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Supplement to $E^{(1)}_{\text{exchange}}$

- As pointed out by Steve Puglia, the exchange integral

$$\boxed{E^{(1)}_{\text{exchange}} = -\frac{g\lambda}{2}\frac{\Omega}{(2\pi)^6}\int d^3k\, d^3q\, \theta(k_F - |\vec{k}+\vec{q}|)\,\theta(k_F - k)}$$

can be evaluated as easily as the direct integral after the change of variables $\vec{q} \to \vec{q}\,' = \vec{q} + \vec{k}$

$$\boxed{\begin{aligned}\Rightarrow E^{(1)}_{\text{exchange}} &= -\frac{1}{g}\frac{\lambda}{2\Omega}\left(\frac{g\Omega}{(2\pi)^3}\int d^3k\, \theta(k_F - k)\right)\left(\frac{g\Omega}{(2\pi)^3}\int d^3q'\, \theta(k_F - q')\right)\\ &= -\frac{1}{g}\frac{\lambda}{2\Omega}N^2\end{aligned}}$$

- The reason this is so simple is that the interaction is a "contact term" (i.e. a delta function). If we had used a finite range interaction, there would have been a function of q in the integral (the fourier transform of the potential) and we would have had to integrate over the more complicated geometry described in the notes.

- To see an example, look at the online selections from Chap. 1 of Fetter and Walecka, where they do the Coulomb interaction.

- The simplicity of the result here, however, is evidence of the power of the effective field theory method.

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Example: non-interacting Fermi gas with degeneracy g in a large box of volume V

$$\Rightarrow \boxed{\epsilon_i \to \epsilon_p = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}}$$

and $\boxed{\sum_i \xrightarrow[\substack{V\to\infty \\ N\to\infty}]{} gV \int \frac{d^3k}{(2\pi)^3}}$

So
$$\boxed{\begin{aligned}\Omega_0(V,T,\mu) &= -\frac{1}{\beta}\sum_i \ln\left(1+e^{-\beta(\epsilon_i-\mu)}\right) \\ &= -\frac{g}{\beta}\frac{V}{(2\pi)^3}\int d^3k \ln\left(1+e^{-\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}\right)\end{aligned}}$$

- note that the integrand is well-defined and bounded at both small and large k:

$$k\to 0,\ k^2\ln\left(1+e^{-\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}\right) \to k^2\ln\left(1+e^{\beta\mu}\right) \to 0$$
$$k\to\infty,\ k^2\ln\left(1+e^{-\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}\right) \to k^2\ln\left(1+e^{-\beta\frac{\hbar^2k^2}{2m}}\right) \to k^2 e^{-\beta\frac{\hbar^2k^2}{2m}} \to 0$$

- It's easier to evaluate the integral with $\epsilon = \frac{\hbar^2k^2}{2m}$ as the integration variable:

$$\Rightarrow d\epsilon = \frac{\hbar^2}{m}k\,dk \quad \text{and} \quad k^2dk = \left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{2m}{\hbar^2}\frac{1}{2}\epsilon^{1/2}d\epsilon$$

$$\Rightarrow \boxed{\Omega_0 = -\frac{g}{\beta}\frac{V}{8\pi^3}\underbrace{4\pi}_{\text{angular integration}}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{1}{2}\int_0^\infty d\epsilon\ \epsilon^{1/2}\ln\left(1+e^{\beta(\mu-\epsilon)}\right)}$$

It is useful to write this in another form by integrating by parts [$v=\ln(1+e^{\beta(\mu-\epsilon)}) \to dv=(1+e^{\beta(\mu-\epsilon)})^{-1}e^{\beta(\mu-\epsilon)}(-\beta)\,d\epsilon$ and $du=\epsilon^{1/2}d\epsilon \to u=\frac{2}{3}\epsilon^{3/2}$ and the surface term vanishes at $\epsilon=0$ and $\epsilon=\infty$]

$$\Rightarrow \boxed{\Omega_0 = PV = \frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{2}{3}\int_0^\infty d\epsilon\ \frac{\epsilon^{3/2}}{e^{\beta(\epsilon-\mu)}+1}}$$

which gives us the pressure directly.

