

Physics 7230: Statistical Mechanics

Lecture set 5: Density Matrix

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Abstract

In this set of lectures, we will introduce and discuss the properties and utility of the *density matrix* - a special quantum mechanical operator whose diagonal elements give the probability distribution for quantum mechanical microstates. It is a generalization of conventional wavefunction formulation of quantum mechanics, and in equilibrium allows computation of the partition function and therefore thermodynamics in quantum statistical mechanics. We will also discuss how thermodynamics (ETH) and in particular entropy – the so-called “entanglement” entropy – arises in a closed quantum system from entanglement of a subsystem with the rest of the system.

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I. DENSITY MATRIX FUNDAMENTALS IN QUANTUM STATISTICAL MECHANICS

A. General basics

Density matrix $\hat{\rho}$ was first introduced by John von Neumann in 1927 and independently by Lev Landau, and as we will see supercedes conventional wavefunction formulation of quantum mechanics.

Given a density matrix characterizing a statistical ensemble of a quantum system and obeying normalization conditions,

$$\text{Tr}[\hat{\rho}] = 1, \quad \text{Tr}[\hat{\rho}^2] \leq 1, \quad (1)$$

the averages of any operator $\hat{O}$ can be computed according to,

$$\langle \hat{O} \rangle = \text{Tr} [\hat{O} \hat{\rho}]. \quad (2)$$

A density matrix is given by a statistical state of a quantum system. Much as a wavefunction, once prepared in an initial state evolves in time according to the time dependent Schrodinger equation (or equivalently according to the evolution operator $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$, $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$), subject to systems Hamiltonian $\hat{H}$, a density matrix evolves according to the von Neumann equation (also known as the Liouville - von Neumann equation),

$$i\hbar\partial_t\hat{\rho} = [\hat{H}, \hat{\rho}], \quad (3)$$

or equivalently, $\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t)$ (not to be confused with the Heisenberg equation for evolution an operator, which has an opposite sign).

The von Neumann entropy

$$S_{vN} = -\text{Tr} [\hat{\rho} \ln \hat{\rho}] = -\langle \ln \hat{\rho} \rangle = -\sum_n \lambda_n \ln \lambda_n, \quad (4)$$

where λ_n are eigenvalues of $\hat{\rho}$ is the quantum mechanical counter-part (generalization) of the Shannon's entropy $S_S = -\sum_q P_q \ln P_q = -\langle \ln P_q \rangle$.

B. Equilibrium density matrix

For a system in thermal equilibrium the density matrix must be stationary and is thus, according to (3) is taken to be a function of the Hamiltonian, with a form special to ensembles discussed in Lectures 2-4,

- Microcanonical

$$\hat{\rho}_{mc} = \frac{1}{\Omega} \delta(E - \hat{H}) \quad (5)$$

- Canonical

$$\hat{\rho}_c = \frac{1}{Z} e^{-\hat{H}/k_B T} \quad (6)$$

- Grandcanonical

$$\hat{\rho}_{gc} = \frac{1}{\mathcal{Z}} e^{-(\hat{H} - \mu \hat{N})/k_B T} \quad (7)$$

Detailed balance of transitions between different states required to attain statistical equilibrium demands that $\hat{\rho}$ is a Hermitian operator.

Focusing on the canonical (equally true for grandcanonical) ensemble, we note that the *unnormalized* part of density matrix $\hat{\rho}_c^u(\beta) = e^{-\hat{H}/k_B T}$ satisfies a useful operator differential equation,

$$\partial_\beta \hat{\rho}_c^u = -\hat{H} \hat{\rho}_c^u(\beta), \quad (8)$$

that can be verified by formal substitution, utilizing a Taylor series in $\hat{H}$ representation of $\hat{\rho}_c^u(\beta)$. One can view this as a time-dependent Schrodinger equation in an imaginary time, $\tau = it$ (where τ ranges from 0 to $\beta\hbar$). Equivalently, when expressed in coordinate representation (see below) one can also view this as an equation in real time for diffusion in a potential.

II. PURE STATES IN QUANTUM MECHANICS

Recall from standard quantum mechanics, that states $|\psi\rangle$ of an isolated quantum system are rays (since normalization creates physical equivalence class) in Hilbert space with expectation values of physical observables, represented by Hermitian operators $\hat{O}$ are given by,

$$\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle.$$

A. Dirac basis-independent representation

It is convenient to introduce a completely equivalent description in terms of the so-called “pure” density matrix

$$\hat{\rho} = |\psi\rangle\langle\psi|, \quad (9)$$

in terms of which we have,

$$\langle\hat{O}\rangle = \langle\psi|\hat{O}|\psi\rangle = \text{Tr}[\hat{O}\hat{\rho}], \quad (10)$$

as given in (2).

One advantage of using $\hat{\rho}$ over states $|\psi\rangle$ is that the overall unphysical phase disappears, so in a sense density matrix is more physical.

