Quantum Monte Carlo Methods.

Not yet. I will start from the alternative formulation of quantum mechanics in terms of path integrals. First, for the two level system, then for the many-body lattice system, then for a particle in the space-time continuum, and finally for a system of interacting particles. In addition I will discuss the interaction representation in quantum mechanics and how it leads to Feynman diagrams. Some quantum Monte Carlo methods are based on this formulation, but certainly there are other methods which are not. This Section sets the stage for the subsequent discussion of MC techniques.

Two level systems.

Suppose you are asked a question: "What are the most important models in quantum physics?" Harmonic oscillator is probably number one in the list. I would give the second place to the two-level system TLS. It is just everywhere: for spins $S = 1/2$ it describes everything, it gives the low-temperature dynamics of any system described by the double-well semiclassical potential (amorphous glasses, SQUIDs, magnetic grains, molecules, defects, etc.), it is extremely important in spectroscopy when a pair of levels is in near resonance with the radiating field, level-crossing phenomena in which a pair of levels is brought to near resonance by a sweeping field is another example, it is also considered as the basic element of quantum computer, a qubit.

Coherent dynamics of the TLS system is very simple to do because all we have to know is how to solve quadratic equations. Let $\mid 1\rangle$ and $\mid 2\rangle$ are the two relevant states we are talking about, and the Hamiltonian matrix in the $1, 2$ representation is

$$H = \xi \hat{\tau}_z - \Delta_0 \hat{\tau}_x \ ,$$

where $\hat{\tau}$ are Pauli matrices.

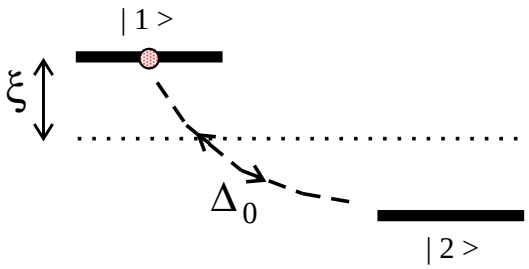
$$\hat{\tau}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \quad \hat{\tau}_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \ , \quad \hat{\tau}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ ,$$

Here I also assume that Δ_0 is a real number, in a more general case one has to write

$$H = \begin{pmatrix} \xi & -\Delta_0 \\ -\Delta_0^* & -\xi \end{pmatrix} \ ,$$

but in what follows we will use the first form for simplicity.

It is conventional to call Δ_0 in this Hamiltonian a transition amplitude, and ξ - an energy bias. Of course, if one "rotates" this matrix by writing it in some other basis set, then the meaning of Δ_0 and ξ will change as well, e.g., in the basis set $|\,a,b\rangle = \frac{1}{\sqrt{2}}(|\,1\rangle \pm |\,2\rangle)$ it is the other way around: Δ_0 is the bias and ξ is the transition amplitude.



In other words we have two states with energies split by 2ξ and the Hamiltonian has a matrix element $-\Delta_0$ to make a transition between them.

The eigenfunction equation is

$$\begin{pmatrix} \xi & -\Delta_0 \\ -\Delta_0 & -\xi \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix} ,$$

and its solution for energy is

$$\det(H - E) = 0 , \qquad \text{or} \qquad E^2 = \Delta_0^2 + \xi^2 , \qquad \text{or} \qquad E_{1,2} = \pm\sqrt{\Delta_0^2 + \xi^2} ,$$

Substituting this into the eigenfunction equation and normalizing the solutions (normalization condition is, of course, $u^2 + v^2 = 1$) we find the ground, $E_g = -E$, and excited, $E_e = +E$ states as

$$|g >= \sin\theta \,|\, 1\rangle + \cos\theta \,|\, 2\rangle , \qquad |e >= \cos\theta \,|\, 1\rangle - \sin\theta \,|\, 2\rangle ,$$

$$\cos\theta = \sqrt{\frac{E + \xi}{2E}} .$$

The dynamics of the system immediately follows from the Schrödinger Equation. If at time $t = 0$ the system was prepared in some state ψ, then at a later time t the probability amplitude, or **transition amplitude**, to find it in the same state is

$$A_{\psi\psi}(t) = \langle\, \psi |\, \psi(t)\rangle = \langle\, \psi |\, e^{-iHt} |\, \psi\rangle .$$

In the eigenfunction basis, this relation may be written as

$$\psi = \sum_{\alpha=g,e} |\,\alpha\rangle\,\langle\,\alpha|\,\psi\rangle\ ;$$

$$A_{\psi\psi}(t) = \sum_{\alpha=g,e} e^{-iE_\alpha}\langle\,\psi|\,\alpha\rangle\,\langle\,\alpha|\,\psi\rangle = \sum_{\alpha=g,e} e^{-iE_\alpha}\,|\langle\,\alpha|\,\psi\rangle|^2\ .$$

This is absolutely general for any quantum system. As an example, consider the probability amplitude for coming back to state $|\,1\rangle$ after time t:

$$A_{11}(t) = \sin^2\theta\, e^{iEt}\ +\ \cos^2\theta\, e^{-iEt}\ ;$$

$$A_{11}(t) = \cos(Et)\ +\ i\frac{\xi}{E}\ \sin(Et)\ .$$

Similarly

$$A_{22}(t) = \cos(Et)\ -\ i\frac{\xi}{E}\ \sin(Et)\ .$$

The partition function in quantum mechanics

$$Z = \sum_a e^{-E_a/T}\ ,$$

can be expressed as a sum over return probability amplitudes $A_{\psi\psi}(\tau)$, where $\{\psi\}$ is some complete basis set and $\tau = -i/T$ is imaginary time

$$Z = \sum_a \left[\sum_\psi |\langle\,a|\,\psi\rangle|^2\right]\ e^{-iE_a(-i/T)} = \sum_\psi \left[\sum_a\ e^{-iE_a(-i/T)}\,|\langle\,a|\,\psi\rangle|^2\right] \equiv$$

$$\sum_\psi A_{\psi\psi}(\tau = -i/T)\ .$$

This equation is general too. Since we have already done probability amplitudes in the basis set $|\,1,2\rangle$, we may use them to get

$$Z_{TLS} = 2\cos(-iE/T) = 2\cosh(E/T)\ ,$$

which is, of course, the correct answer $Z = e^{E/T} + e^{-E/T}$.