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· We can find N directly from

$$\boxed{N = \sum_i n_i^0 = \sum_i \frac{1}{e^{\beta(\epsilon_i-\mu)}+1} \longrightarrow +\frac{gV}{(2\pi)^3}\int d^3k \, \frac{1}{e^{\beta(\epsilon_k-\mu)}+1} = \frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty d\epsilon \, \frac{\epsilon^{1/2}}{e^{\beta(\epsilon-\mu)}+1}}$$

or from $N = -\frac{\partial \Omega_0}{\partial \mu}$ (use the first version with the ln)

To find the energy, we can find S from $S = -\left(\frac{\partial \Omega}{\partial T}\right)_{V\mu}$ (recalling $\beta = 1/k_BT$) and then using $E = TS - PV + \mu N$.
Or we can find it directly (in this case) as we did with N:

$$\boxed{E = \sum_i n_i^0 \epsilon_i \longrightarrow \frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)\int_0^\infty d\epsilon \, \frac{\epsilon^{3/2}}{e^{\beta(\epsilon-\mu)}+1}}$$

Comparing the E and Ω_0 equations, we find the "equation of state"

$$\boxed{PV = \frac{2}{3}E}$$

· See Fetter + Walecka exerpts for details of fermions at low temperature and for bosons.
  · we'll return to the latter, later or in PS.

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Aside: consider the fermion occupation number further

$$\boxed{n_i^0 = \frac{1}{e^{\beta(\epsilon_i-\mu)}+1}}$$

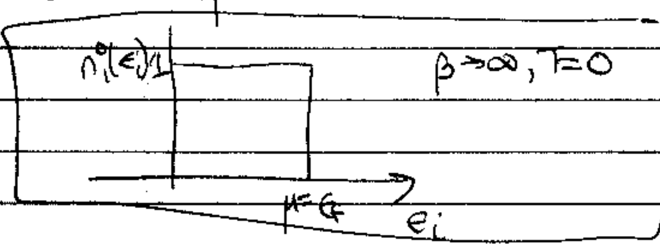
- Since $e^x \geq 0$, $n_i^0 \leq 1$ (which is good, since we're averaging 0's and 1's, but it means that any μ is possible, unlike the boson case).

- Consider the high temperature ($\beta \to 0$) and low temperature ($\beta \to \infty$) limits of n_i^0.

$\beta \to \infty$: if $\epsilon_i - \mu > 0 \Rightarrow e^{\beta(\epsilon_i-\mu)} \to \infty \Rightarrow n_i^0 \to 0$

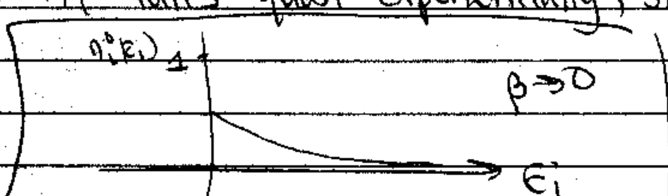
if $\epsilon_i - \mu < 0 \Rightarrow e^{\beta(\epsilon_i-\mu)} \to 0 \Rightarrow n_i^0 \to 1$

so $n_i^0(\epsilon_i) \xrightarrow{\beta\to\infty} \theta(\mu - \epsilon_i)$ and we fill levels up to $\mu = \epsilon_F$

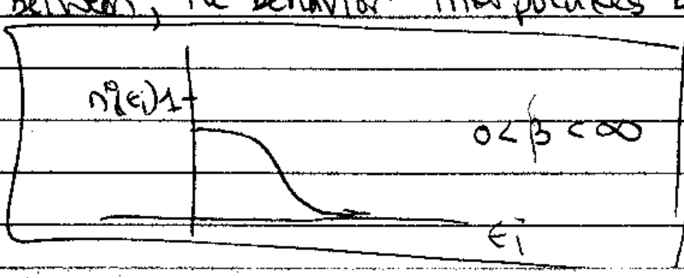


Note that this limit applied to N and E reproduces our previous non-interacting ground state results.

