$\frac{dE}{dt} \sim -\frac{V}{2m}\frac{p^2}{L} = -E\frac{V}{L}.$$

Let us consider a classical particle of velocity v and mass m which hits the wall. An easy exercise in kinematic shows that in the scattering the particle lost an energy 2 m v V. If there are N hits per second the energy loss will be

$$\frac{dE}{dt} = -2\,m\,v\,V\,N.$$

In a second a particle of velocity v hits v/2L times against the wall, then

$$\frac{dE}{dt} = -2\,m\,v\,V\frac{v}{2L} = -2\,E\frac{V}{L}.$$

The factor of 2 is due to the fact that for a stationary states only half of the particles (the right movers) hits against the wall.

A different and instructive derivation of energy variation can be obtained using (12). Taking time derivative and using the definition of S in terms of D we obtain

$$\frac{d}{dt}H^{(L)} = -2\frac{\dot{L}}{L}H^{(L)} + \left(-i\frac{\dot{L}}{L}\right)\left[D,\,H^{(L)}\right] = -2\frac{\dot{L}}{L}H^{(L)} - i\frac{\dot{L}}{L}\left[D,\,H^{(L)}\right].$$

The naive use of commutation relations, see (9) would give zero, but carre must be taken in computing the commutator. On energy eigenstates

$$\langle k\left|\left[D,\,H^{(L)}\right]\right|s\rangle = (E_s - E_k)\langle k\,|\,D\,|\,s\rangle = (E_s - E_k)\frac{1}{2\,i}\langle k\left|x\,\partial_x + \partial_x\,x\right|s\rangle$$

A short calculation shows that

$$\langle k\,|\,D\,|\,k\rangle = 0;\quad \langle k\,|\,D\,|\,s\rangle = i\frac{2\,k\,s}{k^2 - s^2}(-1)^{k-s};\ k \neq s.$$

We are exactly with the same kind of sums considered in previous derivation. We leave to the reader the proof that final result is again (15).

■ **Arbitrary movements for both walls**

The system can be trivially generalized. Let xL, xR the positions of left and right boundaries, and L = xR - xL.

Eigenfunctions and eigenvalues are:

wallbasis2

$$u_k[x;\,L] = \sqrt{\frac{2}{L}}\,\text{Sin}\left[\frac{\pi\,k\,(x - xL)}{L}\right];\quad E_k = \frac{1}{2}\pi^2\frac{k^2}{L^2}. \tag{5.16}$$

The mode expansion becomes

wallequatonsforA2

$$\frac{da_k}{dt} + \sum_s F_{ks}\,a_s = -i\,E_k\,a_k;$$
$$F_{ks} = \int_0^L u_k\,\partial_t u_s = \frac{2\,k\,s}{k^2 - s^2}\left(\frac{\dot{L}}{L}(-1)^{k-s} + \frac{vL}{L}\left(-1 + (-1)^{k-s}\right)\right)\ (k \neq s);\ F_{kk} = 0. \tag{5.17}$$

xL, and xR = xL + L are the boundaries, vL is d(xL)/dt.

Let us note some points

1. The basis (1) has definite parity for reflections around the mid-point xM = (xR+xL)/2, x-xM -> - (x-xM), i.e. x-> 2xM-x, under this operation

$$u_k[x;\,L] \;\rightarrow\; (-1)^{k+1}\,u_k[x;\,L]$$

2. For vR = - vL (a parity preserving movement around the middle of the box) dL/dt = - 2 vL and

$$F_{ks} = -\frac{2\,k\,s}{k^2 - s^2}\,\frac{vL}{L}\,\left(\left(1 + (-1)^{k-s}\right)\right)$$

i.e. only transitions between states with same parity are allowed.

3. For vL = vR we have a rigid traslation of the walls, then the result must follos from Galilean invariance. This is indeed true, the reader can prove it by himself or read the proof below. (The proof is in a closed cell).

Proof

■ Energy conservation and free walls

It is possible to compute both energy and momentum variation as the walla move. The computation proceed as in (14) giving

dEdtanddPdt

$$\begin{aligned}\frac{dE}{dt} &= -\frac{vR}{2}\left|\Psi'[xR]\right|^2 + \frac{vL}{2}\left|\Psi'[xL]\right|^2\\ \frac{dP}{dt} &= -\frac{1}{2}\left(\left|\Psi'[xR]\right|^2 - \left|\Psi'[xL]\right|^2\right).\end{aligned} \tag{5.18}$$