We may stop at this point, but I would like to give another derivation of these answers which is both instructive and more suitable for numerical simulations of interacting lattice systems we are going to discuss later. It may be called a perturbative expansion in Δ_0, or a **discrete path-integral**.

The simplicity of classical MC schemes is largely due to the possibility of writing explicitly the energy of the system. In quantum MC simulations this is no longer true in general: given Hamiltonian H for the macroscopic interacting many-body system we do not know what are system eigenstates $\mid a\rangle$ and eigenvalues E_a. It means, that the eigenstate representation where the evolution operator in imaginary time is purely diagonal $e^{-H/T}\mid a\rangle = e^{-E_a/T} \mid a\rangle$, can not be used (otherwise the problem would be identical to the classical calculation). Instead, we have to calculate statistical averages in some basis set where $e^{-H/T}$ is non-diagonal.

Suppose we use some convenient basis set to describe system states $|\alpha>$. For example, considering particles on a lattice we may choose eigenfunctions of the particle number operator $n(i)$ to describe system states, i.e. $\mid \alpha\rangle = \mid n_1, n_2, \ldots, n_N\rangle$ corresponds to the state which has n_1 particles on the first lattice site, n_2 particles on the second, etc. This basis is also called the **site representation**. The collection of all allowed values of $\{n_i\}$ numbers specifies the basis set to construct the Hilbert space of the system. In this particular case it is discrete. Any other basis set is also allowed, and the only concern at this point is how convenient it is for the subsequent numerical simulation.

From now on we will work in the $\mid 1, 2\rangle$ representation for the TLS. The evolution of the initial state $\mid i\rangle$ can be written as (this expression is often called the τ**-exponent**

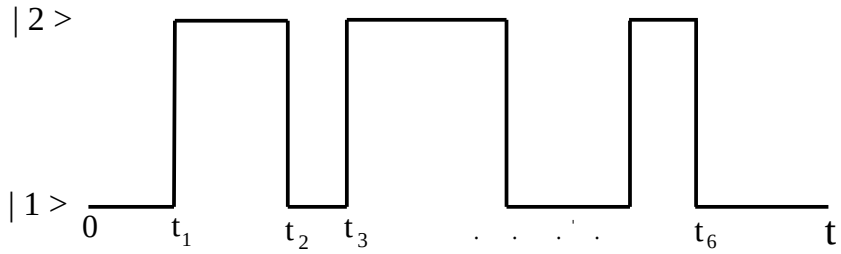
$$e^{-iHt} \equiv e^{-iH\,dt} e^{-iH\,dt} \ldots e^{-iH\,dt} ,$$

where the number of terms in the product $L = t/dt \to \infty$. We now insert sums over complete sets, $\sum_{k=1,2} \mid k\rangle\langle\, k\mid = 1$, between all exponents to get what is called the **path integral** representation of quantum mechanics

$$A_{if} = \sum_{\alpha_1, \alpha_2, \ldots \alpha_{L-1}} \langle\, f\mid e^{-iH\,dt}\mid \alpha_{L-1}\rangle \,\langle\, \alpha_{L-1}\mid e^{-iH\,dt}\mid \quad \ldots \quad \alpha_1\rangle\langle\, \alpha_1\mid e^{-iH\,dt}\mid i\rangle \ .$$

We may formally call $|\alpha_0\rangle = |i\rangle$ and $|\alpha_L\rangle = |f\rangle$. Any sequence $\alpha_0, \alpha_1, \ldots, \alpha_L \equiv$

$\alpha(t)$ is a "trajectory" in the α-space. A typical example is shown below



which literally translates as: "From time 0 to time t_1 the state of the system did not change, i.e. $\alpha(t < t_1) = 1$. At time t_1 there was a transition to another state $\alpha(t_1) = 2$ which remained the same until time t_2, etc." The sum over all possible $\alpha(t)$ means any allowed values of α at any time. In the TLS system this includes arbitrary number of transitions between states $|\,1\rangle$ and $|\,2\rangle$ which may happen at any moments, $0 < t_1 < t_2 < \ldots < t_n < t$ in time.

What is left is the calculation of the matrix elements $\langle\,\alpha'|\,e^{-iHdt}|\,\alpha\rangle$ in the limit $\delta t \to 0$ to get the contribution of a given trajectory to the transition amplitude. For definiteness, I will vaguely call it the trajectory "weight" no matter it is a complex number, in general. In this limit we have $e^{-iHdt} \approx 1 - iHdt$ and immediately see that if $|\,\alpha'\rangle = |\,\alpha\rangle$ then this matrix element is $1 - i\xi dt \approx e^{-i\xi dt}$ for $\alpha = 1$, and $1 + i\xi dt \approx e^{+i\xi dt}$ for $\alpha = 2$. Using short hand notation $\xi_{\alpha=1,2} = \pm\xi$, we can also write it is

$$\langle\,\alpha|\,e^{-iHdt}|\,\alpha\rangle \approx e^{-i\xi_\alpha dt}\ .$$

Moreover, if $|\,\alpha(t)\rangle$ does not change between times t_i and t_{i+1}, then we have to deal with the product of exactly the same diagonal matrix element, i.e. the corresponding piece of trajectory contributes a factor $e^{-i\xi_\alpha(t_{i+1}-t_i)}$ to the trajectory weight. If $|\,\alpha'\rangle \neq |\,\alpha\rangle$ then only the non-diagonal part of the Hamiltonian contributes to the answer and we get $-i(-\Delta_0)dt = i\Delta_0 dt$ factors for each transition between the states. Combining everything together we write the transition amplitude as

$$A_{if}(t) = \sum_{n=0}^{\infty} \int_0^t dt_1 \int_{t_1}^t dt_2 \ldots \int_{t_{n-1}}^t dt_n\,(i\Delta_0)^n\,e^{-i\xi_{\alpha_0}(t_1-0)-i\xi_{\alpha_1}(t_2-t_1)\ldots-i\xi_{\alpha_n}(t-t_n)}\ ,$$

trajectory description **transitions** **diagonal evolution**

where we sum and integrate over all allowed trajectories (n is even only if

$\alpha_0 = \alpha_n$ and n is odd if $\alpha_0 \neq \alpha_n$), and mention explicitly the trajectory weight.

This formulation is much more complex then solving the quadratic equation, but it hardly changes when α takes more than two values, or when we are dealing with a large system of interacting particles (the corresponding generalization follows next), while the matrix diagonalization approach quickly becomes impractical.