$\beta \to 0$: If $\beta\mu \ll 1$, then μ does not have much of an effect, and $n_i^0(\epsilon_i)$ is significant until $\beta\epsilon_i \gg 1$. That means that n_i^0 falls quasi-exponentially, starting at $n_i^0 = .5$:



In between, the behavior interpolates between these extremes



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Functional Integral Formulation

- To both generate the perturbation series in the interaction and to go beyond perturbation theory to construct non-perturbative approximations to the many-body problem, we turn to functional integrals.
  - Our discussion follows the spirit, if not always the details, of chapter 2 in Negele and Orland.
  - We construct the partition function as a path integral (an integral over field configurations)
    - naturally suggests approximations, including numerical approximations
    - provides intuitive physical description of the system, including the simple generation of Feynman diagrams
    - transparently and efficiently incorporates and exploits the symmetries of the system (and is particularly powerful treating spontaneous symmetry breaking).
  - We'll proceed in stages:
    - start with constructing the path integral for the familiar case of a quantum mechanical particle
    - then see how we get the same results with better mathematical behavior by continuing to imaginary time
    - which is then easily connected to the partition function
    - a simple model in zero-dimensional field theory (just an integral) illustrates issues about perturbation theory and generating a diagrammatic expansion
    - finally, we extend our formalism to many-body systems

- Historical note:
  - P.A.M. Dirac suggested the basic idea of path integrals in 1933
  - R.P. Feynman worked out the details in 1948-50.

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We start with a quantum mechanical particle with Hamiltonian $\hat{H}(\hat{p},\hat{x})$.

- The common example is a single particle in a potential:

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

but we should be prepared to consider more general forms, with terms that have mixed $\hat{p}$'s and $\hat{x}$'s.

- Recall that $\hat{H}$ governs the time evolution of the state $|\Psi(t)\rangle$ that satisfies: $\boxed{i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle}$

$$\Rightarrow \boxed{|\Psi(t_f)\rangle = e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|\Psi(t_i)\rangle}$$

which identifies the evolution operator U. The matrix element of U in coordinate space is

$$\boxed{U(x_f t_f, x_i t_i) = \langle x_f|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|x_i\rangle}$$

- This is the object we'll construct a path integral for.

- The game plan is to realize that we can approximate U for small time intervals Δt (making an error of order $(\Delta t)^2$, for example) and that we can break up (t_f-t_i) into enough of these intervals that we have a controlled approximation to U.
  - Note that $\boxed{U(x_2t_2, x_0t_0) = \int dx\, U(x_2t_2, xt)\, U(xt, x_0t_0)}$ for any t (just write out the exponentials and insert $\int dx\, |x\rangle\langle x| = 1$) and in particular for $t_2 < t < t_0$.

- Divide $t_f - t_i$ into M equal steps of size $\Delta t \equiv \epsilon$, so that

$$\boxed{\epsilon = \frac{t_f-t_i}{M}}$$

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We'll label the times in between as t_n:

$$\underset{t_0\ t_1\ t_2\ \cdots\ t_{m-1}\ t_m}{\vdash\!\!-\!\!+\!\!-\!\!+\!\!-\!\!+\!\!-\!\!+\!\!-\!\!+\!\!-\!\!\dashv}$$

so that $\boxed{t_0 \equiv t_i}$ and $\boxed{t_m \equiv t_f}$

and

$$\boxed{t_n = t_0 + n\epsilon} . \qquad n = 0, 1, \cdots, m$$

- For convenience, we label $\boxed{x_0 \equiv x_i}$ and $\boxed{x_m \equiv x_f}$

• Now $\boxed{e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} = \left(e^{-\frac{i\epsilon}{\hbar}\hat{H}}\right)^m}$ and we can insert $\boxed{\int dx\, |x\rangle\langle x| = 1}$ in between each term. ($\hat{H}$ commutes with itself, so this is ok to do.)

