Let's consider all probability measures on R. Think of a prob. measure as being a single random variable by itself. Given two such random variables x, y, we can make them independent and form the random variable $x+y$.

Precisely $x : \Omega \to R$ and $y : \Omega' \to R$ where Ω, Ω' are measure spaces. Then $x+y : \Omega \times \Omega' \to R$. Consider generating functions.

$$Z_x(J) = \int_\Omega e^{Jx} d\mu \qquad J = i\xi \quad \text{if } x \text{ unbounded}$$

$$Z_y(J) = \int_{\Omega'} e^{Jy} d\mu'$$

$$Z_{x+y}(J) = \int_{\Omega\times\Omega'} e^{J(x+y)} d\mu \times d\mu' = Z_x(J)\, Z_y(J).$$

Therefore we get an operation on probability measures on R corresponding to multiplication of the Fourier transforms. This is convolution of the measures. I guess it's known that signed measures $d\mu$ with $\int_R |d\mu| < \infty$ form an algebra under convolution.

The Bochner thm. tells us how to spot Fourier transforms of finite measures as positive-definite continuous functions of ξ. Probality measure have value 1 when $\xi = 0$.

So the probability measures on the line form a monoid under convolution which can be identified with positive definite continuous functions under product $F(\xi)$ with $F(0) = 1$ by the formula $F(\xi) = \int e^{i\xi x} d\mu(x)$

Claim that the invertible elements of this monoid are given by the δ-measures. In effect we know that $|F(\xi)| \leq 1$ with equality $\Leftrightarrow$ $d\mu$ is supported in a set $\{x \mid e^{-i\xi x} = e^{i\xi a}\}$ which is a coset $a + \frac{2\pi}{\xi}\mathbb{Z}$. If F is invertible, then $|F| = 1$, so $d\mu$ has its support a point.

Let's restrict attention to measures having moments. Then the first moment is a homomorphism of the monoid to $\mathbb{R}$, and this homomorphism is an isom. on the subset of δ-measures, so the monoid is a direct product of δ-measures and measures with mean 0. Then the second moment is a homomorphism to the monoid $(\mathbb{R}_{\geq 0}, +)$. The Gaussian measures of mean 0 are mapped isomorphically under this homomorphism, but there is no possibility of splitting them off.

There is a basic theorem which describes the infinitely decomposable elements of this monoid, i.e. those F which are n-th powers in the monoid for any $n \geq 1$. Such an F cannot vanish - here's why. Suppose $F(\xi) = 0$ but $F(\xi/2) \neq 0$. Because F is positive definite we know the matrix $F(\xi_i - \xi_j)$ is positive-semi-definite for any $\xi_1, \ldots, \xi_n$. Take ξ_i to be the sequence $0, \xi/2, \xi$ and let $a = F(\xi/2)$. Then we get the matrix

$$\begin{pmatrix} 1 & a & 0 \\ \bar{a} & 1 & a \\ 0 & \bar{a} & 1 \end{pmatrix}$$

whose determinant is $1 - |a|^2 - |a|^2 = 1 - 2|a|^2$. This must be ≥ 0 so $|a| \leq \frac{1}{\sqrt{2}}$. But if $F(\xi/2) \neq 0$ [redacted] [redacted] and if we can find an $\tilde{F}$ with $\tilde{F}^N = F$, then for N large enough

$$\left|\tilde{F}(\xi/2)\right| = \left|F(\xi/2)\right|^{1/N} > \frac{1}{\sqrt{2}}$$

and we get a contradiction.

Main example of an inf. decomposable prob. measure is Poisson distribution

$$F = \sum_{n \geq 0} e^{-\lambda} \frac{\lambda^n}{n!} \left(e^{aJ}\right)^n = e^{\lambda(e^{aJ} - 1)}$$

Here

$$\log F = \lambda(e^{aJ} - 1) = \sum_{n \geq 1} \frac{J^n}{n!}(\lambda a^n)$$

so the reduced moments of the distribution are λa^n for $n \geq 1$.

A consequence of $F(\xi)$ never vanishing is that $F^{1/N}$ is well-defined char. fn.; it is the unique continuous N-th root of F with value 1 at $\xi = 0$. In fact we can define $\log F$ and

$$F^t = e^{t \log F}$$

for all $t \geq 0$, getting a stochastic process with independent stationary increments.

We've already encountered the Gaussian process with

$$F(\xi, t) = e^{-t\frac{\xi^2}{2}}$$

or

$$d\mu_t = \frac{e^{-\frac{1}{2}\frac{x^2}{t}}}{\sqrt{2\pi t}}\,dx$$

which describes Brownian motion. Let's consider the example of the Poisson process:

$$F^t = e^{\lambda t(e^J - 1)} = \sum e^{-\lambda t} \frac{(\lambda t)^n}{n!} e^{Jn}$$

Thus we get the probability distribution on N given by

$$(*) \qquad p_n(t) = e^{-\lambda t} \frac{\lambda^n t^n}{n!}.$$

Recall how this arises. One is interested in events like telephone calls. Assume the probability of a call in a small time interval dt is λdt, and let $p_n(t)$ be the probability of exactly n calls in time t. Then

$$p_n(t+dt) = p_{n-1}(t)\lambda dt + p_n(t)(1-\lambda dt)$$

or

$$\begin{cases} \dfrac{dp_n}{dt} = \lambda p_{n-1} - \lambda p_n \\ \dfrac{dp_0}{dt} = -\lambda p_0 \end{cases}$$

and the solution is $(*)$.

Alternative derivation: Start from

$$p(x,t) = \int K(x-x', t-t') p(x',t')\, dx'$$

and let $t' \to t$. The probability distribution $K(x, \Delta t)\,dx$ as $\Delta t \to 0$ should approach $\delta(x)\,dx$ + correction proportional to Δt. Let's do this carefully. Take a test function $\phi(x)$

$$\int dx\, \phi(x) p(x,t) = \int dx'\, p(x',t') \int dx\, \phi(x) K(x-x', t-t')$$

Expand $\quad \phi(x) = \phi(x') + \phi'(x')(x-x') + \dfrac{\phi''(x')}{2!}(x-x')^2 + \cdots$

whence $\int dx\, \phi(x)\, K(x-x', t-t')$

$$= \sum \frac{\phi^{(n)}(x')}{n!} \underbrace{\int dx\, (x-x')^n K(x-x', t-t')}_{}$$

n th moment of the probability distribution $K(x, \Delta t)\, dx$

Now we expect

$$\int e^{Jx} K(x, \Delta t)\, dx = e^{\sum' J^n \frac{b_n(\Delta t)}{n!}}$$

where $\frac{b_n(\Delta t)}{\Delta t} \longrightarrow b_n$ as $\Delta t \to 0$. Notice that for small Δt the moments + reduced moments differ by $O((\Delta t)^2)$. Thus

$$\frac{1}{\Delta t} \int dx\, x^n K(x, \Delta t) \longrightarrow b_n$$

and we get in the limit as $\Delta t \to 0$

$$\int dx\, \phi(x) \frac{\partial p}{\partial t}(x,t) = \cancel{\sum_{n\geq 1}' \phi^{(n)}(x}$$

$$= \int dx'\, p(x';t) \sum \frac{\phi^{(n)}(x')}{n!} b_n .$$

Integrating by parts gives the DE

$$\frac{\partial p}{\partial t} = \sum_{n \geq 1}' \frac{b_n}{n!} (-1)^n \frac{\partial^n p}{\partial x^n}$$

For example if all $b_n = \lambda > 0$ we get

$$\frac{\partial p}{\partial t}(x,t) = \lambda \sum_{n\geq 1}' \frac{(-1)^n}{n!} \frac{\partial^n p}{\partial x^n} = \lambda\, p(x-1,t) - \lambda p(x,t)$$

which is our <u>Poisson process</u> on page 27.