Using time-dependent Schrodinger equation for $|\psi(t)\rangle$ we obtain the von Neumann equation for the evolution of $\hat{\rho}(t)$. We can also check that

$$\text{Tr}[\hat{\rho}] = 1, \quad \text{Tr}[\hat{\rho}^2] = 1, \quad (11)$$

and is a defining property of a pure density matrix state, i.e., a density matrix that corresponds to a single quantum mechanical state $|\psi\rangle$, which of course can be a superposition of many other states. This is to be contrasted with the “mixed” density matrix, to be discussed in next subsection.

B. Basis representation

Just like a state $|\psi\rangle = \sum_n c_n |n\rangle$ can be represented in terms of an orthonormal basis as a state vector $\{c_n\}$, so can density matrix can be represented as a basis-dependent matrix ρ_{nm} , where

$$\hat{\rho} = \sum_{n,m} \rho_{nm} |n\rangle\langle m| \quad (12)$$

with matrix elements by definition given by $\rho_{nm} = \langle n|\hat{\rho}|m\rangle = c_n c_m^*$.

In terms of this representation the trace in (10) is easily computed, giving

$$\langle\hat{O}\rangle = \text{Tr}[\hat{O}\hat{\rho}] = \sum_{nm} O_{nm} \rho_{mn} \quad (13)$$

The time evolution is given by matrix version of (3) for H_{nm} and ρ_{nm} . It is convenient to choose $|n\rangle$ to be eigenstates of $\hat{H}$, such that $\hat{H}|n\rangle = E_n|n\rangle$, which then gives,

$$\rho_{nm}(t) = \rho_{nm}(0)e^{-i(E_n - E_m)t/\hbar}, \quad (14)$$

consistent with above $\rho_{nm} = c_n c_m^*$ representation and showing that diagonal matrix elements of $\hat{\rho}$ are stationary in the Hamiltonian basis and the off-diagonal coherences oscillate at frequency set by the difference of energy eigenvalues.

The property (11) is just a reflection of the normalization of $|\psi\rangle$ that pure $\hat{\rho}$ is describing. We also note that a pure density matrix, $\hat{\rho}$ in (9) can be viewed, somewhat perversely in the basis of $|\psi\rangle$ itself. It is then a matrix of all zeros (corresponding to all other states transverse to $|\psi\rangle$) and 1 as $\rho_{\psi\psi} = \langle\psi|\hat{\rho}|\psi\rangle = 1$. From this extremely degenerate, rank 1 matrix many of the above expressions e.g., (11) become obvious.

We next consider a generalization of conventional quantum mechanics to that describing a statistical ensemble of quantum states. Such system is described by a “mixed” density matrix, to be discussed in next subsection.

III. MIXED STATES IN QUANTUM MECHANICS

We now generalize above analysis to “mixed” density matrix that describes a statistical ensemble of pure quantum states, that cannot be represented as any state $|\psi\rangle$. As such, mixed density matrix is not equivalent to conventional states of a single quantum mechanical system.

A. General

Thus we consider a “mixed” density matrix, defined as an ensemble of pure density matrix with probability p_i ,

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad (15)$$

with normalization $\sum_i p_i = 1$, in terms of which we have,

$$\langle \hat{O} \rangle = \sum_i p_i \langle \psi_i | \hat{O} | \psi_i \rangle = \text{Tr}[\hat{O} \hat{\rho}], \quad (16)$$

where there is both a quantum mechanical and statistical averages.

We can also check that

$$\text{Tr}[\hat{\rho}] = 1, \text{Tr}[\hat{\rho}^2] \leq 1, \quad (17)$$

with the second equation being the litmus test for a density matrix describing a mixed state. It can be traced to the fact that $p_i^2 \leq 1$.

B. Thermal equilibrium

In thermal equilibrium $\hat{\rho}(\hat{H})$ take on the form (5)-(7) in the first section, above, with specific form depending on the ensemble. All other properties of mixed density matrix goes through. As an example we focus on the canonical ensemble.

1. Hamiltonian eigenstates representaton

As discussed above $\hat{\rho}$ is a Hermitian operator, generically represented by a corresponding matrix $\rho_{nm} = \langle n | \hat{\rho} | m \rangle$. In the special basis of the Hamiltonian eigenstates, the density matrix simplifies significantly,

$$\hat{\rho} = \frac{1}{Z} \sum_n e^{-E_n/k_B T} |n\rangle \langle n|$$

taking a diagonal form,

$$p_n = \frac{1}{Z} e^{-E_n/k_B T}, \quad \rho_{nm} = \frac{1}{Z} e^{-E_n/k_B T} \delta_{nm} = p_n \delta_{nm},$$

that is quite convenient for many equilibrium computations and makes the quantum statistical mechanics closer to the classical one.