• (Note that $|x\rangle$ can stand for $|\vec{x}\alpha\rangle$ with α a spin index, in which case $\delta(x - x') \equiv \delta_{\alpha\alpha'}\delta^3(\vec{x} - \vec{x}')$ and $\int dx\, |x\rangle\langle x| = \sum_\alpha \int d^3x\, |\vec{x}\alpha\rangle\langle\vec{x}\alpha| = 1$, but we'll generally ignore this here.)

$$\Rightarrow \boxed{\begin{aligned} U(x_f t_f, x_i t_i) &= \langle x_f | \left(e^{-\frac{i\epsilon}{\hbar}\hat{H}}\right)^m | x_i\rangle \\ &= \int \left(\prod_{k=1}^{m-1} dx_k\right) \langle x_m | e^{-\frac{i\epsilon}{\hbar}\hat{H}} | x_{m-1}\rangle\langle x_{m-1} | e^{-\frac{i\epsilon}{\hbar}\hat{H}} | x_{m-2}\rangle \\ &\quad \times \langle x_{m-2}| \cdots\cdots e^{-\frac{i\epsilon}{\hbar}\hat{H}} | x_1\rangle\langle x_1 | e^{-\frac{i\epsilon}{\hbar}\hat{H}} | x_0\rangle \end{aligned}}$$

• If we could get all of the $\hat{p}$'s in $\hat{H}$ to the left and the $\hat{x}$'s to the right, then we can evaluate each of the matrix elements by inserting a complete set of momentum eigenstates $|p_k\rangle$:

$$\boxed{\langle x_n | e^{-\frac{i\epsilon}{\hbar}\hat{H}(\hat{p},\hat{x})} | x_{n-1}\rangle = \int d^3p_n \langle x_n | p_n\rangle\langle p_n | e^{-\frac{i\epsilon}{\hbar}\hat{H}(\hat{p},\hat{x})} | x_{n-1}\rangle}$$

but even $\boxed{\hat{H} = \hat{p}^2/2m + V(\hat{x})}$ doesn't work: $e^{-\frac{i\epsilon}{\hbar}\hat{H}} \neq e^{-\frac{i\epsilon}{\hbar}\frac{\hat{p}^2}{2m}} e^{-\frac{i\epsilon}{\hbar}V(\hat{x})}$ since $[\hat{p}, \hat{x}] \neq 0$. But they are equal up to a commutator of the exponent, which is proportional to ϵ^2.

$\Rightarrow$ we can "normal order" the exponential leaving and make an error of only ϵ^2.

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For generality, we'll define the "normal form" $:\hat{O}(\hat{p},\hat{x}):$ operator $\hat{O}(\hat{p},\hat{x})$ to be the result of moving all the $\hat{p}$'s to the left and the $\hat{x}$'s to the right.

- So $\hat{H}_V(\hat{p},\hat{x}) = \hat{p}^2/2m + V(\hat{x}) = :\hat{H}_V(\hat{p},\hat{x}):$

and

$$\boxed{:e^{-i\frac{\epsilon}{\hbar}\hat{H}_V(\hat{p},\hat{x})}: = \sum_{n=0}^{\infty}\left(-i\frac{\epsilon}{\hbar}\right)^n \sum_{k=0}^{n} \frac{1}{k!(n-k)!}\left(\frac{\hat{p}^2}{2m}\right)^k (V(\hat{x}))^{n-k}}$$

- One can show (see Negele and Orland [2.35]) that the normal form differs from the original $e^{-i\epsilon/\hbar \hat{H}}$ for any $\hat{H}$ by terms of $O(\epsilon^2)$. When acting on a normalizable, differentiable wave function, the difference in these evolution operators should be ϵ^2 times a finite number, so the limit $\epsilon \to 0$ is well behaved (that is, the wave function is correctly evolved).