<u>Digression:</u> $\Gamma(s)\Gamma(1-s) = \dfrac{\pi}{\sin \pi s}$

$$\left|\Gamma\left(\tfrac{1}{2}+iy\right)\right|^2 = \frac{\pi}{\sin\left(\frac{\pi}{2}+i\pi y\right)} = \frac{\pi}{\cos i\pi y} = \frac{2\pi}{e^{\pi y}+e^{-\pi y}}$$

$$\Rightarrow \quad \left|\Gamma\left(\tfrac{1}{2}+iy\right)\right| \sim \sqrt{2\pi}\, e^{-\frac{\pi}{2}y} \qquad \text{as} \quad y \to +\infty.$$

Another derivation:

$$\Gamma\left(s+\tfrac{1}{2}\right) = \int_0^\infty e^{-t}\, t^{s+\frac{1}{2}} \frac{dt}{t} = \int_0^\infty e^{-su} (su)^{s+\frac{1}{2}} \frac{du}{u}$$

$$= s^{s+\frac{1}{2}} \int_0^\infty e^{s\underbrace{(-u+\log u)}_{-1-\frac{1}{2}(u-1)^2+\cdots}} u^{-1/2}\, du$$

$$\sim s^{s+\frac{1}{2}} e^{-s} \int_{-\infty}^{\infty} e^{-\frac{s}{2}v^2} (1+v)^{-1/2}\, dv \quad \left(1+O\left(\tfrac{1}{s}\right)\right)$$

$$\sim s^{s+\frac{1}{2}} e^{-s} \frac{\sqrt{2\pi}}{\sqrt{s}} \left(1+O\left(\tfrac{1}{s}\right)\right)$$

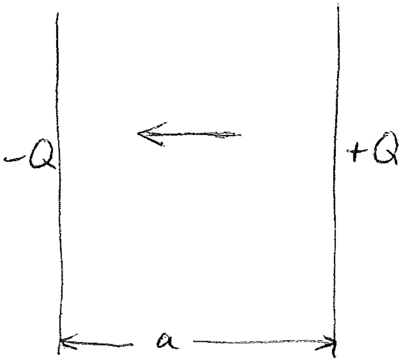
$$\therefore \quad \boxed{\Gamma\left(s+\tfrac{1}{2}\right) = s^s e^{-s} \sqrt{2\pi} \left(1+O\left(\tfrac{1}{s}\right)\right)}$$

$\log \Gamma\left(\tfrac{1}{2}+iy\right) =$ [redacted] $iy \underbrace{\log(iy)}_{\log y + i\frac{\pi}{2}} - iy + \log\sqrt{2\pi}$

$$\therefore \log\left|\Gamma\left(\tfrac{1}{2}+iy\right)\right| = -\frac{\pi}{2}y + \log\sqrt{2\pi} + O\left(\tfrac{1}{y}\right)$$

actually an exponential error

Dielectric behavior of a gas. Treat gas as ideal and dilute so that the molecules don't interact with each other. Review the dielectric formalism: Consider a parallel plate condenser. If a voltage V is



applied charge is pumped from one plate to the other, so that one has charge $+Q$ on one plate and charge $-Q$ on the other. The capacitance is

$$Q = CV.$$

According to Gauss law, the electric field is zero outside the condenser and is constant inside

$$E = \frac{4\pi Q}{A} \qquad \text{e.s. units}$$

pointing from + plate to − plate. Here A is the area of the plate. On the other hand

$$V = aE = \frac{4\pi a}{A} Q$$

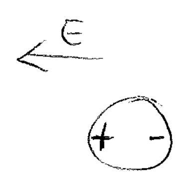
so therefore

$$C = \frac{A}{4\pi a}$$

for a vacuum inside the plates.

Next suppose we have a dielectric medium inside. Then the electric field induces a dipole moment per unit volume

$$\vec{P} = \chi \vec{E}$$



These dipoles cancel inside the condenser except for a surface charge σ. Clearly we can compute the total dipole moment by using the surface charge $\pm\sigma$ separated by the distance a.

$$\vec{P} \cdot aA = \sigma \cdot a \qquad \text{or} \qquad \sigma = PA = \chi E A$$

Then Gauss gives

$$E = \frac{4\pi}{A}(Q - \sigma)$$

so

$$= \frac{4\pi}{A}(Q - \chi E A) = \frac{4\pi Q}{A} - 4\pi \chi E$$

$$(1 + 4\pi\chi)E = \frac{4\pi Q}{A}$$

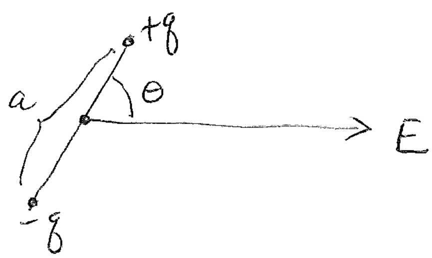
$$V = aE = \frac{4\pi a}{A(1 + 4\pi\chi)} Q$$

so the capacitance is

$$\varepsilon = (1 + 4\pi\chi)$$

$$C = (1 + 4\pi\chi)\frac{A}{4\pi a} \qquad \cancel{\varepsilon = \frac{1}{1+4\pi\chi}}$$

Now suppose the medium in our condenser is a gas of polar molecules.



The electostatic energy of the molecule in the field E is

$$-\vec{\mu} \cdot \vec{E}$$

where μ is the dipole moment. If there were no thermal agitation the molecules would line up with minimum energy pointing in the direction of $\vec{E}$, and the dipole moment of the molecule would be $\mu_0 = aq$.