Problem. Find the solution for $A_{11}(t)$ within the path-integral formulation using Laplas transforms: $A(p) = \int_0^\infty e^{-pt} A(t) dt$

If $\xi = 0$ the answer follows immediately since the time ordered integral equals

$$\int_0^t dt_1 \int_{t_1}^t dt_2 \ldots \int_{t_{2n-1}}^t dt_{2n} = t^{2n}/(2n)! \; ,$$

and thus

$$A_{11} = \sum_{n=0}^{\infty} \frac{(-1)^n (\Delta_0 t)^{2n}}{(2n)!} = \cos(\Delta_0 t) \; ,$$

in agreement with the previous solution.

Lattice path-integral for a single particle system.

Our discussion of the TLS can be readily generalized to the case when a particle hops over the d-dimensional lattice, not just two sites

$$H = -\Delta_0 \sum_{<ij>} (b_i^\dagger \, b_j + h.c.) \; + \; \sum_i \xi_i n_i \; , \tag{1}$$

It is written in the site representation, thus n_i is the particle number on the lattice site i (in the single-particle case only one site may have non-zero $n_i = 1$), ξ_i is the energy of the particle state on site i, and Δ_0 is the transition amplitude between the nearest neighbor sites. By definition, operator b_i **annihilates** the particle from the corresponding site, and $b_i^\dagger$ **creates** the particle on the site. At this point it does not matter whether creation and annihilation operators are describing bosons or fermions. Literally, the first term says "the matrix element to move particle from site j to site i is $-\Delta_0$", and may be considered as a short-hand notation for writing the Hamiltonian matrix in the site-representation.

We may now divide the system Hamiltonian into two terms, one diagonal in the representation $\mid \alpha\rangle$, let's call it U, and the other non-diagonal, let's denote it K. Thus we have

$$H = K + U \; ; \qquad U \mid \alpha >= U_\alpha \mid \alpha > \; ; \tag{2}$$

and

$$K \mid \alpha\rangle = \sum_\gamma K_{\gamma\alpha} \mid \gamma\rangle \; ; \qquad K_{\alpha\alpha} = 0 \; . \tag{3}$$

This is absolutely general since any matrix element of the Hamiltonian in a given basis set is either diagonal or non-diagonal. In our case U is the second term in (1), K is the first one, and the basis states are characterized as $\alpha = \{n_i\}$, or, just $\mid i\rangle$ where i is the only site with the non-zero occupation number.

We may now repeat all steps of the lattice path-integral derivation from the previous paragraph. Let's restrict ourselves to the subject of statistical mechanics, i.e. consider only diagonal transition amplitudes in imaginary time $\tau = -i\beta$:

$$A_{\alpha_0,\alpha_0}(-i\beta) = \langle\, \alpha_0 \mid e^{-\beta H} \mid \alpha_0\rangle = \langle\, \alpha_0 \mid \prod_{k=1}^{L} e^{-d\tau H} \mid \alpha_0\rangle \quad \text{with} \quad d\tau L = \beta \; , \tag{4}$$

or,

$$Z = \sum_{\{\alpha_i\},\alpha_L=\alpha_0} \langle\, \alpha_L \mid e^{-d\tau H} \mid \alpha_{L-1}\rangle \ldots \langle\, \alpha_1 \mid e^{-d\tau H} \mid \alpha_0\rangle \; . \tag{5}$$

As before, a collection of states at all times forms a trajectory, i.e. system state evolution in time, which we may also call a space-time system configuration (for future MC use) $\nu = \alpha(t) \equiv i(t) \equiv [\alpha_0, \alpha_1, \ldots, \alpha_L]$ with $\alpha_L = \alpha_0$. The other reason for calling it a trajectory, in analogy with the TLS, is the correspondence between the system state and particle location at different times.

The last thing to do is the configuration weight. For quantum statistics it is given by the product of evolution operators between the time slices. Again, in the limit of $d\tau \to 0$, we may approximate

$$e^{-d\tau\, H} \approx 1 - d\tau\, K \; - \; d\tau\, U + O(\Delta\tau^2)$$

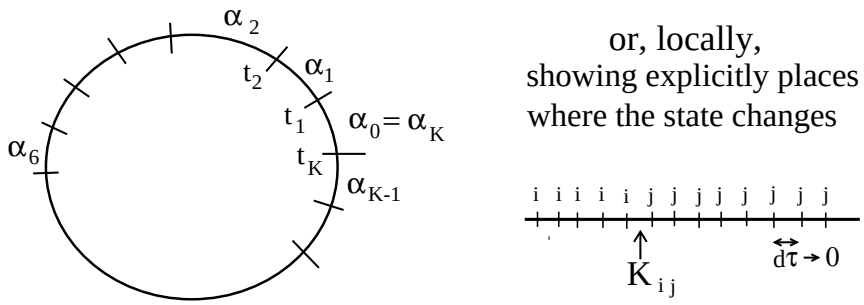
so that

$$\langle\, \alpha \mid e^{-d\tau\, H} \mid \alpha\rangle \approx e^{-d\tau\, U_\alpha} \; , \tag{6}$$

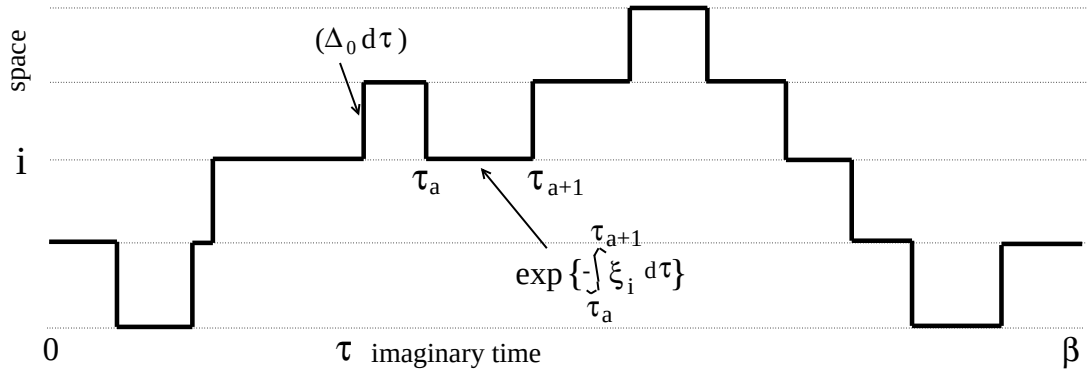
$$\langle\, \alpha |\, e^{-d\tau\, H} |\, \alpha' \neq \alpha \rangle \approx -d\tau\, K_{\alpha\alpha'}\ , \tag{7}$$