We use the symbols E, P, to denote mean values in this section. vL and vR are the velocities of left and right walls, and in terms of mode coefficients

$$\Psi'[xL] = \sum_k a_k \sqrt{\frac{2}{L}}\,\frac{\pi}{L}\,k; \qquad \Psi'[xR] = \sum_k a_k \sqrt{\frac{2}{L}}\,\frac{\pi}{L}\,k\,(-1)^k;$$

The derivation is proposed as an exercise to the reader, a direct proof is also given below (*closed cell*),

For vR = vL= V (rigid movements) dL/dt = 0, and the result is proportional to energy change and we obtain the expected relation between energy end momentum (this is just a consequence of Galilei invariance)

$$\frac{dP}{dt} = \frac{1}{V}\,\frac{dE}{dt}; \qquad \frac{dE}{dt} = V\,\frac{dP}{dt}.$$

In general

devrel

$$\begin{aligned}&\frac{dE}{dt} = V\,\frac{dP}{dt} - \frac{1}{4}\,v_{rel}\left(\left|\Psi'[xR]\right|^2 + \left|\Psi'[xL]\right|^2\right);\\ &vR = V + \frac{1}{2}\,v_{rel}; \quad vL = V - \frac{1}{2}\,v_{rel};\end{aligned} \tag{5.19}$$

These expressions allow to pose the following problem. Suppose that thet wo wall have a large mass M and are completely free, how they move? We can obtain the movement by energy and momentum conservation.

dedpandmovingwalls

$$\begin{aligned}&M\,\frac{d\,vR}{dt} + M\,\frac{d\,vL}{dt} + \frac{dP}{dt} = 0;\\ &M\,vR\,\frac{d\,vR}{dt} + M\,vL\,\frac{d\,vL}{dt} + \frac{dE}{dt} = 0.\end{aligned} \tag{5.20}$$

These equation in principle determine the movement. The "force" acting on the walls is very complicated and velocity dependent, remember that L[t] and vL[t] enter in the expression for the evolution of expansion coefficients a_k.

In idealized case is when left and right walls are identified,the equation in this case describe a motion on a ring. Clearly in this case vL = vR, the length of the ring is fixed by its initial value. The simplified equations read in this case (dL/dt = 0), and are reduced to those for P (equation for E follows from V dP/dt = dE/dt):

$$M \frac{dV}{dt} + \frac{dP}{dt} = 0;$$

$$\frac{da_k}{dt} + \frac{V}{L} \sum_s B_{ks} a_s = -i E_k a_k;$$

$$B_{ks} = \frac{2 k s}{k^2 - s^2} \left(-1 + (-1)^{k-s}\right); \quad (k \neq s);$$

$$\frac{dP}{dt} = -\frac{\pi^2}{L^3} \left(\left| \sum_k a_k k (-1)^k \right|^2 - \left| \sum_k a_k k \right|^2 \right);$$

Proof of (18)

The variation of energy of the quantum state for both walls moving proceed exactly as in (14)

$$\frac{dE}{dt} = -2 \frac{\dot{L}}{L} E - \frac{\pi^2}{2 L^2} \sum_{ks} \left(k^2 - s^2\right) a_k^* F_{ks} a_s.$$

The only difference is in the F matrix. Inserting (4) and remembering the for k=s F_{ks} is zero we have (the deduction is similar to that following eq.(14)):

$$\frac{dE}{dt} = -2 \frac{\dot{L}}{L} E - \frac{\pi^2}{2 L^2} \sum_{k \neq s} a_k^* a_s 2 k s \left((-1)^{k-s} \left(\frac{\dot{L}}{L} + \frac{vL}{L} \right) - \frac{vL}{L} \right) =$$

$$-\frac{\pi^2}{L^2} \frac{vR}{L} \left| \sum_k a_k k (-1)^k \right|^2 + \frac{\pi^2}{L^2} \frac{vL}{L} \left| \sum_k a_k k \right|^2.$$

We have introduced the velocity of the right wall, $vR = vL + \dot{L}$. Using expansion in the basis (1)

$$\frac{d\Psi}{dx} = \sum_k a_k \sqrt{\frac{2}{L}} \operatorname{Cos}\left[\frac{\pi k (x - xL)}{L}\right] \frac{\pi}{L} k;$$

$$\Psi'[xL] = \sum_k a_k \sqrt{\frac{2}{L}} \frac{\pi}{L} k; \qquad \Psi'[xR] = \sum_k a_k \sqrt{\frac{2}{L}} \frac{\pi}{L} k (-1)^k;$$

then we can also write the generalization of (15):

$$\frac{dE}{dt} = -\frac{vR}{2} \left| \Psi'[xR] \right|^2 + \frac{vL}{2} \left| \Psi'[xL] \right|^2$$