At non-zero temperature we want the effective dipole moment. Thus we have to average $\mu_0 \cdot \vec{\varepsilon}$ where ε runs over all unit vectors weighted by the Bolzmann factor $e^{+\beta\mu_0 \vec{\varepsilon}\cdot\vec{E}}$.

$$Z = \frac{1}{2}\int_0^{\pi} e^{\beta\mu_0|E|\cos\theta} \sin\theta \, d\theta = \left[-\frac{e^{\beta\mu_0|E|\cos\theta}}{2\beta\mu_0|E|} \right]_0^{\pi}$$

$$= \frac{e^{\beta\mu_0|E|} - e^{-\beta\mu_0|E|}}{2\beta\mu_0|E|}$$

$$\langle \mu_0 \cdot \vec{\varepsilon} \rangle = \frac{1}{\beta}\frac{\vec{\partial}}{\partial E} \log Z$$

$$= \frac{1}{\beta}\frac{\vec{\partial}}{\partial E}\left\{ -\log|E| + \log\left(e^{\beta\mu_0|E|} - e^{-\beta\mu_0|E|}\right) \right\}$$

$$= \frac{1}{\beta}\left\{ -\frac{E}{|E|^2} + \frac{e^{\beta\mu_0|E|} + e^{-\beta\mu_0|E|}}{e^{\beta\mu_0|E|} - e^{-\beta\mu_0|E|}} \beta\mu_0 \frac{E}{|E|} \right\}$$

$$= \mu_0 \underbrace{\left\{ \frac{e^{\beta\mu_0|E|} + e^{-\beta\mu_0|E|}}{e^{\beta\mu_0|E|} - e^{-\beta\mu_0|E|}} - \frac{1}{\beta\mu_0|E|} \right\}}_{\mathcal{L}(\beta\mu_0|E|)} \frac{E}{|E|}$$

where $\mathcal{L}$ is the Langevin fn.

$$\mathcal{L}(y) = \frac{e^y + e^{-y}}{e^y - e^{-y}} - \frac{1}{y} = \frac{1 + \frac{y^2}{2} + \frac{y^4}{4!}}{y + \frac{y^3}{3!} + \frac{y^5}{5!}} - \frac{1}{y}$$

$$= \frac{1}{y}\left[\left(1 + \frac{y^2}{2} + \frac{y^4}{24} + \right)\left(1 + \frac{y^2}{6} + \frac{y^4}{120} + \right)^{-1} - 1 \right]$$

$$\boxed{\mathcal{L}(y) = \frac{1}{3}y - \frac{1}{45}y^3 + \cdots}$$

Thus the average dipole moment is for small E

$$\langle \vec{\mu} \rangle = \mu_0 \frac{1}{3} \beta \mu_0 |E| \frac{E}{|E|} = \frac{1}{3}\beta\mu_0^2 \cdot E$$

so $\quad \chi = \frac{1}{3}\beta\mu_0^2 \quad$ for 1 -molecule.

For the gas

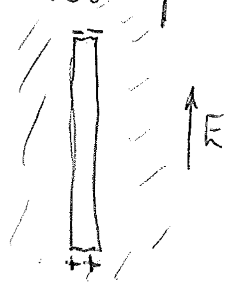
$$\chi = \rho \frac{1}{3}\beta\mu_0^2$$

and so the dielectric constant is

$$\varepsilon = 1 + 4\pi \frac{\rho}{3}\beta\mu_0^2$$

In the above we assumed that the electric field seen by the molecule is the constant macroscopic electric field corresponding to the voltage between the plates. This ignores the obvious atomic variation. In order to take this variation into account one removes the atom and looks for the field in the remaining hole. The field depends on the shape of the hole.

Ex 1. Thin slit parallel to E. The surface charges at the ends of the slit are negligible, so the field inside the slit is the same as the field E in the dielectric

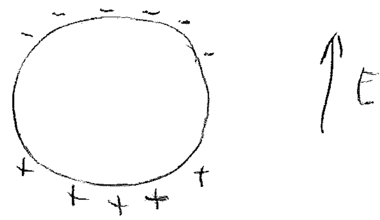


Ex 2. Thin slit perpendicular to E

Here the field inside the slit is

$$D = E + 4\pi P$$

Ex. 3 Circular hole.



In this case computation shows the field [redacted] in the hole to be

$$\tilde{E} = E + \frac{1}{3} 4\pi P.$$

The idea is that we want to use $\tilde{E}$ to compute the polarization:

$$P = \chi \tilde{E}$$

$$\therefore \ P = \chi E + \frac{4\pi\chi}{3} P$$

$$P = \frac{\chi}{1 - \frac{4\pi\chi}{3}} E$$

Recall

$$E = \frac{4\pi}{A}(Q - PA) = \frac{4\pi}{A} Q - 4\pi P$$

$$\frac{4\pi}{A} Q = E + \frac{4\pi\chi}{1 - \frac{4\pi\chi}{3}} E \qquad E = \frac{V}{a}$$

$$Q = \frac{4\pi A}{a}\left(1 + \frac{4\pi\chi}{1 - \frac{4}{3}\pi\chi}\right) V$$

Thus the dielectric constant is

$$\varepsilon = 1 + \frac{4\pi\chi}{1 - \frac{1}{3}4\pi\chi}$$

which gives

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{4\pi}{3}\chi$$

and Clausius - Mossotti

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{4\pi}{3}\left(\frac{\rho \mu_0^2}{kT} + \rho\alpha\right) \qquad \rho = \text{density}$$

polar part depending on temperature | this is normal susceptibility of the molecule which exists for non-polar molecule. temperature independent

August 14, 1980

Neutron Scattering by a crystal (or liquid or gas). The free neutron is described by the Hamiltonian

$$\frac{p^2}{2M} \qquad p = \frac{\hbar}{i}\nabla$$

acting on L^2(space); we ignore spin. [redacted] The neutron interacts with only the nuclei of the solid and the interaction is of very short range (10^{-13} cm. as opposed to atomic dimensions $\sim 1A^\circ = 10^{-8}$ cm.)

Let R_i run over the positions of the nuclei in the solution and let $V(R-R_i)$ denote the potential energy of the neutron located at R and [redacted] solid atom as R_i. Then the interaction Hamiltonian is

$$\sum_i V(R-R_i)$$

Next we need a [redacted] description of the "solid". There are two possible simple models.

1. Crystal: Here one has a generalized harmonic oscillator:

$$H = \sum_i \frac{p_i^2}{2m} + \text{quadratic fn. of } R_i - R_i^\circ = q_i$$

so one knows the Hilbert space is a boson Fock space with single particles called phonons described by wave vectors + polarization.

2. Ideal gas: The Hilbert space is a Fock space (either boson or fermion) with single particles described by

$$\frac{p^2}{2m} \qquad p = \frac{\hbar}{i}\nabla \qquad \text{on } L^2(\text{space}).$$

So let's look at the case of the gas. Fix the number of particles to be N. The Hilbert space of states for the neutron + gas is the tensor product

$$\mathcal{H}_{neutron} \otimes \Lambda^N \qquad \text{(suppose fermions)}$$

so a state is described by a wave function $f(Q, x_1, \dots, x_N)$ antisymmetric in the x_j. ~~we take~~ The interaction energy is the operator of multiplying by

$$(*) \qquad \sum_{j=1}^{N} V(Q - x_j)$$

So now take the direct sum over all N and we get the Hilbert space

$$\mathcal{H}_{neutron} \otimes \underset{\text{(fermion Fock space)}}{\Lambda}$$