- We can use the normal form directly in our integral:

$$\boxed{\begin{aligned}\langle x_n | :e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})}: | x_{n-1}\rangle &= \int d^3p_n \langle x_n | p_n\rangle\langle p_n | :e^{-i\frac{\epsilon}{\hbar}\hat{H}(\hat{p},\hat{x})}: | x_{n-1}\rangle \\ &= \int \frac{d^3p_n}{(2\pi\hbar)^3} e^{i p_n(x_n - x_{n-1})} e^{-i\frac{\epsilon}{\hbar}H(p_n, x_{n-1})}\end{aligned}}$$

where the $\hat{p},\hat{x}$ operators are replaced by their c-number eigenvalues and re-exponentiated.

- (Note: For simplicity we're dropping spin – assume spin independent)

- For H_V we get:

$$\boxed{\begin{aligned}\langle x_n | e^{-i\frac{\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)} | x_{n-1}\rangle &= \langle x_n | :e^{-i\frac{\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)}: | x_{n-1}\rangle + O(\epsilon^2) \\ &= \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\frac{p}{\hbar}(x_n - x_{n-1}) - i\frac{\epsilon}{\hbar}\frac{p^2}{2m} - i\frac{\epsilon}{\hbar}V(x_{n-1})} + O(\epsilon^2) \\ &= \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{3/2} e^{\frac{i}{\hbar}\left(\frac{m}{2\epsilon}(x_n - x_{n-1})^2 - \epsilon V(x_{n-1})\right)} + O(\epsilon^2)\end{aligned}}$$

Fresnel integral ⇒ [complete the square]

Aside: Doing the Fresnel integral by "completing the square."

- This is one of the frequently used manipulations with functional integrals

$$\boxed{\int \frac{d^3p}{(2\pi\hbar)^3}\, e^{-i\frac{\epsilon}{\hbar}\frac{p^2}{2m} + i\frac{p}{\hbar}(x_n - x_{n-1})} \equiv F(x_n, x_{n-1})}$$

is the integral we want to do. We care most about the dependence on x_k — how can we isolate it?

- The idea is to add and subtract a term independent of p to the exponent so that the exponent is a perfect square. Then we can switch to p' that decouples the x and p' dependence:

$$-\frac{i}{\hbar}\frac{\epsilon}{2m}\left(p^2 - \frac{2m}{\epsilon}p(x_n - x_{n-1})\right)$$

$$= -\frac{i}{\hbar}\frac{\epsilon}{2m}\left(p^2 - \frac{2m}{\epsilon}p(x_n - x_{n-1}) + \frac{m^2}{\epsilon^2}(x_n - x_{n-1})^2\right) + \frac{i}{\hbar}\frac{\epsilon}{2m}\frac{m^2}{\epsilon^2}(x_n - x_{n-1})^2$$

$$= -\frac{i}{\hbar}\frac{\epsilon}{2m}\Big(\underbrace{p - \frac{m}{\epsilon}(x_n - x_{n-1})}_{\equiv p'}\Big)^2 + \frac{i}{\hbar}\frac{m}{2\epsilon}(x_n - x_{n-1})^2$$

- The Jacobian is 1 in changing variables to p' ($d^3p = d^3p'$)

$$\Rightarrow \boxed{F(x_n, x_{n-1}) = e^{\frac{i}{\hbar}\frac{m}{2\epsilon}(x_n - x_{n-1})^2} \int \frac{d^3p'}{(2\pi\hbar)^3}\, e^{-\frac{i}{\hbar}\frac{\epsilon p'^2}{2m}}}$$

- The Gaussian integral over p' just gives factors depending on ϵ, m, and $\hbar$. We will often cancel it against an identical factor, for example from a noninteracting evolution operator or partition function, in which case we're done.

- This approach will later be generalized to integrals over functions.