Let us now consider momentum. We can imagine that this momentum is usual momentum in presence of an infinitely high barriers simulated by the walls, so we use usual definition for it. On a energy eigenstates

$$P \mid k\rangle = \mid s\rangle \langle s \mid P \mid k\rangle;$$

$$\langle s \mid P \mid k\rangle = \frac{1}{i} \frac{1}{L} \frac{2 k s}{k^2 - s^2} \left((-1)^{k-s} - 1 \right) = \frac{i}{L} \frac{2 k s}{s^2 - k^2} \left((-1)^{k-s} - 1 \right) \equiv \frac{i}{L} B_{sk}; \quad (k \neq s)$$

We note that matrix B is a part of matrix F, the one proportional to vL. For an arbitrary state

$$\langle \Psi \mid P \mid \Psi\rangle = \frac{i}{L} \sum_{ks} a_s^* B_{sk} a_k.$$

Taking the derivative and using equation of motion for a_k

$$\frac{dP}{dt} = -\frac{\dot{L}}{L} P + \frac{i^2}{L} \sum_{ks} a_s^* (E_s - E_k) B_{sk} a_k - \frac{i}{L} \sum_{ks} a_s^* [B, F]_{sk} a_k$$

The first sum is treated in the usual way:

$$\sum_{k\neq s} a_s^* (E_s - E_k) B_{sk} a_k = \frac{\pi^2}{2L^2} \sum_{k\neq s} a_s^* \frac{s^2-k^2}{s^2-k^2} 2ks\left((-1)^{k-s}-1\right) a_k =$$

$$\frac{\pi^2}{L^2} \sum_{k\neq s} a_s^* k s \left((-1)^{k-s}-1\right) a_k =$$

$$\frac{\pi^2}{L^2} \left|\sum_k k a_k (-1)^k\right|^2 - \frac{\pi^2}{L^2}\left|\sum_k k a_k\right|^2 = \frac{L}{2}\left|\Psi'[xR]\right|^2 - \frac{L}{2}\left|\Psi'[xL]\right|^2$$

$$\frac{dP}{dt} = -\frac{\dot{L}}{L} P - \frac{1}{2}\left(\left|\Psi'[xR]\right|^2 - \left|\Psi'[xL]\right|^2\right) - \frac{i}{L}\sum_{ks} a_s^* [B, F]_{sk} a_k$$

F matrix is composed of two parts, the second being proportional to matrix B, we pose

$$F_{ks} = \frac{\dot{L}}{L} A_{ks} + \frac{vL}{L} B_{ks}; \quad A_{ks} = \frac{2ks}{k^2-s^2}(-1)^{k-s}; \quad B_{ks} = \frac{2ks}{k^2-s^2}\left(-1+(-1)^{k-s}\right).$$

$$\frac{dP}{dt} = -\frac{\dot{L}}{L} P - \frac{1}{2}\left(\left|\Psi'[xR]\right|^2 - \left|\Psi'[xL]\right|^2\right) - \frac{i\dot{L}}{L^2}\sum_{ks} a_s^* [B, A]_{sk} a_k$$

The commutator can be computed and gives $-B_{sk}$ and cancel exactly the first term

$$\frac{dP}{dt} = -\frac{\dot{L}}{L} P - \frac{1}{2}\left(\left|\Psi'[xR]\right|^2 - \left|\Psi'[xL]\right|^2\right) + \frac{i}{L}\frac{\dot{L}}{L}\sum_{ks} a_s^* B_{sk} a_k =$$

$$-\frac{1}{2}\left(\left|\Psi'[xR]\right|^2 - \left|\Psi'[xL]\right|^2\right).$$

Computation of the commutator

Only the term with -1 in B gives a contribution to the commutator:

$$-[B, A]_{sk} = \sum_m{}' \frac{2sm}{s^2-m^2}\frac{2mk}{m^2-k^2}(-1)^{m-k} - \frac{2sm}{s^2-m^2}(-1)^{s-m}\frac{2mk}{m^2-k^2} =$$

$$\sum_m{}' \frac{4skm^2}{s^2-m^2}\frac{1}{m^2-k^2}(-1)^m\left((-1)^k-(-1)^s\right) =$$

$$4sk\left((-1)^k-(-1)^s\right)\frac{1}{k^2-s^2}\sum_m{}' \left(\frac{k^2(-1)^m}{k^2-m^2} - \frac{s^2(-1)^m}{s^2-m^2}\right)$$

In the sum are excluded *both* m=s and m=k terms.