The interaction energy is an operator on this tensor product. If we give a basis for $\mathcal{H}_{neut.}$, then we get a matrix of operators on Λ. So if we take the basis $|Q\rangle$ for $\mathcal{H}_{neut}$, we get a diagonal matrix, and the operator on Λ corresponding to position Q is $(*)$. This is the one-particle operator associated to the function $x \mapsto V(Q-x)$ and hence can be written

$$\int dx\, \psi(x)^* V(Q-x) \psi(x).$$

(Recall that $\psi(x)^* \psi(y)$ form a basis for the 1-particle operators on Λ). Thus our interaction operator is

$$H_{int} = \int dQ \; |Q\rangle \int dx\, \psi(x)^* V(Q-x) \psi(x) \; \langle Q| \, ,$$

We want to convert this to momentum basis using

$$\langle x | k \rangle = e^{ikx} \qquad \int \frac{dk}{2\pi} |k\rangle\langle k| = id$$

$$\langle Q | K \rangle = e^{iKQ} \qquad \int \frac{dK}{2\pi} |K\rangle\langle K| = id$$

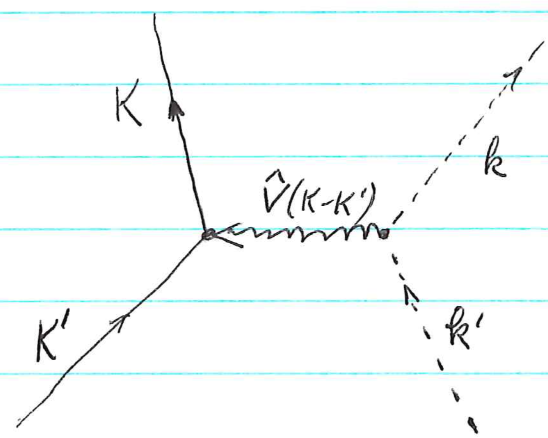
$$H_{int} = \int \frac{dK}{2\pi}\frac{dK'}{2\pi}\frac{dk}{2\pi}\frac{dk'}{2\pi} \int dQ\,dx\; |K\rangle\langle K|Q\rangle\, \psi_k^* \langle k|x\rangle$$

$$\times\, V(Q-x)\, \langle x|k'\rangle\, \psi_{k'}\, \langle Q|K'\rangle\langle K'|$$

$$= \int \frac{dK\,dK'\,dk\,dk'}{(2\pi)^4} |K\rangle \psi_k^* \psi_{k'} \langle K'| \underbrace{\int dQ\,dx\; e^{-iKQ-ikx+ik'x+iK'Q}\, V(Q-x)}_{\int dQ\,dx\, \hat{V}(Q)\, e^{-iK(Q+x)-ikx+ik'x+iK'(Q+x)}}$$

$$2\pi\,\delta(-K - k + k' + K')\, \hat{V}(K-K')$$

It appears that the diagrams belonging to this interaction are



where momentum is conserved: $k' + K' = k + K$.

Next we should see how this changes when our gas is replaced by a crystal.

Let's compute the matrix elements of H_{int} relative to the basis $|K\rangle$ for $\mathcal{H}_{neut}$.

$$\langle K | H_{\text{[redacted]}\,int} | K' \rangle = \langle K | \sum_j V(Q - x_j) | K' \rangle$$

$$= \int dQ \; e^{-iKQ} \sum V(Q - x_j) \, e^{iK'Q}$$

$$= \sum_j \int dQ \; e^{-i(K-K')(Q+x_j)} \, V(Q \cancel{-x_j})$$

$$= \underbrace{\left(\sum_j e^{-i(K-K')x_j} \right)}_{\text{this is an operator on } \mathcal{H}_{solid}} \hat{V}(K-K')$$

Nice situation. What we are trying to understand is inelastic scattering of the neutron by a bunch of particles. One might obtain simpler models by having a single particle with position x which is tied down by a potential. Then the neutron might knock this particle into a higher state.

The simplest example of this type might be the [redacted] X-ray problem. Here the Hilbert space is

$$\mathcal{H}_{neut} \otimes \mathbb{C}^2$$

where $\mathbb{C}^2$ is a 2-state system.

August 16, 1980

Let's work out the motion of Gaussian wave packets in time, no forces acting.

$$\psi(x,t) = \int \frac{dk}{2\pi}\, e^{i(kx - \omega_k t)}\, \Psi(k)$$

$$\hbar\omega_k = \frac{(\hbar k)^2}{2m} \qquad \omega_k = \frac{\hbar}{m}\frac{k^2}{2}$$

and $\Psi(k)$ will be a Gaussian function

$$\Psi(k) = e^{-\alpha\frac{k^2}{2} + \beta k} \cdot \text{Const.} \qquad \text{Re}(\alpha) > 0$$

By translating w.r.t. x, t we can assume α, β are real, so let's suppose

$$\Psi(k) = e^{-a\frac{k^2}{2} + bk} \qquad a > 0,\ b \text{ real.}$$

The average momentum of this packet is

$$\langle p \rangle = \frac{\int \frac{dk}{2\pi}\, \hbar k\, |\Psi(k)|^2}{\int \frac{dk}{2\pi} |\Psi(k)|^2}$$

If we center

$$-a\frac{k^2}{2} + bk = -a\frac{\left(k - \frac{b}{a}\right)^2}{2} + \frac{b^2}{2a}$$

then we see that $|\Psi(k)|^2 = e^{-a\left(k - \frac{b}{a}\right)^2} \cdot \text{const.}$

defines a Gaussian distribution with mean $\frac{b}{a}$. Thus

$$\langle p \rangle = \hbar\frac{b}{a}$$

Now

$$\psi(x,t) = \int \frac{dk}{2\pi}\, e^{-\left(a + i\frac{\hbar}{m}t\right)\frac{k^2}{2} + i(x - ib)k}$$

$$= \frac{1}{\sqrt{2\pi\left(a+i\frac{\hbar}{m}t\right)}}\, e^{-\frac{1}{\left(a+i\frac{\hbar}{m}t\right)}\frac{(x-ib)^2}{2}}$$

$$\frac{1}{\left(a+i\frac{\hbar}{m}t\right)}\frac{(x-ib)^2}{2} = \frac{a-i\frac{\hbar}{m}t}{a^2+\frac{\hbar^2}{m^2}t^2}\left(\frac{x^2}{2}-ibx-\frac{b^2}{2}\right)$$

We are interested in the real part of this exponent which gives the probability distribution for finding the particle

$$+\ \text{Re part} = \frac{a}{a^2+\left(\frac{\hbar}{m}t\right)^2}\frac{x^2}{2} - \frac{\frac{\hbar}{m}tb}{a^2+\left(\frac{\hbar}{m}t\right)^2}\,x \quad + \text{const}$$

This has a minimum at

$$ax = \frac{\hbar}{m}tb \quad \text{or} \quad x = \underbrace{\frac{\hbar b}{a}}_{\langle p\rangle}\frac{1}{m}t$$

so the mean position is $\langle x\rangle = \frac{\langle p\rangle}{m}t$.
The variance of this Gaussian packet is

$$\langle x^2\rangle - \langle x\rangle^2 = \frac{a^2+\left(\frac{\hbar}{m}t\right)^2}{2a}$$

(The 2 comes from the fact that $|\psi(x,t)|^2 = e^{-\frac{2a}{a^2+\left(\frac{\hbar}{m}t\right)^2}\frac{x^2}{2}+\cdots}$.
Hence the standard deviation of the wave packet is

$$\sqrt{\langle x^2\rangle-\langle x\rangle^2} = \sqrt{\frac{a^2+\left(\frac{\hbar}{m}t\right)^2}{2a}} \sim \frac{1}{\sqrt{2a}}\frac{\hbar}{m}|t|$$

for large $|t|$.