2. Position representaton

Another useful and important basis is the position/coordinate basis, $|x\rangle$ that are eigenstates $\hat{x}|x\rangle = x|x\rangle$ of the position operator $\hat{x}$, with eigenvalue x . The canonical ensemble unnormalized density matrix in this representation is given by,

$$\rho^u(x, x'; \beta) = \langle x | e^{-\beta \hat{H}} | x' \rangle = \sum_{nm} \langle x | n \rangle \langle n | e^{-\beta \hat{H}} | m \rangle \langle m | x' \rangle, \quad (18)$$

$$= \sum_n \psi_n(x) \psi_n^*(x') e^{-\beta E_n}, \quad (19)$$

expressed purely in terms of the Hamiltonian eigenfunctions and eigenvalues. We note the close relation of $\rho^u(x, x'; \beta)$ to the evolution operator in quantum mechanics $U(x, x'; t)$, identifying the former as the evolution operator in imaginary time $t = -i\tau = -i\beta\hbar$ (note the units are indeed that of time), converting (i.e., analytically continuing) $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ to $\hat{\rho}^u(\beta) = e^{-\hat{H}\tau/\hbar}$, with $\hat{\rho}^u(\beta) = \hat{U}(-i\beta\hbar)$.

Recalling an operator differential equation satisfied by equilibrium (canonical) density matrix, Eq.(8), in coordinate representation it takes the form,

$$\partial_\beta \rho^u(x, x', \beta) = -H(\hat{p}, x) \rho^u(x, x', \beta), \quad (20)$$

where $\hat{p} = -i\hbar\partial_x$, i.e., giving the coordinate representation Schrodinger equaiton in imaginary time.

Thinking about the fundamental definition of $\hat{\rho}^u$ in (6), (7) or equivalently the evolution equation (20), we also note that $\rho^u(x, x', \tau)$ satisfies an important “propagator” property,

$$\rho^u(x_2, x_0; \tau_1 + \tau_2) = \int dx_1 \rho^u(x_2, x_1; \tau_2) \rho^u(x_1, x_0; \tau_1), \quad (21)$$

in analogy with a quantum mechanical propagator.

The corresponding expectation value of an operator $\hat{O}$ is given in coordinate space

$$\langle \hat{O} \rangle = \int dx dx' O(x, x') \rho(x', x), \quad (22)$$

an extension of the general result (13) to coordinate representation.

3. Path-integral representation

As discussed in earlier lectures, Hamiltonian approach to computation of thermodynamic averages for quantum systems requires (in comparison to classical statistical mechanics) an additional step of a diagonalization of the Hamiltonian to obtain E_n . We mention here for completeness that an alternative approach invented by Richard Feynman[14, 15], allows one to bypass the diagonalization step, but at the cost of working with a path-integral over (imaginary) time-dependent microscopic degrees of freedom $\{q_n(\tau)\}$, with an exponential of the corresponding Euclidean classical action (obtained from standard action by replacing $t = -i\tau$), $S_E[\{q_n(\tau)\}] = \int_0^{\beta\hbar} d\tau L[\{q_n(\tau)\}]$ as the counter-part of the Boltzmann weight, with $L[\{q_n(\tau)\}]$ the classical Lagrangian. This is not surprising, given the connection we have already seen in Eq.(20). Namely, for a quantum system the coordinate-space density matrix can be written as partition function can be written as a path-integral[15],

$$\rho^u(x, x'; \beta) = \int_{x(0)=x, x(\beta\hbar)=x'} [dx(\tau)] e^{-S_E[x(\tau)]/\hbar}, \quad (23)$$

and the associated partition function is the trace,

$$Z = \sum_{\{q_n(\tau)\}} e^{-S_E[\{q_n(\tau)\}]/\hbar}, \quad (24)$$

$$= \int dx \rho^u(x, x; \beta), \quad (25)$$

$$= \int_{-\infty}^{\infty} dx \int_{x(0)=x, x(\beta\hbar)=x} [dx(\tau)] e^{-S_E[x(\tau)]/\hbar}, \quad (26)$$

where the imaginary time ranges over a finite interval, $0 \leq \tau \leq \beta\hbar$, with periodic boundary conditions $x(0) = x(\beta\hbar)$.

This thereby reduces quantum statistical mechanics of a point (0d) particle described by $\hat{q} \equiv \hat{x}$, (i.e., zero-dimensional “field”) to a classical statistical mechanics of a fluctuating closed “curve” - “polymer string”, described by a 1d closed curve $q(\tau)$ with the effective classical Hamiltonian given by

$$H_{\text{eff}}[q(\tau)] \equiv S_E[q(\tau)]/\hbar.$$

In passing we note that this nicely extends to quantum field theory of a d -dimensional system with field operators $\hat{\phi}(\mathbf{x})$ to a $d + 1$ -dimensional path-integral formulation over commuting field degrees of freedom, $\phi(\mathbf{x}, \tau)$, whose description can be viewed as an effective classical statistical field theory over fields $\phi(\mathbf{x}, \tau)$.

We also note that in the limit of high temperature (much higher than any natural frequencies of the system), $q(\tau)$ are τ independent and the Euclidean action reduces to $\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau L[q(\tau)] \rightarrow \beta H(q)$, and the partition function reduces to the classical one.

We note that the above path-integral representation of d -dimensional quantum statistical mechanics in terms of $(d + 1)$ -dimensional classical statistical mechanics is a direct imaginary time analog of Feynman's representation of the Schrodinger quantum mechanics, $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$ written in terms of the evolution operator $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ in terms of the path-integral in real time[14], where in coordinate representation it is given by, $U(x, x'; T) = \int_{x(0)=x, x(T)=x'} [dx(t)] e^{iS[x(t)]/\hbar}$.