With these approximations the configuration weight with K places where the state of the system has changed from α_a to $\alpha_{a+1} \neq \alpha_a$ is

$$W_\nu = exp\left\{ -\int_0^\beta d\tau U_{\alpha(\tau)} \right\} \prod_{a=1}^{K} \Big(-\, d\tau\, K_{\alpha_a \alpha_{a+1}} \Big)\ , \tag{8}$$



This picture is a little "abstract", i.e. it is absolutely general and may be used for any Hamiltonian. The picture below is more specific because it takes into account properties of the Hamiltonian (1) which include (i) only one particle on the lattice, and (ii) non-diagonal transitions happen only between the n.n. sites. For the particle hopping on a lattice, $U_{\alpha(t)} \equiv \xi_{i(t)}$, and $-K_{\alpha_a \alpha_{a+1}} = \Delta_0$.



Its advantage is in telling us clearly in graphical terms what exactly one of the allowed sequences $[\alpha_0, \alpha_1, \ldots, \alpha_L]$ is. The similarity with the TLS is

obvious. The partition function is the sum over all possible trajectories

$$Z = \sum_{K=0}^{\infty} \int_0^\beta d\tau_1 \ldots \int_{\tau_{K-1}}^\beta d\tau_K \sum_{\alpha_0,\ldots,\alpha_K=\alpha_0} \times \prod_{a=1}^{K} \Big(- K_{\alpha_a \alpha_{a+1}} \Big) \exp\Big\{ - \sum_{a=1}^{K} \int_{\tau_{a-1}}^{\tau_a} U_{\alpha_a} d\tau \Big\} . \quad (9)$$

Here, by definition, $\tau_0 = \tau_K$, on the imaginary time circle shown above. Again, this general form simplifies to

$$Z = \sum_{K=0}^{\infty} (\Delta_0)^K \int_0^\beta d\tau_1 \ldots \int_{\tau_{K-1}}^\beta d\tau_K \sum_{i_{CP}(\tau)} \exp\Big\{ - \sum_{a=1}^{K} \int_{\tau_{a-1}}^{\tau_a} \xi_{i(\tau)} d\tau \Big\} , \quad (10)$$

for the Hamiltonian (1). I underlined that the $i(t)$ trajectory is a closed path (CP) because $i(0) = i(\beta)$.

Lattice path-integral for the many-body system.

It is getting a little boring to continue. The many body lattice Hamiltonian is different from (1) by interaction terms of the form

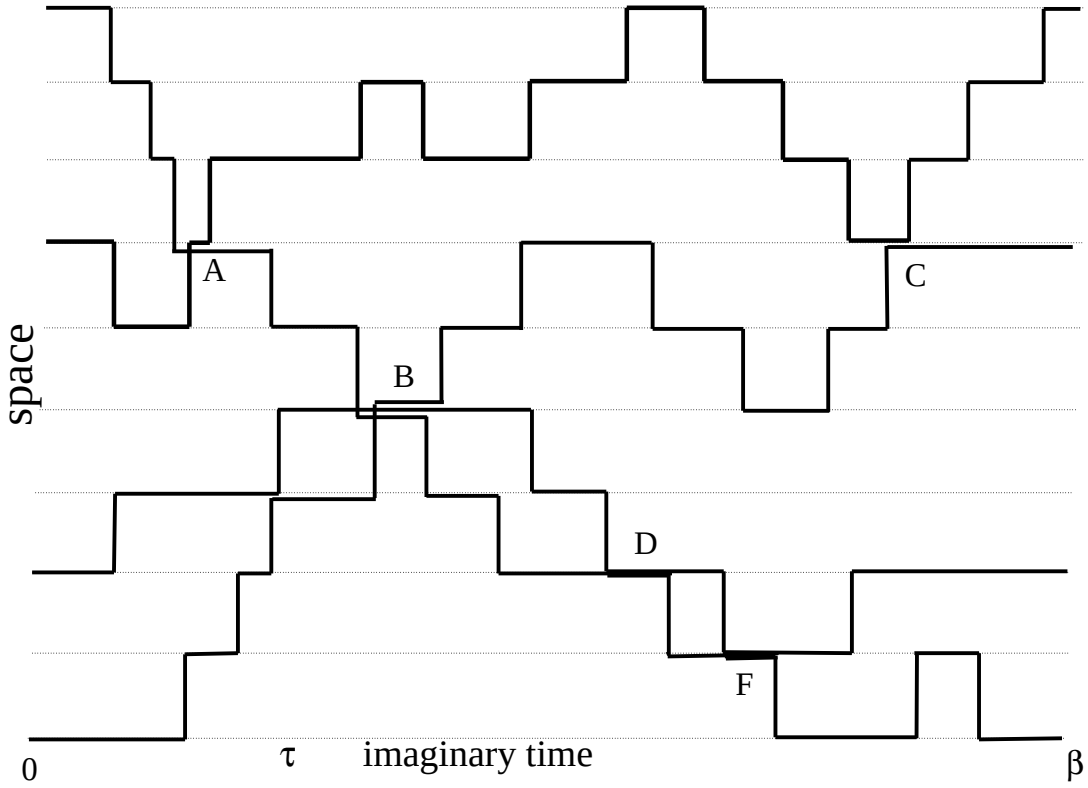
$$\frac{1}{2} \sum_{i,j} U(i,j)\, n_i n_j \ ,$$

which is diagonal in the site representation. If only on-site interactions are present, then we recover the **Hubbard model**)

$$H = -\Delta_0 \sum_{<ij>} (b_i^\dagger\, b_j + h.c.) + \frac{U}{2} \sum_i n_i^2 + \sum_i \xi_i n_i \ , \quad (11)$$

(compare it to the $|\psi|^4$ model). The other (I would call it "technical" only) difference is that now matrix elements $\Delta_0 \langle\, n_i + 1, n_j - 1 |\, b_i^\dagger\, b_j |\, n_i, n_j \rangle$ depend on n_i and n_j. [For bosons it is $\Delta_0 \sqrt{n_j (n_i + 1)}$; for fermions it is non-zero and equal $\pm\Delta_0$ only when the Pauli principle is satisfied (more on the sign later)]. Nothing at all changes in the derivation of the path-integral for this system, and Eqs. (2-9) remain valid without modification (this is the reason why I

was trying to keep notations as general as possible). The picture behind Eq. (9) is now