<u>Notice</u>: For heat flow + random walk, the standard deviation is proportional to $\sqrt{t}$.

Question: Is there a thermal side to classical scattering?

It's not clear what this might mean. You could try to describe a beam of classical particles (e.g. bullets) as some sort of distribution on phase space.

Remarks on scattering by a potential from the classical viewpoint. Suppose the potential is central: $V(r)$. Then angular momentum is conserved, and for a given angular momentum the motion is governed by a radial equation which is motion in an effective potential. Recall

$$L \text{ [redacted] } = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - V(r)$$

$$p_r = m\dot{r} \qquad p_\theta = mr^2\dot{\theta}$$

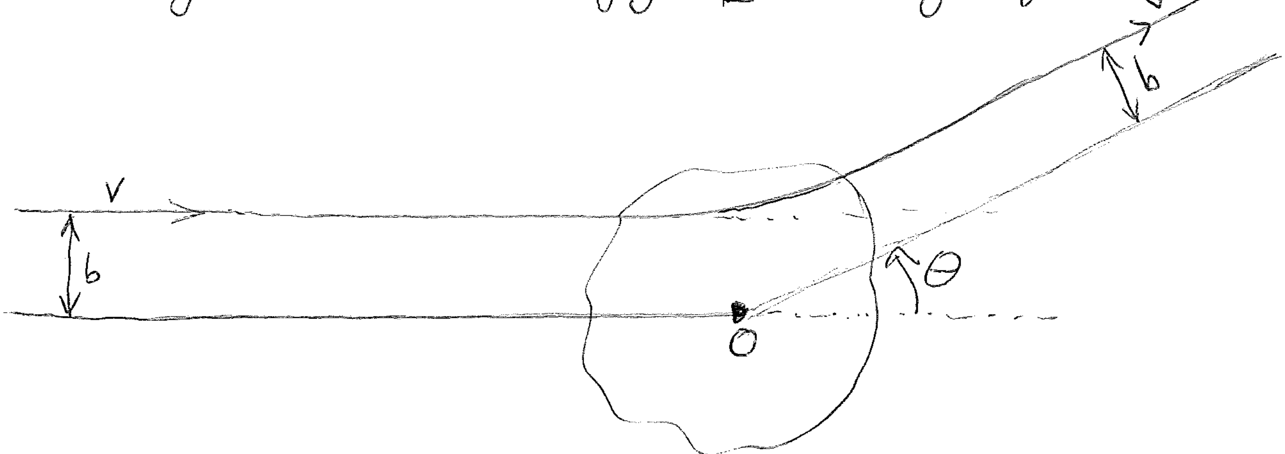
$$H = \frac{1}{2}m\left(\frac{p_r^2}{m^2} + r^2\left(\frac{p_\theta}{mr^2}\right)^2\right) + V$$

$$= \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + V(r) \qquad \dot{p}_\theta = 0 \quad \therefore p_\theta = J \text{ const.}$$

so

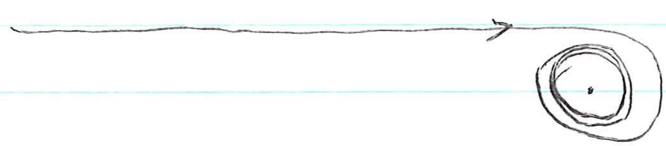
$$\dot{p}_r = -\frac{\partial H}{\partial r} = -\frac{\partial}{\partial r}\underbrace{\left(\frac{J^2}{2mr^2} + V(r)\right)}_{V_{eff}(r)}$$

[redacted] Suppose that we consider a V of finite range and fix the angular momentum J. Then what does the scattering amount to classically? One gives the energy [redacted] away from the scatterer

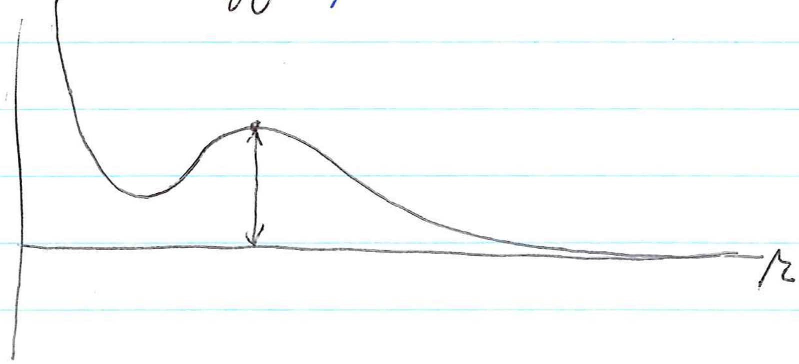


Then the velocity is known and $J = vb$ where b is the impact parameter. Quantities of interest are the scattering angle and the "sojourn time". The sojourn time can be defined as the extra time taken by the scattering. Look radially; pick a large R and compare the time [redacted] taken to go in from a distance R, scatter and come out to distance R, and do this both with V and [redacted] without.

Notice that there may exist orbits which get trapped:

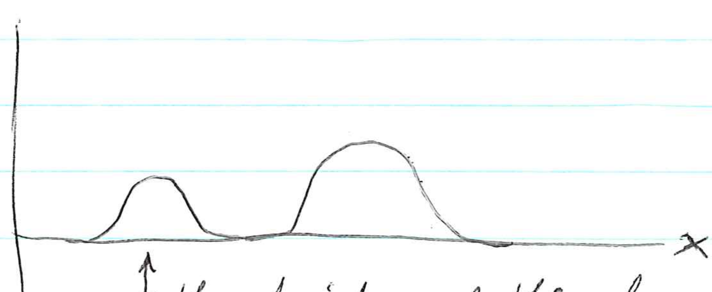


e.g. where the eff. potential looks as follows:



If the energy is exactly the height of the first hump we will get such a spiral.

Suppose one looks at 1-diml scattering on the half-line.



the position of this hump cannot be located by classical scattering data

We have

$$\frac{m}{2}\left(\frac{dx}{dt}\right)^2 + V(x) = E \qquad \text{Put } m=2$$

$$\frac{dx}{dt} = \pm\sqrt{E - V(x)}$$

$$dt = [redacted] \frac{dx}{\sqrt{E - V(x)}}$$

Hence [redacted] if $E > \sup V(x)$, the time taken to go from R to O and back is

$$T(E) = 2\int_0^R \frac{dx}{\sqrt{E - V(x)}}$$

This can be expanded in a series

$$\left(E - V(x)\right)^{-1/2} = E^{-1/2}\left(1 - \frac{V}{E}\right)^{-1/2}$$

$$= E^{-1/2}\left(1 + \frac{1}{2}\frac{V}{E} + \frac{3}{8}\frac{V^2}{E^2} + \cdots\right)$$

and so $T(E)$ is effectively equivalent to the moments

$$\int_0^R V(x)^n \, dx$$

These do not determine V in general, e.g. we can translate. [redacted] Even if lower energies are allowed, one can't locate the position of a hump hidden behind a potential wall.