IV. DENSITY MATRIX EXAMPLES

We will now present a few sample density matrices in various representations and examine their properties.

Given a state $|\psi\rangle$ we can always construct a pure density matrix as described above. A mixed density matrix depends on the statistical ensemble characterized by probability distribution $\{p_i\}$ can also be constructed for any specific situation. In equilibrium the density matrix is completely determined by the Hamiltonian of the system, given by Eqs.5,6,7, with the corresponding E , T , μ , depending on the ensemble of choice.

A. Spin-1/2 states

- **Pure state $|+, \hat{n}\rangle$ of spin 1/2** polarized along $\hat{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$:

Such state can be written in the $|\uparrow\rangle, |\downarrow\rangle$ basis, the eigenstates of $\hat{S}_z$, $|+, \hat{n}\rangle = \cos \frac{\theta}{2} e^{-i\phi/2} |\uparrow\rangle + \sin \frac{\theta}{2} e^{i\phi/2} |\downarrow\rangle$.

The corresponding pure density matrix is given by

$$\hat{\rho}^{\text{pure}, \hat{n}} = |+\rangle\langle+| = \cos^2 \frac{\theta}{2} |\uparrow\rangle\langle\uparrow| + \sin^2 \frac{\theta}{2} |\downarrow\rangle\langle\downarrow| + \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{-i\phi} |\uparrow\rangle\langle\downarrow| + \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{i\phi} |\downarrow\rangle\langle\uparrow|, \quad (27)$$

that has matrix elements given by

$$\rho_{\sigma, \sigma'}^{\text{pure}, \hat{n}} = \begin{pmatrix} \cos^2 \frac{\theta}{2} & \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{-i\phi} \\ \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{i\phi} & \sin^2 \frac{\theta}{2} \end{pmatrix}. \quad (28)$$

In the $|+, \hat{n}\rangle, |-, \hat{n}\rangle$ basis its matrix elements are given by,

$$\rho_{\sigma, \sigma'}^{\text{pure}, \hat{n}} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (29)$$

In the case of photons such pure state describes perfectly polarized light. This density matrix can be straightforwardly demonstrated to satisfy normalization, $\text{Tr}[\hat{\rho}] = 1$, purity condition $\text{Tr}[\hat{\rho}^2] = 1$, and gives $\hbar/2$ for the expectation values of $\hat{n} \cdot \vec{S}$. For $\theta = \pi/2, \phi = 0$, we find 0 for $\hat{S}_z$ and $\hbar/2$ for $\hat{S}_x$.

For latter choice of quantization axis, $\theta = \pi/2, \phi = 0$, it is an eigenstate of $\hat{S}_x$, and reduces to,

$$\hat{\rho}^{\text{pure}, \hat{x}} = \frac{1}{2} (|0\rangle + |1\rangle) (\langle 0| + \langle 1|), \quad (30)$$

$$= \frac{1}{2} (|0\rangle\langle 0| + |1\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 1|). \quad (31)$$

with the matrix representation given by

$$\rho_A = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad (32)$$

and we used another common notation of $|0\rangle, |1\rangle$ basis (used in quantum information), isomorphic to up/down spin basis.

- **Mixed state at infinite temperature:**

If instead we consider an ensemble state that is an equal statistical mixture of all quantization axes, $\hat{n}$ uniformly distributed over 4π steradians (for photons we would call this “unpolarized” light from eg., an incandescent light bulb), the density matrix is given by,

$$\rho_{\sigma,\sigma'}^{\text{mixed}} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}, \quad (33)$$

which can be straightforwardly obtained by averaging $\rho_{\sigma,\sigma'}^{\text{pure},\hat{n}}(\theta, \phi)$ over $\hat{n}$ on a surface of Stokes sphere. The diagonal elements correspond to equal probabilities for the spin up and spin down states. We note that all off-diagonal quantum mechanical coherences average out.

It can be seen that this mixed state satisfies $\text{Tr}[\hat{\rho}_{\text{mixed}}^2] = 1/2 < 1$, and

$$\langle \vec{S} \rangle = \text{Tr}[\hat{\rho} \vec{S}] = 0.$$

This incoherent state with all spin components vanishing is clearly very different from the above pure state for $\theta = \pi/2$, for which although $\langle S_z \rangle = 0$, there is perfect polarization along $\hat{x}$.

Comparing this mixed density matrix to the canonical density matrix at $\beta = 0$, we see that this mixed state corresponds to an infinite temperature state, for which in equilibrium all states are equally likely, with this case $p_{\text{up/down}} = 1/2$.

We note that it is *impossible* to describe this (and any other) mixed state in terms of any state $|\psi\rangle$. Do *not* confuse a mixed state (where there is an incoherent statistical ensemble of many quantum mechanical systems), with a pure density matrix of a state that is a superposition of many pure states!