Formally, in the lattice model there is no way to tell what is the continuation of the line if the site occupation number is > 1, either way is equally OK because particles are identical. I deliberately show one of the many **equivalent** interpretations in places A,B,C, and refuse to make any "interpretation" at all in places D and F. The "interpretation" of points A,B,C is done for pedagogical reason— you see that the system state at $\tau = 0$ is the same as at time $\tau = \beta$ because one line ends exactly where the other line starts and particles are identical. If we "glue" the right and left ends of the figure (as if it is drawn on the β-cylinder) then certain interpretations will look as large loops which wind around the β-cylinder several times before they close. In continuous $d \geq 2$ space, however, two trajectories have zero chances to come to the same space time point, and there is no ambiguity in following a contin-

uous line. Again, graphical pictures are convenient because they visualize a particular configuration. The partition function sums/integrates all possible trajectories which satisfy $\alpha(\tau = 0) = \alpha(\tau = \beta)$.

Remarks

d-dimensional quantum $\Longrightarrow$ (d+1)-dimensional classical mapping
There are no operators, commutation relations, and other "scary" quantum mechanics notions in Eq. (9); it is written entirely in terms of well defined sums and integrals of simple functions. It is no different from what we have studied in the classical MC Section, especially if we keep $\Delta\tau$ finite and replace all integrals with sums over time slices. One may imagine now a $d+1$-dimensional classical system which has a classical state α_0=(collection of d-dimensional lattice occupation numbers at time-slice 0) for the first d-dimensional layer, α_1 for the second d-dimensional layer, etc., up to L-th layer. The corresponding (d+1)-dimensional configuration has a weight defined by Eq. (8). At this point one may immediately start the simulation using standard MC techniques (after we discuss what are MC estimators for energy, density, etc. in this representation). If all W_ν are positive definite we may even pretend that there is some "classical energy", $E_\nu^{(class.)}$, and "effective classical temperature", T_{eff} formally defined by the relation

$$E_\nu^{(class.)} = -T_{eff}\ \ln\Big(W_\nu\Big)\ .$$

Of course, $E^{(class.)}$ has noting to do with the true energy, and T_{eff} has nothing to do with the true temperature (which is here the system size in the imaginary time direction!). This might be very instructive since we have a well developed intuition for classical models.

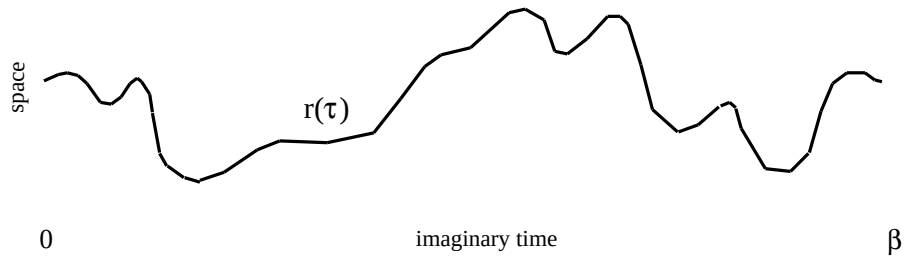
Sign problem
It is transparent in (8) that if the product of $-K_{\alpha_a\alpha_{a+1}}$ is alternating in sign, then the configuration weight is not always positive definite and we face the sign-problem. To avoid it, we'd better have all matrix elements of $-K$ positive, or, always have an even number of negative matrix elements of $-K$ so that their product is positive. Obviously this is a severe restriction. Many frustrated systems (they carry this name for a reason!) have sign alternating $K_{\alpha\alpha'}$ and do not allow efficient MC simulations. Same for the majority of fermionic systems where sign alternation of $K_{\alpha\alpha'}$ comes from anticommutation relations between the fermionic operators. For fermions,

two particles with the same spin can not be found on the same site, and thus there is no confusion in "interpreting" the flow of trajectories—the reading of the graph is unique. The sign of the trajectory is given by $Sign_\nu = (-1)^P$, where P is the number of pairwise permutations required to convert $i_1(0), i_2(0), \ldots i_N(0)$ set of fermionic coordinates into $i_1(\beta), i_2(\beta), \ldots i_N(\beta)$ set where $i_1(\beta), i_2(\beta), \ldots i_N(\beta)$ is prepared by following fermionic trajectories. When W_ν is not positive definite, we may not introduce the notions of the classical energy and effective temperature—and thus our classical intuition is of little help.

Path-integral for one particle in continuous space.

We are fully prepared to do the derivation of the continuous space path-integral. Mathematically involved people may question some points in the derivation by asking questions about integral "measures". I will ignore this issue completely (and I believe rigorously) by saying that "In quantities which are based on ratios of path integrals (statistical averages are of this kind) such ill-defined measures cancel between the numerator and denominator. Also, all measures are well-defined in lattice model—take the limit of very small lattice constant at the end of the lattice calculation."

I will start from the picture which is easy to believe considering what we did above.



Now, instead of trajectory jumping between lattice sites we have a "continuous" line (it may be as rough as you want, in fact it is diffusive-like at very short time scales). The partition function has to integrate them all with the proper weights. So, lets find the corresponding weights with a little less of talking about details which are familiar. The Hamiltonian is

$$H = \hat{K} + \hat{U} \; = \; p^2/2m + U(r) \; . \tag{12}$$

The probability amplitude of return in time $-i\beta$, and partition function are

$$A_{rr}(-i\beta) = \langle\, r|\, e^{-\beta H}|\, r\rangle\ . \quad Z = \mathrm{Tr}\, e^{-\beta H} = \int dr A_{rr}(-i\beta)\ . \tag{13}$$

Write the evolution operator as a product of exponentials with $d\tau \to 0$ and $d\tau L = \beta$

$$A_{rr} = \langle\, r|\, \prod_{i=1}^{L} e^{-d\tau H}|\, r\rangle\ ,$$

Since $d\tau \to 0$ we may decompose different terms in the Hamiltonian as follows

$$e^{-\hat{K}d\tau - \hat{U}d\tau} \approx e^{-\hat{K}d\tau}\, e^{-\hat{U}d\tau} + O(d\tau^2)\ .$$