August 18, 1980

Feynman's inequality: $F \leq F_0 + \langle H - H_0 \rangle_0$.
Here we have a perturbation situation

$$H = H_0 + V \qquad\qquad V = H - H_0$$

and F, F_0 are the actual + unperturbed free energies:

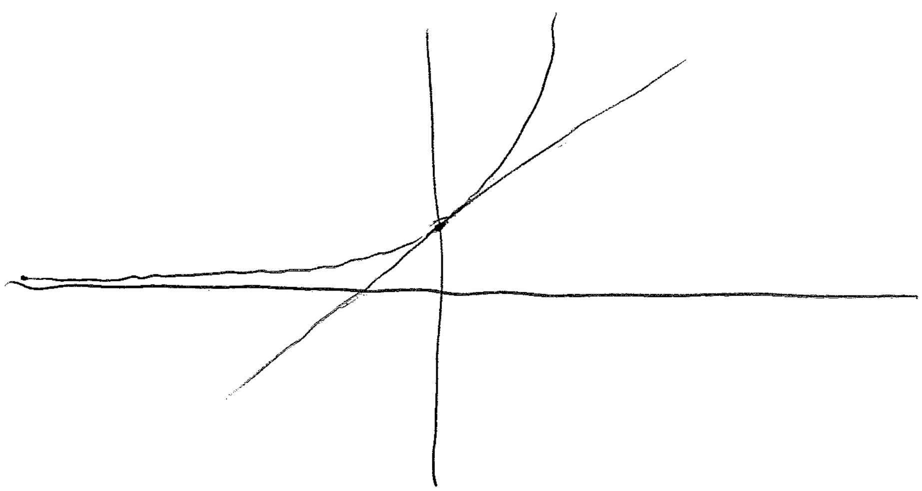
$$e^{-\beta F} = tr\left(e^{-\beta H}\right) \qquad \text{(also with } 0\text{)}$$

and
$$\langle A \rangle_0 = tr\left(e^{-\beta H_0} A\right) \Big/ tr\left(e^{-\beta H_0}\right).$$

Proof in a classical situation.

$$\frac{e^{-\beta F}}{e^{-\beta F_0}} = \frac{\int e^{-\beta(H_0 + V)}}{\int e^{-\beta H_0}} = \langle e^{-\beta V} \rangle_0$$

Now $e^x \geq 1 + x$



so that [redacted]

$$e^{-\beta(V - \langle V \rangle_0)} \geq 1 - \beta(V - \langle V \rangle_0)$$

$$\Rightarrow \quad \left\langle e^{-\beta(V - \langle V \rangle_0)} \right\rangle_0 \geq 1 \Rightarrow \langle e^{-\beta V} \rangle_0 \geq e^{-\beta \langle V \rangle_0}$$

Taking logarithms

$$-\beta F + \beta F_0 \geq -\beta \langle V \rangle_0$$

and so Feynman's inequality results since $\beta > 0$.

Another proof can be based upon

$$H_\lambda = H_0 + \lambda V \qquad 0 \leq \lambda \leq 1.$$

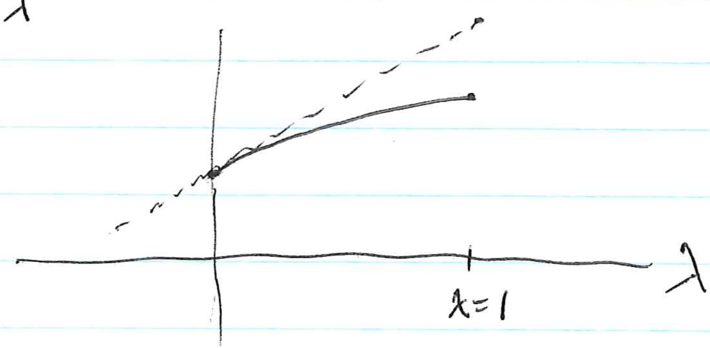
To simplify, set $\beta = 1$. [redacted].
Then

$$F_\lambda = -\log \int e^{-H_0 - \lambda V}$$

$$\frac{dF_\lambda}{d\lambda} = \frac{\int V e^{-H_0 - \lambda V}}{\int e^{-H_0 - \lambda V}} = \langle V \rangle_\lambda$$

$$-\frac{d^2 F_\lambda}{d\lambda^2} = \langle V^2 \rangle_\lambda - \langle V \rangle_\lambda^2 \geq 0.$$

Thus F_λ is concave downward



so

$$F_\lambda \leq F_0 + \underbrace{\lambda \left.\frac{dF_\lambda}{d\lambda}\right|_{\lambda=0}}_{\langle V \rangle_0}$$

which is the Feynman inequality.

In the quantum situation it is no longer

true that
$$e^{-\beta(H_0+V)} = e^{-\beta H_0}\, e^{-\beta V}$$
and so we have to work more carefully.

The basic question is whether [redacted]
$$F_\lambda = -\log\left(\operatorname{tr} e^{-(H_0+\lambda V)}\right)$$
is concave downward. It's enough to see that $\frac{d^2F}{d\lambda^2} \le 0$ at $\lambda = 0$. This is a 2nd order matter in perturbation theory. Dyson equation
$$e^{+H_0} e^{-H_0-V} = 1 - \int_0^1 dt_1\, V(t_1) + \int_0^1 dt_1 \int_0^{t_1} dt_2\, V(t_1)V(t_2) - \cdots$$
where $\quad V(t) = e^{+tH_0} V e^{-tH_0}$.

$$\frac{\operatorname{tr}\left(e^{-(H_0+V)}\right)}{\operatorname{tr}\left(e^{-H_0}\right)} = \left\langle e^{H_0} e^{-(H_0+V)} \right\rangle_0$$
$$= 1 - \int_0^1 dt_1 \langle V(t_1)\rangle_0 + \int_0^1 dt_1 \int_0^{t_1} dt_2 \langle V(t_1)V(t_2)\rangle_0 - \cdots$$

$$\langle V(t)\rangle_0 = \frac{\operatorname{tr}\left(e^{-H_0} e^{tH_0} V e^{-tH_0}\right)}{\operatorname{tr}\left(e^{-H_0}\right)} = \frac{\operatorname{tr}\left(e^{-H_0} V\right)}{\operatorname{tr}\left(e^{-H_0}\right)} = \langle V\rangle_0$$
is independent of t.