- **Pure N -spin $1/2$ states:**

We can also consider N -spin states. For example

- *unentangled - product states:* An illustrative simple examples of product 2-spin

states are given below,

$$|\psi_z\rangle = |\uparrow\rangle|\uparrow\rangle, \quad (34)$$

$$|\psi_+\rangle = |+\rangle|-\rangle = \frac{1}{2}(|\uparrow\rangle + |\downarrow\rangle)(|\uparrow\rangle - |\downarrow\rangle). \quad (35)$$

While (34) looks simpler in the $\hat{S}_z$ basis than (35), this is just a choice of the basis. In the $\hat{S}_x$ basis the reverse is true.

– *entangled*:: Illustrative simple examples of entangled 2-spin states are given below,

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\uparrow\rangle + |\downarrow\rangle|\downarrow\rangle), \quad (36)$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|+\rangle|-\rangle + |-\rangle|+\rangle), \quad (37)$$

$$|\psi_{\text{cat}1}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\dots\rangle - |\downarrow\downarrow\downarrow\dots\rangle). \quad (38)$$

These are entangled 2-spin and N -spin states, with the last one for obvious reasons sometimes referred to as “cat” state - superposition of a “dead” and “alive cat”. On the next homework, we will work out density matrices for such multi-spin states, utilizing above construction of a pure density matrix from a state $|\psi\rangle$.

B. Free particle

As an example we now consider coordinate-space representation of the density matrix for a free particle in d -dimensions, modeled by $\hat{H}_0 = \hat{\mathbf{p}}^2/2m$. Using our discussion of a general unnormalized $\rho^u(\mathbf{x}, \mathbf{x}'; \beta)$ above, for a free particle with momentum eigenstates $|\mathbf{k}\rangle$, we find

$$\rho_0^u(\mathbf{x}, \mathbf{x}'; \beta) = \langle \mathbf{x} | e^{-\beta \hat{H}_0} | \mathbf{x}' \rangle \quad (39)$$

$$= \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{x}) \psi_{\mathbf{k}}^*(\mathbf{x}') e^{-\beta E_{\mathbf{k}}}, \quad (40)$$

$$= \left(\frac{m}{2\pi\beta\hbar^2} \right)^{d/2} e^{-\frac{1}{2}m(\mathbf{x}-\mathbf{x}')^2/(\beta\hbar^2)} = \frac{1}{\lambda_T^d} e^{-\pi(\mathbf{x}-\mathbf{x}')^2/\lambda_T^2}, \quad (41)$$

where $\lambda_T = h/\sqrt{2\pi m k_B T}$ and the prefactor arises from eigenstates' normalization. We also note that in the $\beta \rightarrow 0$ limit, the density matrix reduces to a δ -function $\rho_0^u(\mathbf{x}, \mathbf{x}'; 0) = \delta(\mathbf{x}-\mathbf{x}')$

as expected for a fully incoherent state at infinite temperature with vanishing coherences, i.e., a classical particle.

C. Harmonic oscillator

As another example we consider coordinate-space representation of the density matrix for a particle in 1d harmonic potential, modeled by $\hat{H}_{\text{ho}} = \hat{p}^2/2m + \frac{1}{2}m\omega^2\hat{x}^2$. As we did for a free particle, above, $\rho_{\text{ho}}^u(x, x'; \beta)$ can be obtained by utilizing eigenstates of a harmonic oscillator, namely, the Hermite polynomials $H_n(x)e^{-\frac{1}{2}x^2}$ and performing a sum in (19).

Alternatively, and simpler, we can use either a solution of the imaginary-time Schrodinger equation (20), or a path-integral formulation (23). We thereby find a somewhat complicated (but famous) expression for the unnormalized (no factor of $1/Z$) density matrix,

$$\rho_{\text{ho}}^u(x, x'; \beta) = \left(\frac{m\omega}{2\pi\hbar \sinh(\beta\hbar\omega)} \right)^{1/2} e^{-\frac{m\omega}{4\hbar} [(x+x')^2 \tanh(\beta\hbar\omega/2) + (x-x')^2 \coth(\beta\hbar\omega/2)]}, \quad (42)$$

$$(43)$$

where the partition function is directly obtained,

$$Z = \frac{1}{2 \sinh(\beta\hbar\omega/2)}, \quad (44)$$

consistent with our result from earlier lecture and homework. From this we obtain for normalized density matrix $\rho = \rho^u/Z$,

$$\rho_{\text{ho}}(x, x'; \beta) = \left(\frac{m\omega \tanh(\beta\hbar\omega/2)}{\pi\hbar} \right)^{1/2} e^{-\frac{m\omega}{2\hbar \sinh(\beta\hbar\omega)} [(x^2+x'^2) \cosh(\beta\hbar\omega) - 2xx']}. \quad (45)$$

As we will explore on the homework, this density matrix has rich behavior satisfying all the expected limits.