Next we insert sums of complete sets

$$1 \equiv \int dr_i\, |\, r_i\rangle\langle\, r_i|\ , \quad \text{and} \quad 1 \equiv \int dp_i\, |\, p_i\rangle\langle\, p_i|\ ,$$

(where $|\, r\rangle = \delta(r)$ and $|\, p\rangle$ is the plane wave e^{ipr}) in between all the exponents to get (notice that $e^{-\hat{U}d\tau}|\, r\rangle = e^{-U(r)d\tau}|\, r\rangle$ and $e^{-\hat{K}d\tau}|\, p\rangle = e^{-(p^2/2m)d\tau}|\, p\rangle$)

$$Z = \int \ldots \int (dr_0\, dr_1\, \ldots dr_L)\, \delta(r_0 - r_L) \int \ldots \int (dp_1\, \ldots dp_L)$$

$$e^{-U(r_0)d\tau}\langle\, r_0|\, p_1\rangle\, e^{-(p_1^2/2m)d\tau}\langle\, p_1|\, r_1\rangle\, e^{-U(r_1)d\tau}\langle\, r_1|\, p_2\rangle\, e^{-(p_2^2/2m)d\tau}\langle\, p_2|\, r_2\rangle$$
$$\ldots\ e^{-U(r_1)d\tau}\langle\, r_{L-1}|\, p_L\rangle\, e^{-(p_L^2/2m)d\tau}\langle\, p_L|\, r_L\rangle\ , \tag{14}$$

We see a difference here with what we did before. In particular, we treat kinetic and potential energy terms on equal footing, and have sandwiched each exponential separately. We have to do it, because the momentum operator is $-i\nabla$ and there is no simple way of writing its non-diagonal matrix elements in the space representation. Now, there is no problem in going further. The advantage is that we get rid of operators and may now enjoy numbers. The integrals $\langle\, r|\, p\rangle = e^{ipr}$ and we simply combine all terms into one exponential

$$Z = \int \ldots \int (dr_0\, dr_1\, \ldots dr_L)\, \delta(r_0 - r_L) \int \ldots \int (dp_1\, \ldots dp_L)$$

$$\exp\Big\{ -\sum_{i=1}^{L} U(r_i)d\tau - \sum_{i=1}^{L} \Big[(p_i^2/2m)d\tau + ip_i(r_i - r_{i-1}) \Big] \Big\}\ , \tag{15}$$

It is looking better already. Finally, we take Gaussian integrals over momenta (by completing squares) and get the exponential as

$$\exp\Big\{ -\sum_{i=1}^{L} U(r_i) d\tau - \sum_{i=1}^{L} m(r_i - r_{i-1})^2/2d\tau \Big\} , \tag{16}$$

In the limit of $d\tau \to 0$ we may introduce a short-hand definition $dr_i/d\tau = \dot{r}_i \approx (r_i - r_{i-1})/d\tau$ and replace sums over i with the integrals to get the famous Feynman's path-integral

$$Z = \oint \mathcal{D}r \exp\Big\{ -\int_0^\beta \Big[m\dot{r}^2(\tau)/2 + U(\, r(\tau)\,) \Big] d\tau \Big\} , \tag{17}$$

where the following short-hand notation is used for the integration over all possible trajectories which form closed loops in time $r(\tau = 0) = r(\beta)$

$$\oint \mathcal{D}r \equiv lim_{L\to\infty,\, d\tau L = \beta} \int dr_0 \ldots \int dr_L \, \delta(r_0 - r_L) \, .$$

Simple, elegant, and suitable for MC simulations! If you are confused what does the integration over all possible continuous lines means, and whether time derivatives are properly defined for arbitrary lines, simply consider these integrals and derivatives as limiting cases of the sums and finite differences, **by definition**.

One last projection. If we convert imaginary time back to real time $\tau \to it$, and consider the quantum mechanical transition amplitude for the particle to go from point r_a to point r_b in time t then it is given by

$$A_{ba}(t) = \int_{r_a}^{r_b} \mathcal{D}r \; e^{i\int d\tau \, [M\dot{r}^2/2 - U(r)]} = \int_{r_a}^{r_b} \mathcal{D}r \; e^{i\int d\tau \, \mathcal{L}(r,\dot{r})} \, ,$$

where

$$\mathcal{L}(r,\dot{r}) = \frac{M\dot{r}^2}{2} - U(r) \, ,$$

is the system Lagrangian, and $\int d\tau \, \mathcal{L}(r,\dot{r}) = S[r(t)]$ is the system **action**. Amazingly, Feynman formulated quantum mechanics in classical terms, including particle motion over classical trajectories. However, all of this is not "real" yet unless we sum over all possible trajectories and include each trajectory into the integral with the phase equal to the trajectory action. This is were things go bizarre and against classical intuition (in certain cases).

Many-body path-integral in continuous space.

Nothing to derive. The only difference with the previous section is that we have N trajectories for N particles. To simplify notations let me introduce $\mathbf{R}$ = set of coordinates $r_1, r_2, \ldots r_N$ to specify positions of all N particles at a given moment of time. Then for

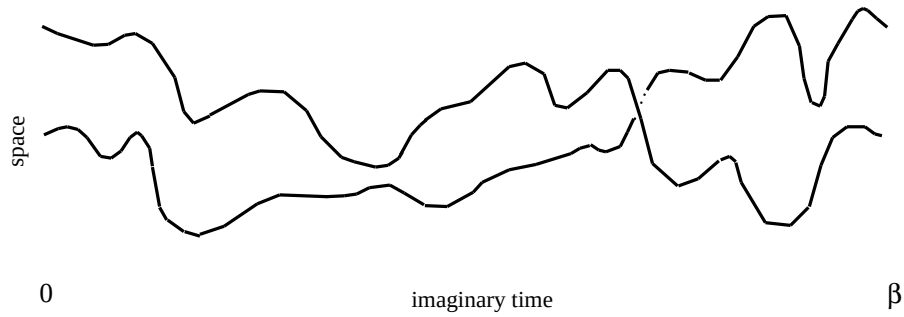
$$H = \hat{K} + \hat{U} \; = \; \sum_{i=1}^{N} p_i^2/2m_i + \sum_{i=1}^{N} U(r_i) + \frac{1}{2}\sum_{i\neq j}^{N} V(r_i - r_j) \; , \qquad (18)$$

the path-integral expression to calculate the partition function is

$$Z = \oint \mathcal{D}\mathbf{R} \exp\left\{ -\int_0^\beta \left[\sum_{i=1}^{N} m_i \dot{r}_i^2(\tau)/2 + \sum_{i=1}^{N} U(r_i(\tau)) + \frac{1}{2}\sum_{i\neq j}^{N} V(r_i(\tau) - r_j(\tau)) \right] d\tau \right\} , \qquad (19)$$

Same note as before. The notion of a closed trajectory in $\mathbf{R}$ in the many-body system is that the set of coordinates $r_1(0), r_2(0), \ldots r_N(0)$ is the same as the set $r_1(\beta), r_2(\beta), \ldots r_N(\beta)$, while the oder of coordinates may be arbitrary. For example, (2.1, 3.5, 6.) set is the same as the (3.5, 6., 2.1) set and the two-particle trajectory in the picture below IS allowed.