The sum can be evaluated in the following way. First let us sum on all values but in the form (verify the sum with *Mathematica*):

$$\sum_{L=1}^{\infty} \frac{(-1)^L}{x^2-L^2} = \frac{-1+\pi x \operatorname{Csc}[\pi x]}{2x^2}$$

For x→ k pose x = k + z. Series expansion gives

$$\frac{(-1)^k}{2kz} + \left(-\frac{1}{2k^2} - \frac{(-1)^k}{2k^2}\right) + O(z)$$

The pole term is what must be subtracted, it is in fact the limit of the series term as x→ k,

$$\frac{(-1)^k}{(k+z)^2-k^2} \simeq \frac{(-1)^k}{2kz} - \frac{(-1)^k}{4k^2}$$

After multiplication by k^2we have for the whole sum

$$\left(-\frac{1}{2} - \frac{1}{4}(-1)^k\right).$$

We have now to subtract the term with m = s, as a risult the first sum is

$$-\left(\frac{1}{2} + \frac{1}{4}(-1)^k\right) - \frac{k^2}{k^2-s^2}(-1)^s$$

The second sum is obtained interchanging the roles of s and k, then

$$-[B, A]_{sk} = 4\,s\,k\left((-1)^k - (-1)^s\right)\frac{1}{k^2 - s^2}\left(\frac{1}{s^2 - k^2}\,s^2\,(-1)^k - \frac{1}{k^2 - s^2}\,k^2\,(-1)^s + \frac{(-1)^s - (-1)^k}{4}\right)$$

The first two term, once multiplied by the sign in the prefactor, become

$$\frac{1}{s^2 - k^2}\,s^2\left(1 - (-1)^{k+s}\right) - \frac{1}{k^2 - s^2}\,k^2\left((-1)^{s+k} - 1\right) = -(-1)^{k+s} + 1$$

The two last terms:

$$\left((-1)^k - (-1)^s\right)\left((-1)^s - (-1)^k\right) = 2\left((-1)^{k+s} - 1\right)$$

and

$$-[B, A]_{sk} = \frac{4\,k\,s}{k^2 - s^2}\left((-1)^{k+s} - 1\right)\left(-\frac{1}{2}\right) = \frac{2\,k\,s}{s^2 - k^2}\left((-1)^{k+s} - 1\right) = B_{sk}$$

■ **Oscillations**

If movement of the walls is periodic there is a possibility to produce a resonance phenomenon between particle states. The general equations for a_k coefficients:

p5wallequatonsforAoscill

$$\frac{da_k}{dt} + \sum_s F_{ks}\,a_s = -i\,E_k\,a_k\,; \tag{5.21}$$

are known to produce resonance for external periodic perturbation. let us recall briefly the theory. Extracting the "free evolution", i.e. time dependence due to $E_k$with the change of variables

$$a_k = c_k[t]\,\mathrm{Exp}\left[-i\int_0^t E_k\,dt\right] \equiv c_k[t]\,\mathrm{Exp}[-i\,\delta_k[t]]$$

equations (21) take the form

p5transitionc

$$\frac{dc_k}{dt} + \sum_s \mathrm{Exp}[i\,(\delta_k - \delta_s)]\,F_{ks}\,c_s = 0, \tag{5.22}$$

well suited for an iterative solution. If we start with a system in a state α, i.e. $c_\alpha = 1$, all other c's zero, a perturbative corrections to c_k, for $k \neq \alpha$, is readily obtained

p5transition0order

$$\frac{dc_k}{dt} + \mathrm{Exp}[i\,(\delta_k - \delta_\alpha)]\,F_{k\alpha}\,c_\alpha = 0;\ \Rightarrow c_k \simeq -\int_0^t \mathrm{Exp}[i\,(\delta_k - \delta_\alpha)]\,F_{k\alpha} \tag{5.23}$$

At first order in the "small" perturbation due to F matrix only the term with s=α has been extracted, because at zero order only $c_\alpha$is not zero. Usually the right hand side of (23) is a rapid oscillating function, keeping small the value of the integral, This is the usual perturbation theory (see text). The exception being if in F is present a frequency which cancel the factor $\delta_k - \delta_\alpha$ in this case there is not depression and the amplitude for transition can be large. If we limit to the case of one frequency and assume that approximatively the energy are fixed this happens when the external frequency is near a difference E_β- E_α. We can approximatively restrict our attention to the two system level α-β but we can try to resolve exactly eq.(22) for this reduced system

$$\frac{dc_\beta}{dt} + \mathrm{Exp}[i\,(\delta_\beta - \delta_\alpha)]\,F_{\beta\alpha}\,c_\alpha = 0;\qquad \frac{dc_\alpha}{dt} + \mathrm{Exp}[i\,(\delta_\alpha - \delta_\beta)]\,F_{\alpha\beta}\,c_\beta = 0.$$