I need
$$\int_0^1 dt_1 \int_0^{t_1} dt_2\, e^{\alpha(t_1-t_2)} = \int_0^1 dt_1\, e^{\alpha t_1} \underbrace{\left[\frac{e^{-\alpha t_2}}{-\alpha}\right]_0^{t_1}}_{\frac{1-e^{-\alpha t_1}}{\alpha}}$$
$$= \int_0^1 dt\, \frac{e^{\alpha t}-1}{\alpha} = \left[\frac{e^{\alpha t}}{\alpha^2} - \frac{t}{\alpha}\right]_0^1 = \frac{e^\alpha - 1}{\alpha^2} - \frac{1}{\alpha} = \begin{cases} \dfrac{e^\alpha - 1 - \alpha}{\alpha^2} & \alpha \neq 0 \\[2mm] \dfrac{1}{2} & \text{if } \alpha = 0 \end{cases}$$

$$\langle V(t_1)V(t_2)\rangle_0 = \operatorname{tr}\left(e^{-H_0}e^{t_1H_0}Ve^{-t_1H_0}e^{t_2H_0}Ve^{-t_2H_0}\right)\Big/ \underbrace{\operatorname{tr}(e^{-H_0})}_{Z}$$

$$= \frac{1}{Z}\operatorname{tr}\left(e^{-H_0+(t_1-t_2)H_0}Ve^{-(t_1-t_2)H_0}V\right)$$

$$= \frac{1}{Z}\sum_{m,n} e^{-E_m+(t_1-t_2)E_m}\langle m|V|n\rangle e^{-(t_1-t_2)E_n}\langle n|V|m\rangle$$

$$\int_0^1 dt_1\int_0^{t_1} dt_2 \langle V(t_1)V(t_2)\rangle_0 = \frac{1}{Z}\sum_{m,n} e^{-E_m}|\langle m|V|n\rangle|^2 \begin{cases} \left(e^{\varepsilon_{mn}}-1-\varepsilon_{mn}\right)/\varepsilon_{mn}^2 \\ \frac{1}{2} & \text{if } E_m=E_n \end{cases}$$

where $\varepsilon_{mn} = E_m - E_n$

To establish the inequality I want there is no harm in supposing the energy levels of H_0 are non-degenerate. Thus the above integral is

$$(*)\quad \frac{1}{Z}\sum_m e^{-E_m}|\langle m|V|m\rangle|^2\cdot\frac{1}{2} + \frac{1}{Z}\sum_{m\neq n} e^{-E_m}|\langle m|V|n\rangle|^2\,\frac{e^{\varepsilon_{mn}}-1-\varepsilon_{mn}}{\varepsilon_{mn}^2}$$

Also we have

$$\int_0^1 dt_1\langle V(t_1)\rangle_0 = \langle V\rangle_0 = \frac{1}{Z}\sum e^{-E_m}\langle m|V|m\rangle$$

What I want to determine is the 2nd degree term in V of

$$\log\frac{\operatorname{tr}(e^{-(H_0+V)})}{\operatorname{tr}(e^{-H_0})} = \log\left(1-\int_0^1 dt\langle V(t)\rangle_0 + \int_0^1 dt_1\int_0^{t_1}dt_2\langle V(t_1)V(t_2)\rangle_0 - \cdots\right)$$

$$= -\langle V\rangle_0 - \frac{1}{2}\langle V\rangle_0^2 + \int_0^1 dt_1\int_0^{t_1}dt_2\langle V(t_1)V(t_2)\rangle_0 + O(V^3)$$

~~It is obvious that this 2nd degree term is ≥ 0, since $\langle V(t)\rangle_0 = \langle V\rangle_0$, hence it can be written~~

$$\cancel{\int_0^1 dt_1\int_0^{t_1} dt_2 \langle V(t_1)}$$

Notice that if V is diagonal i.e. all $\langle m|V|n\rangle = 0$ for $m \neq n$, then we know

$$\int_0^1 dt_1 \int_0^{t_1} dt_2 \, \langle V(t_1) V(t_2) \rangle_0 = \frac{1}{2} \langle V^2 \rangle_0 \geq \frac{1}{2} \langle V \rangle_0^2$$

But the explicit expression ⊛ shows that the non-diagonal part of V contribute a positive quantity to the $\int_0^1 dt_1 \int_0^{t_1} dt_2 \, \langle V(t_1) V(t_2) \rangle_0$. So it's clear we have

$$\frac{d^2}{d\lambda^2} \log\left(\frac{\operatorname{tr} e^{-(H_0 + \lambda V)}}{\operatorname{tr} e^{-H_0}} \right) \Bigg|_{\lambda = 0} \geq 0$$

and this is enough to establish the Feynman inequality in the quantum case.

This is the same as the proof in Feynman's book. He notes that

$$e^{-E_m} \frac{e^{\varepsilon_{mn}} - 1 - \varepsilon_{mn}}{\varepsilon_{mn}^2} + e^{-E_n} \frac{e^{\varepsilon_{nm}} - 1 - \varepsilon_{nm}}{\varepsilon_{nm}^2}$$

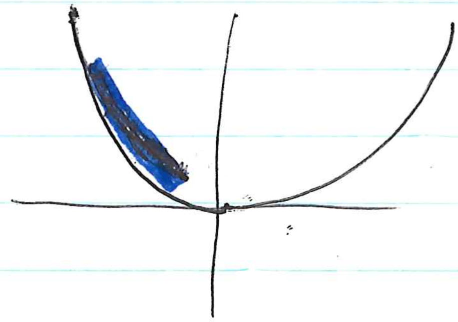
$$= - \frac{e^{-E_m} - e^{-E_n}}{E_m - E_n}$$

so that

$$\int_0^1 dt_1 \int_0^{t_2} dt_2 \, \langle V(t_1) V(t_2) \rangle_0 = \frac{1}{Z} \sum_{m,n} |\langle m|V|n\rangle|^2 \frac{e^{-E_m} - e^{-E_n}}{-E_m + E_n}$$

We now should be in a good position to understand [redacted] the effective potential in a quantum situation. I want to consider motion on the line with the potential U. Fix an inverse temp. β. The Hamiltonian is

$$H_0 = \frac{p^2}{2m} + U(x)$$



and I should think of U as: The simplest example is the harmonic oscillator potential $U(x) = \frac{1}{2}\kappa x^2$.

At the inverse temperature β, the expected position of the particle is

$$\langle x \rangle = \frac{tr\left(e^{-\beta H_0} x\right)}{tr\left(e^{-\beta H_0}\right)} = \frac{\sum_m e^{-\beta E_m} \langle m | x | m \rangle}{\sum e^{-\beta E_m}}$$

[redacted] To get the pseudo-potential we add a "source" term, i.e. a constant force J, to get

$$H_J = \frac{p^2}{2m} + U(x) - Jx$$

and then

$$\langle x \rangle (J) = \frac{tr\left(e^{-\beta H_J} x\right)}{tr\left(e^{-\beta H_J}\right)}$$

The pseudo-potential explains the force J required to achieve a given value of $\langle x \rangle$.

$$\langle x \rangle = \frac{tr\left(e^{-\beta H_J} x\right)}{tr\left(e^{-\beta H_J}\right.} = \frac{1}{\beta}\frac{d}{dJ}\log\left(\frac{tr\left(e^{-\beta H_J}\right)}{[redacted]}\right)$$