V. APPROXIMATE METHODS

It is a rare example that an interesting problem in physics is exactly solvable. So most of the time we must resort to an approximate solution, that hopefully can be justified in the limit of interest. Here we will discuss two such methods. I note that presentations below are

tailored for a special case of classical statistical mechanics or more generally when various components of the Hamiltonian (e.g., H_0, H_1 , and H, H_{tr} below) commute. We will utilize these two methods to solve few problems on the homework.

A. Perturbation theory

Often we are faced with solving a problem for a Hamiltonian $H = H_0 + H_1$, where the problem is only exactly solvable for H_0 . Namely, in the context of statistical mechanics, we can compute all the observables and in particular can calculate the partition function $Z_0 = \text{Tr} [e^{-\beta H_0}]$. However, we are unable to calculate the partition function $Z = \text{Tr} [e^{-\beta(H_0+H_1)}]$. How do we make progress?

Much like in other fields, e.g., quantum mechanics, in the case of a weak perturbation $H_1 \ll H_0$ we can compute Z perturbatively in a controlled expansion in H_1/H_0 . Namely we simply Taylor expand in H_1 , by assumption above, allowing us to calculate exactly term by term to some order of interest,

$$Z = \text{Tr} [e^{-\beta(H_0+H_1)}] \approx \text{Tr} \left[e^{-\beta H_0} \left(1 - \beta H_1 + \frac{1}{2!} \beta^2 H_1^2 + \dots \right) \right], \quad (46)$$

$$= Z_0 \left[1 - \beta \langle H_1 \rangle_0 + \frac{1}{2!} \beta^2 \langle H_1^2 \rangle_0 + \dots \right], \quad (47)$$

where all the averages are done with the solvable probability distribution $e^{-\beta H_0}/Z_0$. Thus, every term can in principle be computed to a desired order.

B. Variational theory

Another quite general approximate treatment is the variational theory, where the upper bound for the free energy, F is computed using a minimized variational free energy, F_{var} computed with a trial Hamiltonian, H_{tr} . To see how this upper bound is established we approximate the partition function,

$$\begin{aligned} Z &= \text{Tr} [e^{-\beta H}] = e^{-\beta F}, \\ &= \text{Tr} [e^{-\beta(H-H_{\text{tr}})} e^{-\beta H_{\text{tr}}}] = \langle e^{-\beta(H-H_{\text{tr}})} \rangle_{\text{tr}} e^{-\beta F_{\text{tr}}}, \\ &\geq e^{-\beta \langle H-H_{\text{tr}} \rangle_{\text{tr}}} e^{-\beta F_{\text{tr}}} \equiv e^{-\beta F_{\text{var}}}, \end{aligned} \quad (48)$$

where the variational free energy

$$F_{\text{var}} = F_{\text{tr}} + \langle H - H_{\text{tr}} \rangle_{\text{tr}} \geq F,$$

provides the upper bound for the actual free energy F of interest, and H_{tr} is the trial Hamiltonian, with respect to which the above expectation value is computed. In above we used the convex property of the e^{-x} function to conclude that $\langle e^{-x} \rangle \geq e^{-\langle x \rangle}$, as illustrated in Fig.1

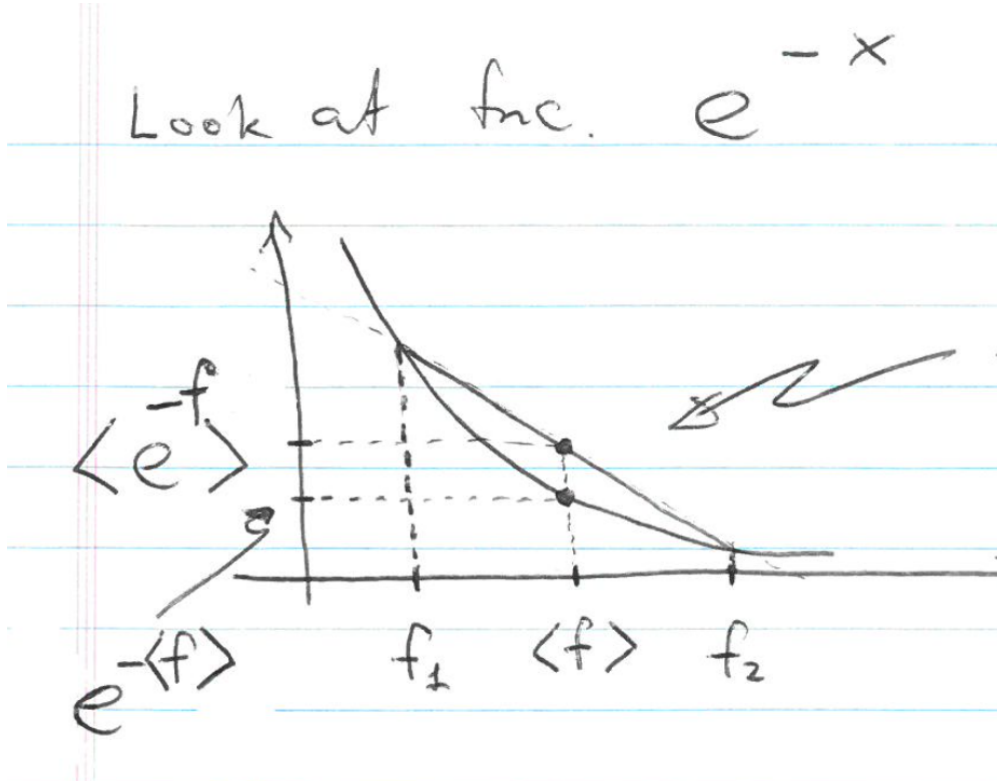


FIG. 1: Illustration of convexity property of e^{-x} .