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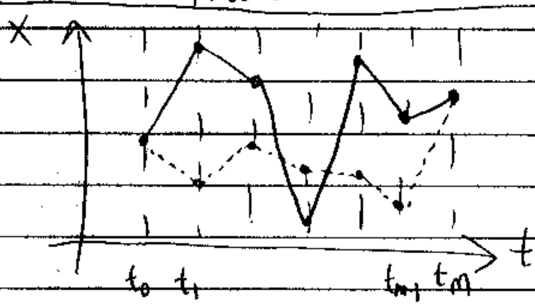
- What about other discretizations? Would it matter?
  - $1 - i\frac{\epsilon}{\hbar}(\hat{p}^2/2m + V(\hat{x}))$ has also an $\mathcal{O}(\epsilon^2)$ error but the momentum integrations diverge.
  - in contrast, $e^{-i\frac{\epsilon}{\hbar}p^2/2m}$ and $e^{-\frac{\epsilon}{\hbar}\frac{p^2}{2m}}$ are bounded, so both real and imaginary time versions are well behaved (the exponential without the i more so!).
  - We still have freedom of where to evaluate V, e.g. $V(x_{n-1})$ vs. $V(x_n)$ vs. $\frac{1}{2}(V(x_{n-1}) + V(x_n))$, which can make a difference in some applications (see Negele and Orland Chapter 8).
  - The issue of operator ordering ($\hat{p}$'s and $\hat{x}$'s in this case) shows up in the path integral formulation in the different discretization possibilities (see Negele and Orland problem 2.5), unlike the previous bullet where V could be evaluated anywhere in the $\epsilon \to 0$ limit.

Ok, putting together the matrix elements

$$\boxed{U(x_f t_f, x_i t_i) = \lim_{M\to\infty} \int dx_1 \cdots dx_{M-1} \left(\frac{m}{2\pi i \epsilon \hbar}\right)^{\frac{3M}{2}} e^{\frac{i}{\hbar}\epsilon \sum_{k=1}^{M}\left(\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 - V(x_{k-1})\right)}}$$



typical trajectories

- A "trajectory" is defined by the set $\{x_0, x_1, \ldots, x_M\}$, which we call $x(t)$ with $x(t_i) = x_i$ and $x(t_f) = x_f$ in the $M\to\infty$ limit.
  - but don't be fooled by the notation: $x(t)$ is not continuous or differentiable in general (as $t_1 \to t_0$, nothing says $x_1 \to x_0$!).
- Similarly, we replace $\boxed{\frac{x_k - x_{k-1}}{\epsilon} \to \frac{dx}{dt} \text{ or } \dot{x}}$ with similar caveats. Always return to the discrete definition when in doubt!

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So, in this notation,

$$\boxed{\epsilon \sum_{k=1}^{M} \frac{m}{2}\left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 \rightarrow \int_{t_i}^{t_f} dt\, \frac{m}{2}\left[\frac{dx}{dt}\right]^2} \qquad \boxed{\epsilon \sum_{k=1}^{M} V(x_{k-1}) \rightarrow \int_{t_i}^{t_f} dt\, V(x(t))}$$

so finally we have

$$\boxed{U(x_f t_f, x_i t_i) = \int_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\, \left(\frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x(t))\right)} = \int_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)]\, e^{i/\hbar\, S[x(t)]}}$$

where the scary measure is hidden as

$$\boxed{\int_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)] = \lim_{M\to\infty} \int \left(\prod_{k=1}^{M-1} dx_k\right) \left(\frac{m}{2\pi i \epsilon \hbar}\right)^{\frac{3M}{2}}}$$

and the action is

$$\boxed{S[x(t)] = \int_{t_i}^{t_f} dt\; L[x(t)]}$$

with Lagrangian

$$\boxed{L[x(t)] = \frac{1}{2} m \left(\frac{dx}{dt}\right)^2 - V(x(t))}$$

In summary, we find the matrix element of the evolution operator between $|x_i\rangle$ and $|x_f\rangle$ by summing over all "paths" starting at x_i at time t_i and ending at x_f at time t_f, with each path "weighted" by the exponential of $i/\hbar$ times the action.