Thus put
$$F(J) = -\frac{1}{\beta}\log \operatorname{tr}(e^{-\beta H_J}) \qquad \frac{dF}{dJ} = -\langle x\rangle$$
and then the pseudo-potential is the Legendre transform
$$\Gamma(\langle x\rangle) = \langle x\rangle J + F(J)$$

I need some examples:

Harmonic oscillator: $U(x) = \frac{1}{2}Kx^2$. Then
$$U(x) - Jx = \frac{1}{2}Kx^2 - Jx$$
$$= \frac{1}{2}K\left(x - \frac{J}{K}\right)^2 - \frac{J^2}{2K}$$
so all we've done is to shift the position; more precisely we get a harmonic oscillator centered at $x = \frac{J}{K}$. Thus
$$\langle x\rangle = \frac{J}{K}$$
so up to a constant
$$\Gamma(\langle x\rangle) = \frac{1}{2}K\langle x\rangle^2$$

August 19, 1980

To understand a bit about the effective potential for quantum motion on the line. Start with the Hamiltonian

$$H = \frac{p^2}{2m} + V(x)$$

and put

$$Z(J) = \frac{tr\left(e^{-\beta(H-Jx)}\right)}{tr\left(e^{-\beta H}\right)}$$

so that

$$\frac{d}{dJ}\frac{\log Z}{\beta} = \frac{tr\left(e^{-\beta(H-Jx)}x\right)}{tr\left(e^{-\beta H}\right)} = \langle x \rangle$$

One thing that might be interesting to know is whether there is a probability measure on the line for which $Z(J)$ is the generating function. It seems this follows from the path integral formula which we now recall.

$$e^{-\beta H} = \text{[redacted]} \lim_{n\to\infty}\left(e^{-\Delta t\left(\frac{p^2}{2m}\right)} e^{-\Delta t V}\right)^n$$

with $\Delta t = \frac{\beta}{n}$

$$\langle x | e^{-\Delta t \frac{p^2}{2m}} | x' \rangle = \int \frac{dp}{2\pi\hbar} e^{i\frac{p}{\hbar}(x-x') - \Delta t \frac{p^2}{2m}}$$

$$= \int \frac{dk}{2\pi} e^{ik\Delta x - \Delta t \frac{\hbar^2}{2m}k^2}$$

$$= \frac{1}{\sqrt{2\pi\hbar^2\Delta t/m}} e^{-\frac{m}{\hbar^2 \Delta t}\frac{(\Delta x)^2}{2}}$$

which leads to a path integral expression

$$tr(e^{-\beta H}) = \int_{x(0)=x(\beta)} \mathcal{D}x(t)\, e^{-\int_0^\beta \left[\frac{1}{\hbar^2}\frac{m}{2}\left(\frac{dx}{dt}\right)^2 + V(x)\right]dt}$$

and hence

$$Z(J) = \frac{tr\left(e^{-\beta(H-Jx)}\right)}{tr\left(e^{-\beta H}\right)} = \frac{\int \underbrace{\mathcal{D}x\, e^{-\int_0^\beta \left[\frac{1}{\hbar^2}\frac{m}{2}\dot{x}^2 + V(x)\right]dt}}\; e^{J\int_0^\beta x\, dt}}{\int\left(\qquad\qquad\right)}$$

From the theory of Wiener measure one can interpret

$$\mathcal{D}x(t)\, e^{-\int_0^\beta \left[\frac{1}{\hbar^2}\frac{m}{2}\left(\frac{dx}{dt}\right)^2 + V(x)\right]dt} \Big/ \int \text{same}$$

as a probability measure on continuous paths. Thus we see that $Z(J)$ is the generating function for the random variable

$$x(t) \longmapsto \int_0^\beta x\, dt$$

In order to really understand this business you need some examples where you can compute various limiting cases: $\beta \to \infty$ or $\hbar \to 0$.

Actually in view of the Feynman inequality, it is reasonable to ask if

$$\lambda \longmapsto \frac{tr\left(e^{-H_0 - \lambda V}\right)}{tr\left(e^{-H_0}\right)}$$

is the generating function of a probability measure on the line, i.e. of the form

$$\int e^{\lambda x}\, d\mu(x) \qquad ?$$

August 20, 1980

Consider

$$\mathrm{tr}\left(e^{-(H_0+\lambda V)}\right) = \lim_{n\to\infty} \mathrm{tr}\left(\left(e^{-\frac{1}{N}H_0}\, e^{-\frac{1}{N}\lambda V}\right)^N\right).$$

Fix N and introduce variables $\lambda_1, \ldots, \lambda_N$. Then

$$\mathrm{tr} \prod_{j=1}^{N}\left(e^{-\frac{1}{N}H_0}\, e^{-\frac{1}{N}\lambda_j V}\right)$$

is a linear combination of exponentials

$$e^{-\frac{1}{N}\sum_1^N \lambda_j v_{\alpha_j}}$$

where $v_{\alpha_1}, \ldots, v_{\alpha_N}$ are all eigenvalues of V.

Let's simplify by replacing $\frac{1}{N}(H_0+V) \longmapsto H_0+V$.

$$\mathrm{tr}\left(\prod_1^N \left(e^{-H_0} e^{-\lambda_j V}\right)\right) = \mathrm{tr}\left(\prod_1^{N-1}\left(e^{-H_0}e^{-\lambda_j V}\right)\cdot e^{-H_0} \sum_\alpha |\alpha\rangle e^{-\frac{\lambda_N}{N} v_\alpha}\langle\alpha|\right)$$

$$= \sum_\alpha e^{-\lambda_N v_\alpha} \left\langle \alpha \left| \prod_1^{N-1}\left(e^{-H_0}e^{-\lambda_j V}\right) e^{-H_0} \right| \alpha \right\rangle$$

The coefficient of $e^{-\lambda_1 v_{\alpha_1} - \lambda_2 v_{\alpha_2} - \cdots - \lambda_N v_{\alpha_N}}$ is

$$\langle \alpha_1 | e^{-H_0} | \alpha_2\rangle \langle \alpha_2 | e^{-H_0} | \alpha_3 \rangle \cdots \langle \alpha_N | e^{-H_0} | \alpha_1 \rangle$$

and this doesn't have to be ≥ 0, or even real for $N=3$. However it might be true that if we set all $\lambda_j = \lambda$, and considered all possible permutations of the sequence $\alpha_1, \ldots, \alpha_N$, then the sum is ≥ 0.

No. Suppose $\alpha_1, \alpha_2, \alpha_3$ are distinct, and put $\langle \alpha_i | e^{-H_0} | \alpha_j \rangle = A_{ij}$. Then $e^{-\lambda(\alpha_1+\alpha_2+\alpha_3)}$ has the coeff.

$$3A_{12}A_{23}A_{31} + 3A_{13}A_{32}A_{21}$$

But we can obviously arrange to find a pos. def. matrix e^{-H_0} whose off-diagonal entries are < 0.

So we conclude that

$$tr\left(\left(e^{-H_0} e^{-\lambda V}\right)^N \right)$$

is not <u>necessarily the generating function</u> of a measure.

The problem of whether

$$f(s) = tr\left(e^{-(H_0 + sV)} \right)$$

is the generating function for a measure still remains.