The use of the variational method is a bit of an art in selecting a convenient H_{tr} , so it approximates well the Hamiltonian H of interest. We pick H_{tr} to be characterized by adjustable variational parameters to minimize F_{var} , as to give a tighter bound on F of interest. . If one picks too many variational parameters then the computation is too difficult. On the other hand, picking too few parameters does not give tight enough bound on F . The good news is that the better the choice of H_{tr} , the closer is the approximate solution F_{var} to the exact free energy F .

VI. THERMODYNAMICS FROM PURE CLOSED QUANTUM SYSTEM

We next turn to a discussion of emergence of thermodynamics and in particular of the “entanglement entropy” in a closed quantum system.

A. Eigenstate Thermalization Hypothesis (ETH)

Amazingly, microcanonical description is believed to extend to a generic closed quantum many-body system in a *single* eigenstate, a postulate known as the Eigenstate Thermalization Hypothesis (ETH), put forth in early 90s by Mark Srednicki[8] and independently by Josh Deutsch[9]. As consequence ETH posits that a quantum mechanical average of an observable $\hat{O}$ for a system in a generic quantum many-body state $|\Psi(t)\rangle$, under unitary evolution, in a long time limit “relaxes” to equilibrium, described by the microcanonical ensemble at energy $E = \langle \Psi | \hat{H} | \Psi \rangle$,

$$\frac{1}{t} \int_0^t dt' \langle \Psi(t') | \hat{O} | \Psi(t') \rangle_{t \rightarrow \infty} = \langle \hat{O} \rangle_{P_{\text{equilibrium}}} \quad (49)$$

and by equivalence of ensembles can also be calculated using canonical/grandcanonical ensemble. To see this we can express $|\Psi(t)\rangle$ in terms of many-body eigenstates $|n\rangle$ and consider expectation value at time t of a *local* operator $\hat{O}$,

$$\langle \Psi(t') | \hat{O} | \Psi(t') \rangle = \sum_{nm} O_{nm} c_m c_n^* e^{-i(E_m - E_n)t/\hbar}. \quad (50)$$

We note a first crucial property that the off-diagonal $n \neq m$ terms oscillate with gaps of the spectrum. In a generic many-body system (in contrast to a special simple, i.e., integrable single-body problem), the spectrum is complex and incommensurate, and thus in the long time limit, these off-diagonal terms exhibit fast incommensurate oscillations, dephasing and averaging out to zero after some time (set by minimum gaps) in the $t \rightarrow \infty$ limit.

Thus, above expectation value “relaxes” (equilibrates) to a stationary time-independent state, determined by diagonal components of the density matrix,

$$\frac{1}{t} \int_0^t dt' \langle \Psi(t') | \hat{O} | \Psi(t') \rangle_{t \rightarrow \infty} = \sum_n O_{nn} |c_n|^2 = \sum_n O_{nn} \rho_{nn}^{\text{diagonal}}. \quad (51)$$

At this point one may celebrate having found that long-time averaged expectation value is determined by a stationary density matrix in the so-called diagonal ensemble.

However, to declare the validity of Eq.49, that would allow one to replace time averages in a pure state by a thermal equilibrium ensemble average, a serious issue of principle remains. Namely, the diagonal components of the density matrix $|c_n|^2$ and therefore the expectation value of $\hat{O}$, $\sum_n |c_n|^2 O_{nn}$ appear to depend on the details of the initial state $|\Psi(0)\rangle$ through the initial expansion coefficients, c_n , not just on its average energy density, $\mathcal{E} = E/V = \langle \Psi | \hat{H} | \Psi \rangle / V \equiv k_B \bar{T}$ as in an thermal ensemble on the right hand side of (49). Eigenstate Thermalization Hypothesis (ETH) proposes that for generic state with a finite excitation energy density (not a ground state) $\mathcal{E} = E/V$, diagonal matrix elements of a local operator are independent of n , depending only on $\mathcal{E}$. Thus O_{nn} can be taken out of the sum, which then reduces to 1, with the result reducing to the microcanonical ensemble around the state n set by E . Namely, in a long time limit the expectation value relaxes to an ensemble average of O_{nn} over eigenstates around energy E in a range of fixed energy density $\mathcal{E}$.

It appears somewhat paradoxical that a closed quantum system evolving under purely unitary, norm-preserving evolution, nevertheless exhibits “relaxation”, with accompanying growth of sub-system’s entanglement entropy (see below). The resolution of this apparent “paradox” is that local observables gets “dressed” and thereby spread into operators that are nonlocal in coordinate and in operator space. Thus, while there is no loss of information or many-body norm, under growth of entanglement the information delocalizes and thereby becomes unobservable through local low-order operators measured in typical experiments. Thus, from the perspective of experimentally accessible local observables, the system relaxes to equilibrium value of these observables.