- as $\hbar \to 0$, it would be natural to apply a stationary phase approximation $\Rightarrow$ nearby paths interfere destructively unless the phase $i/\hbar S$ doesn't change (variation is zero)
  $\Rightarrow$ this is the condition for the classical trajectory

- The measure is a problem when $\epsilon \to 0$. One fix is to normalize U to a reference problem we know the answer to. For example, when $V = 0$,

$$\boxed{U_0(x_f t_f, x_i t_i) = \langle x_f | e^{i/\hbar \frac{\hat{p}^2}{2m}(t_f - t_i)} | x_i \rangle = \left[\frac{m}{2\pi i \hbar (t_f - t_i)}\right]^{3/2} e^{i \frac{m}{2\hbar} \frac{(x_f - x_i)^2}{t_f - t_i}}}$$

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To get the Lagrangian form of the path integral, we used the fact that the dependence on p was quadratic. More generally we have the Hamiltonian form

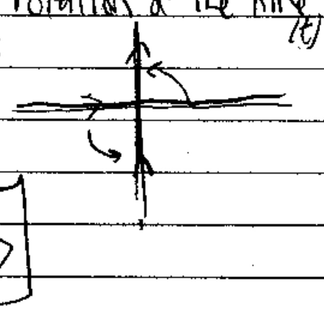
$$\boxed{\begin{aligned} U(x_f t_f, x_i t_i) &= \lim_{M\to\infty} \int dx_1 \cdots dx_{M-1} \int \frac{dp_1 \cdots dp_M}{(2\pi\hbar)^{3M}}\, e^{\frac{i}{\hbar}\sum_{k=1}^{M}\left[p_k(x_k - x_{k-1}) - \epsilon\frac{p_k^2}{2m} - \epsilon V(x_{k-1})\right]} \\ &\longrightarrow \int_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)]\,\mathcal{D}[p(t)]\, e^{i/\hbar \int_{t_i}^{t_f} dt\left[p(t)\frac{\partial}{\partial t}x(t) - H(p(t),x(t))\right]} \end{aligned}}$$

- The $x(t)$ have the same x_i and x_f boundary conditions
- The $p(t)$ have no boundary conditions.

- The "weighting" function is imaginary in our formulation. It would be cleaner to have a nice positive-definite weighting function.
  - This can be achieved by the variable transformation

$$\boxed{t = -i\tau}$$

  - This is often called a "Wick rotation", because we can think of the continuation to "imaginary" time as a rotation of the time integration contour in the complex t-plane:



- The Euclidean evolution operator

$$\boxed{U_E(x_f\tau_f, x_i\tau_i) = \langle x_f| e^{-(\tau_f - \tau_i)\hat{H}/\hbar} |x_i\rangle}$$

can be evaluated by precisely the same steps as before, dividing $\tau_f - \tau_i$ into M intervals of width ϵ.
  - once again, we can neglect commutators that contribute at order ϵ^2.

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In particular,

$$\boxed{\begin{aligned}
U_E(x_f\tau_f, x_i\tau_i) &= \lim_{M\to\infty}\int\left(\prod_{k=1}^{M-1} dx_k\right)\prod_{k=1}^{M}\langle x_k|e^{-\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})}|x_{k-1}\rangle \\
&= \lim_{M\to\infty}\int\left(\prod_{k=1}^{M-1} dx_k\right)\left(\prod_{k=1}^{M} d^3p_k\right)\langle x_k|p_k\rangle\langle p_k|:e^{-\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})}:+O(\epsilon^2)|x_{k-1}\rangle \\
&= \lim_{M\to\infty}\int\left(\prod_{k=1}^{M-1} dx_k\right)\prod_{k=1}^{M}\frac{d^3p_k}{(2\pi\hbar)^3}\, e^{\sum_{k=1}^{M}\left[\frac{ip_k}{\hbar}(x_k-x_{k-1})-\frac{\epsilon}{\hbar}\left(\frac{p_k^2}{2m}+V(x_{k-1})\right)\right]} \\
&= \lim_{M\to\infty}\int\left(\prod_{k=1}^{M-1} dx_k\right)\left(\frac{m}{2\pi\epsilon\hbar}\right)^{3M/2} e^{-\frac{\epsilon}{\hbar}\sum_{k=1}^{M}\left[\frac{m}{2}\frac{(x_k-x_{k-1})^2}{\epsilon^2}+V(x_{k-1})\right]} \\
&= \int_{(x_i,\tau_i)}^{(x_f,\tau_f)} \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar}\int_{\tau_i}^{\tau_f} d\tau\left(\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2+V(x(\tau))\right)} \\
&= \int_{(x_i,\tau_i)}^{(x_f,\tau_f)} \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar}\int_{\tau_i}^{\tau_f} d\tau\, S_E[x(\tau)]}
\end{aligned}}$$