Moreover, the difference between the bosonic and fermionic system is only(!) in the relevance of the parity of the number of pairwise permutations required to convert $r_1(0), r_2(0), \ldots r_N(0)$ set into $r_1(\beta), r_2(\beta), \ldots r_N(\beta)$ set (obtained by following the trajectories). If this number P is odd then the configuration sign is no-longer positive for fermions, i.e. $Sign_\nu = (-1)^P$. The picture below shows one of the allowed trajectories with the pairwise permutation of two particles.



Interaction representation in quantum mechanics and Feynman diagrams.

Here I would like to present another derivation of the lattice path integral as a particular case of the more general method known as Feynman diagrams in the interaction representation. We start from the same initial setup Eqs. (2) and (3) and write formally the evolution operator in imaginary time β as

$$e^{-H\beta} \equiv e^{-\beta U} T_\tau e^{-\int_0^\beta d\tau K(\tau)} , \tag{20}$$

where, by construction, $K(\tau) = e^{\tau U}\, K\, e^{-\tau U}$ is the non-diagonal part of the Hamiltonian. This decomposition is also known as **interaction representation**. Again, the way how H is split into U and K is arbitrary and is motivated only by the convenience of working in some basis set. It can be that U and K are potential and kinetic energy terms correspondingly (if the basis set is real space), but it can be also another way around, i.e. U and K are kinetic and potential energy terms correspondingly (if the basis set is momentum space). To prove this formula we may go back to the Schrödinger Eq. in imaginary time

$$\dot{\Psi}(t) = -(U + K)\Psi$$

and substitute $\Psi(t) = e^{-\tau U}\psi(t)$. The Eq. for $\psi(t)$ is now

$$\dot{\psi}(t) = -e^{tU}\, K\, e^{-tU}\psi(t) = -K(t)\, \psi(t) , \tag{21}$$

with the solution in the form of

$$\psi(\beta) = T_\tau e^{-\int_0^\beta d\tau K(\tau)}\, \psi(0) .$$

The T_τ symbol in front of the exponent says that in the Taylor series expansion of the exponent all $K(\tau)$ operators are "time-ordered". In other words

$$T_\tau e^{-\int_0^\beta d\tau K(\tau)} = 1 - \int_0^\beta d\tau K(\tau) +$$

$$\frac{1}{2}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \Big[K(\tau_2)K(\tau_1)|_{\tau_2>\tau_1} + K(\tau_1)K(\tau_2)|_{\tau_1>\tau_2} \Big] + \dots$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \dots \int_0^\beta d\tau_n\, T_\tau \Big[K(\tau_1)K(\tau_2)\dots K(\tau_n) \Big] ,$$

were all $K(\tau)$ operators in the string are arranged in the time increasing order from right to the left. One may get rid of the $n!$ factors by making time integrals ordered explicitly (in the expression above there are $n!$ identical terms obtained by exchanging n time variables places)

$$= \sum_{n=0}^{\infty} (-1)^n \int_0^\beta d\tau_1 \int_{t_1}^\beta d\tau_2 \ldots \int_{t_{n-1}}^\beta d\tau_n K(\tau_n) \ldots K(\tau_2) \ldots K(\tau_1) \; .$$

This rule immediately follows if we try to solve Eq. (21) in small time steps

$$\psi(\beta) = \Big[1 - K(\tau) d\tau\Big] \ldots \Big[1 - K(d\tau) d\tau\Big] \Big[1 - K(\tau = 0) d\tau\Big] \, \psi(0) \; .$$

Why all this trouble? Because $K(\tau)$ operators do not commute for different times and one can not treat them the same way one treats numbers.

We may now use the interaction expression to write the partition function as

$$Z = \sum_{n=0}^{\infty} (-1)^n \int_{\tau_1 < \tau_2 < \ldots < \tau_n}^\beta d\tau_1 \ldots d\tau_n \sum_\alpha \langle \alpha | e^{-\beta U} K(\tau_n) \ldots K(\tau_2) \ldots K(\tau_1) | \alpha \rangle \; . \tag{22}$$

Eq. (9) immediately follows from it after we put all indices in place for the product of the K matrices

$$\langle \alpha | e^{-\beta U} K(\tau_n) \ldots K(\tau_2) \ldots K(\tau_1) | \alpha \rangle = e^{-\beta U_\alpha} \sum_{\alpha_1 \ldots \alpha_{n-1}} K_{\alpha \alpha_{n-1}}(\tau_n) \ldots K_{\alpha_2 \alpha_1}(\tau_2) K_{\alpha_1 \alpha}(\tau_1)$$

where

$$K_{\alpha\beta}(\tau) = e^{\tau U_\alpha} \, K_{\alpha\beta} \, e^{-\tau U_\beta}$$

You may say "This derivation is identical to the previous one!". True, but now I was not using time slices etc. to get it.