Consider for simplicity E_k constants and assume $E_\beta > E_\alpha$. The resonant term in $F_{\beta\alpha}$ is of the form

$$F_{\beta\alpha} = \mathcal{F}\,\mathrm{Exp}[-i\,\Omega\,t];\qquad F_{\alpha\beta} = -\mathcal{F}\,\mathrm{Exp}[i\,\Omega\,t];\qquad \Omega \simeq E_\beta - E_\alpha.$$

The form of $F_{\alpha\beta}$has been deduced from antihermiticity of the matrix F . The equations can be solved and simplify greatly at exact resonance. For $c_\alpha[0] = 0,\ c_\beta[0] = 1$:

$$\frac{dc_\beta}{dt} + \mathcal{F}\,c_\alpha = 0;\quad \frac{dc_\alpha}{dt} - \mathcal{F}\,c_\beta = 0;\quad c_\beta[t] = \mathrm{Cos}[\mathcal{F}\,t];\quad c_\alpha[t] = \mathrm{Sin}[\mathcal{F}\,t].$$

The system oscillated with period $2\pi/\mathcal{F}$. Populations of the levels, $|c_k|^2$ become 1 with period $\pi/\mathcal{F}$.

In the present case the matrix F has the general form (4) p5fksoscill

$$F_{ks} = \int_0^L u_k \partial_t u_s = \frac{2\,k\,s}{k^2 - s^2}\left(\frac{\dot{L}}{L}(-1)^{k-s} + \frac{vL}{L}\left(-1 + (-1)^{k-s}\right)\right)(k \neq s)\;;\; F_{kk} = 0. \tag{5.24}$$

Consider for instance an oscillating box with

$$L = L_0 \,(1 + A\,\mathrm{Cos}[\Omega\, t])$$

The system (24) allows resonance transtions. We can excite the system in two different ways: take fixed one of the walls, the left for definitess, of move both of them in opposite directions, in the last case vR = - vL, vL = - 1/2 dL/dt. In the two cases w ehave respectively

p5fksresonance

$$\begin{aligned} F_{ks} &= \frac{2\,k\,s}{k^2 - s^2}\,\frac{\Omega\,A\,\mathrm{Sin}[\Omega\, t]}{L_0\,(1 + A\,\mathrm{Cos}[\Omega\, t])}\,(-1)^{k-s}\;; \\ F_{ks} &= \frac{2\,k\,s}{k^2 - s^2}\,\frac{\Omega\,A\,\mathrm{Sin}[\Omega\, t]}{L_0\,(1 + A\,\mathrm{Cos}[\Omega\, t])}\,\frac{1}{2}\left((-1)^{k-s} + 1\right) \end{aligned} \tag{5.25}$$

In the first case all transitions are allowed, in the second case only transitions without change of parity. For small oscillations amplitudes, decomposing the trigonometric functions, we see that the "strength factor" $\mathcal{F}$ is given in the two cases by the same expression, as the sum ($1 + (-1)^{k-s}$) cancel the factor 1/2 in the second case:

$$\mathcal{F} = \frac{1}{2}\,\frac{2\,k\,s}{k^2 - s^2}\,\frac{\Omega\,A}{L_0}.$$

Matrices (25) allow resonances induced by higner harmonics, in fact expanding the denominator a whole series of frequencies appear. Another kind of nonlinear resonances can be induced if the transition $k \to s$ can be achieved by $k \to i \to s$, this would correspond to a correction to the model of two states system, or inperturbation theory to higher orders. If corections are just induced by higher harmonics in the perturbation they are simply computed, for example in (25) we have, expanding the denominator

$$\frac{2\,k\,s}{k^2 - s^2}\,\frac{\Omega\,A\,\mathrm{Sin}[\Omega\, t]}{L_0\,(1 + A\,\mathrm{Cos}[\Omega\, t])} \simeq \frac{2\,k\,s}{k^2 - s^2}\,\frac{\Omega\,A}{L_0}\left(\mathrm{Sin}[\Omega t] - A\,\frac{1}{2}\,\mathrm{Sin}[2\,\Omega\, t] + \ldots\right).$$

Passing from trigonometric functions to exponentials this is seen to correspond to an effective strength

$$\mathcal{F}_2 = \frac{k\,s}{k^2 - s^2}\,\frac{\Omega\,A^2}{L_0}\,\frac{1}{2}\,.$$