which defines the Euclidean action S_E. Note the change in sign, from $\frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x)$ to $\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)$, which effectively "flips" the potential (more later!).

- This formulation can be made mathematically rigorous.
- With the new weighting, we can put this on a computer!

- There's no need to get metaphysical about what imaginary time means; just regard it as a useful trick to extract physical observables.
  - Note that U and U_E have the same content in terms of wavefunctions and energies; insert complete sets of energy eigenfunctions $1 = \sum_n |\psi_n\rangle\langle\psi_n|$ with eigenvalues E_n (so $H|\psi_n\rangle = E_n|\psi_n\rangle$ and $\langle x|\psi_n\rangle = \psi_n(x)$):

$$\boxed{\begin{aligned}
U(x_f t_f, x_i t_i) &= \langle x_f|e^{-\frac{i\hat{H}}{\hbar}(t_f-t_i)}|x_i\rangle = \sum_n \psi_n(x_f)\psi_n^*(x_i)\, e^{-\frac{iE_n(t_f-t_i)}{\hbar}} \\
U_E(x_f\tau_f, x_i\tau_i) &= \langle x_f|e^{-\frac{i\hat{H}}{\hbar}(\tau_f-\tau_i)}|x_i\rangle = \sum_n \psi_n(x_f)\psi_n^*(x_i)\, e^{-\frac{E_n(\tau_f-\tau_i)}{\hbar}}
\end{aligned}}$$

so either object has the info we want.

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· These decompositions are called "spectral representations".

· If we take $\tau_i = 0$, $\tau_f = T$ and take $T \to \infty$, the ground state dominates the sum in U_E, and we can project out E_0 by taking the ln and dividing by T. The dependence on x_i, x_f drops out!

· In the path integral form, this yields the "Feynman-Kac formula":

$$\boxed{E_0 = \lim_{T \to \infty} \left(-\frac{\hbar}{T} \ln \int_{(x_i,0)}^{(x_f,T)} \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar}\int_0^T d\tau \left\{ \frac{m\dot{x}^2}{2} + V(x) \right\}} \right)}$$

· Finally, consider the partition function for a single particle, with the trace evaluated in the coordinate basis:

$$\boxed{Z = \mathrm{Tr}\, e^{-\beta \hat{H}} = \int dx \langle x | e^{-\beta \hat{H}} | x \rangle}$$

· This is just a sum over $U_E(x_f \tau_f, x_i \tau_i)$ with $x_i = x_f$ ("diagonal") and $\tau_f - \tau_i = \beta\hbar$.

· Note that there is no chemical potential for this one-particle problem.

$$\Rightarrow \boxed{\begin{aligned} Z &= \int dx \int_{x(0)=x}^{x(\beta\hbar)=x} \mathcal{D}(x(\tau))\, e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left(\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V(x(\tau)) \right)} \\ &\equiv \int_{x(\beta\hbar)=x(0)} \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left(\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x(\tau)) \right)} \end{aligned}}$$

So we get the partition function by summing over all <u>periodic</u> trajectories of period $\beta\hbar$.

· The last line stresses that the x_M integration is the same as all of the internal x_k integrations.

· Before going on to many-body systems, we'll pause and think about approximations to Z based on a simple analogy.