We have seen already how lattice path integrals follow from this expansion. The only other example I am going to demonstrate is how Eq. (22) naturally generates Feynman diagrams for the many-body system in continuous real space which formally look differently from the path integral. So we switch gears and use kinetic energy as U and potential energy as K (not convenient notation for this derivation but it will not take long). I will use real space representation as an eigenvalue basis though it is not the eigenvalue basis for U. Below $R = (r_1, r_2, \ldots, r_N)$ is the collection of N particle coordinates, and

$$G_i = G(R_{i+1}, R_i, \tau_{i+1} - \tau_i) = \langle R_{i+1} | e^{-(\tau_{i+1} - \tau_i) U} | R_i \rangle \sim \exp\left\{ - \frac{m (R_{i+1} - R_i)^2}{2(\tau_{i+1} - \tau_i)} \right\} \; ,$$

is the free system evolution between points R_i and R_{i+1} in time $\tau_{i+1} - \tau_i$. It is simply a product of single particle propagators

$$G(R', R, \tau) = \prod_{j=1}^{N} g(r'_j, r_j, \tau) \ , \quad g(r', r, \tau) \sim \exp\left\{ - \frac{m(r'-r)^2}{2\tau} \right\}$$

For convenience of notations I will use $\tau_0 = 0$ and $\tau_{n+1} = \beta$. We then have

$$Z = \sum_{n=0}^{\infty} (-1)^n \int_{\tau_1 < \tau_2 < \ldots < \tau_n}^{\beta} d\tau_1 \ldots d\tau_n \sum_{R_0 \ldots R_n} G_n K_{R_n} G_{n-1} K_{R_{n-1}} \ldots K_{R_1} G_0 \ .$$

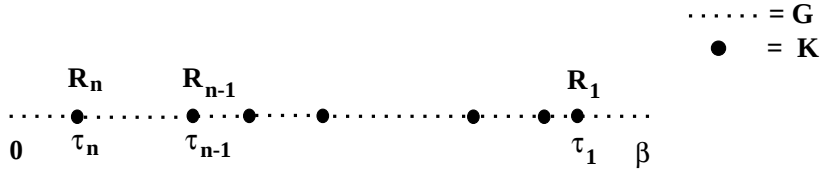
The summation over R_0 involves only free particle propagators and can be removed

$$\begin{aligned} \sum_{R_0} G_n G_0 &= \sum_{R_0} G(R_1, R_0, \tau_1) G(R_0, R_n, \beta - \tau_n) \equiv G(R_1, R_n, \tau_1 + \beta - \tau_n) \\ &\equiv G(R_1, R_n, MOD_\beta(\tau_1 - \tau_n)) \ . \end{aligned} \tag{23}$$

In what follows I will always understand the difference of two time variables as being MOD_β without mentioning this explicitly. Thus

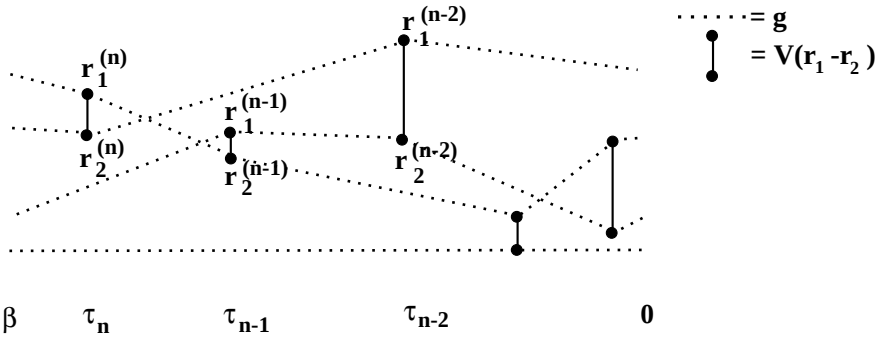
$$Z = \sum_{n=0}^{\infty} (-1)^n \int_{\tau_1 < \tau_2 < \ldots < \tau_n}^{\beta} d\tau_1 \ldots d\tau_n \sum_{R_1 \ldots R_n} G(R_1, R_n, \tau_1 - \tau_n) K_{R_n} \ldots G(R_2, R_1, \tau_2 - \tau_1) K_{R_1} \ .$$

The graphical structure of what we have is given below

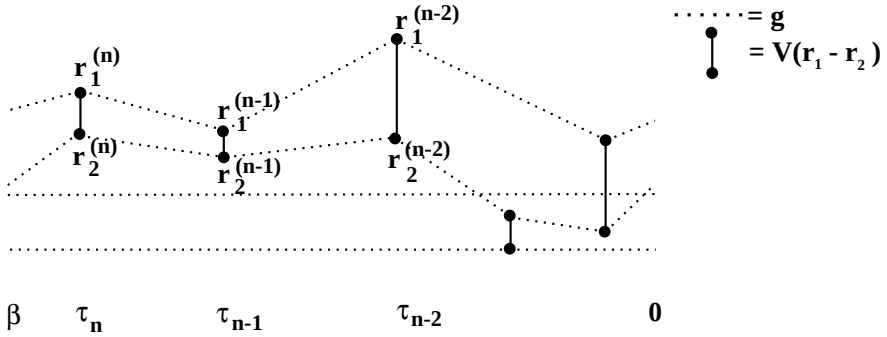


To complete the picture we notice that $K = \sum_{j_1 < j_2} V(r_{j_1} - r_{j_2})$ is the sum over all particle pairs. It means that in each diagram shown above we may specify only two single particle coordinates for each time τ_i. This gives us

the canonical Feynman diagram in the real space representation



Note, that we do not have to mention other particle coordinates apart from a pair coupled by $V(r_1(i) - r_2(i))$ because these coordinates can be integrated out analytically and we end up saying that other particles carry their free propagators to the next point in time, see Eq. (23). Since particles are identical the connection of interaction points on the β-circle may "convert" particle "ID"s when we formally follow the propagator lines. The same structure of interaction points in space-time may be connected by propagators in a **factorial number** of ways and an example of differently connected diagram is shown below.



In the partition function we should sum over all diagrams like the last one. The summation will include such parameters as the number of interaction vertices, n, their times and coordinates, and all allowed ways of connecting interaction points

$$Z = \sum_{n=0}^{\infty} (-1)^n \int_{\tau_1<\tau_2<\ldots<\tau_n}^{\beta} d\tau_1 \ldots d\tau_n \left(\prod_i \int \int dr_1^{(i)} dr_2^{(i)} \right) \sum_{connections} W^{(conn)} \Big[\{\tau_i\}; \{r_1^{(i)}, r_2^{(i)}\} \Big] .$$

where

$$W = \prod_{i=1}^{n} V(r_1^{(i)} - r_2^{(i)}) \ \times gggg \ldots ggg$$

You probably see already that it is easier to draw diagrams and explain what they mean then to write down the formal mathematical expression for it with all indices mentioned! That is why I skip mentioning indices of all g-functions which may be easily restored from the drawing. Note, that in this formulation you do **not** have to perform path-integral integration, and always deal with conventional integrals.

Tired of quantum mechanics? We are done for a while.