There are notable exceptional closed quantum systems (typically in the presence of local random heterogeneities, i.e., “quenched disorder”), that are not ergodic. They do not equilibrate and thus violate ETH, exhibiting the so-called “many-body localization” (MBL)[11], that is currently vigorously studied[12]. More generally, “integrable” systems have infinite number of conserved quantities, that (thereby cannot relax) violate ETH, with MBL being only one example where such integrability is emergent.

B. “Entanglement entropy” in closed quantum systems

We next discuss a concept of entropy in a closed quantum mechanical system in a (normalized) state $|\Psi\rangle$, characterized by a pure density matrix $\hat{\rho} = |\Psi\rangle\langle\Psi|$. It is easy to see that the von Neumann entropy of the total system vanishes identically and is independent of time. This underscores the fact that the total system is in a pure state.

However, imagine splitting this full closed system A+B into subregions A and B and tracing over degrees of freedom in region B (spanned by basis $|\psi_B\rangle$). Physically this represents the fact that in practice we only have access to local operators, with support in some subregion A, and thus it is only the “reduced density matrix” for subsystem A, that is involved,

$$\hat{\rho}_A = \text{Tr}_B [\hat{\rho}] \equiv \sum_{\psi_B} \langle \psi_B | \hat{\rho} | \psi_B \rangle, \quad (52)$$

Even more explicitly, matrix elements of $\hat{\rho}_A$ are given by

$$\rho_{\sigma_A \sigma'_A} \equiv \langle \sigma_A | \hat{\rho}_A | \sigma'_A \rangle = \sum_{\psi_B} \langle \psi_A, \psi_B | \hat{\rho} | \psi'_A, \psi_B \rangle. \quad (53)$$

Generically, this $\hat{\rho}_A$ will be a *mixed* density matrix, i.e., $\text{Tr} [\rho_A^2] < 1$. Correspondingly, we can define the “entanglement entropy”,

$$S_E = -k_B \text{Tr} [\hat{\rho}_A \ln \hat{\rho}_A], \quad (54)$$

that is a quantum-mechanical analog of the thermodynamic entropy, and will generically be nonzero if $\hat{\rho}_A$ is indeed a mixed state.

As we will work out explicitly on the homework:

- **$\hat{\rho}_A$ is pure for:**

A and B *unentangled*, i.e., $|\psi_A \psi_B\rangle = |\psi_A\rangle |\psi_B\rangle$, i.e., a product state, and $S_E = 0$.

- **$\hat{\rho}_A$ is mixed for:**

A and B *entangled*, i.e., $|\psi_A \psi_B\rangle \neq |\psi_A\rangle |\psi_B\rangle$, i.e., not expressible as a product state, and $S_E > 0$.

Thus S_E measures the extent of entanglement between regions A and B. For example, for a fully entangled two-spin singlet state $|\Psi\rangle = \frac{1}{\sqrt{2}} [|\uparrow\rangle_A |\downarrow\rangle_B - |\downarrow\rangle_A |\uparrow\rangle_B]$, leads to a mixed ρ_A with the entanglement entropy that is maximum, $S_E = k_B \ln 2$, quantifying the fact that in such a state there is no local information about a single spin, only quantum correlations between the two spins. In contrast, a fully unentangled product state $|\Psi\rangle = |\uparrow\rangle_A |\downarrow\rangle_B$ gives a pure ρ_A and has a vanishing entanglement entropy, $S_E = 0$. For a more general case of an N spin-chain, starting with an initial state that is unentangled, the initial entropy $S_E(t = 0, L_A) = 0$, but will evolve in time in an ergodic ETH system to $S_E(t \gg t_{equil}, L_A) = L_A s$, that is extensive and given by the thermodynamic entropy. We note that since $S_E(L) = 0$, $S_E(L_A) = S_E(L - L_A)$, maximized at $L_A = L/2$.

VII. RELATION TO INFORMATION THEORY

Amazingly, as was first discussed by “the father” of information theory, Claude Shannon in his landmark 1948 paper, “A Mathematical Theory of Communication”, thermodynamic entropy as defined by the microcanonical ensemble is intimately related to information contained in e.g., a transmitted signal or text of a book. The profound Shannon’s assertion is that “information” (Shannon entropy) is the von Neumann entropy of the signal or data, viewed as stochastic data characterized by probability distribution.

To see this more explicitly, we consider a binary signal of N bits of 0s and 1s

$$\dots 0001101111000110000 \dots \quad (55)$$

with probability p_0 of a 0 bit and $p_1 = 1 - p_0$ of a 1 bit appearing in the signal. We then would like to define “Information” to be consistent with the colloquial intuition, namely, the most predictable signal of, e.g., all 1s, $p_1 = 1$ carrying no, i.e., zero information (since each bit is completely predictable to be a 1) and the least predictable signal of random 0s and 1s, $p_0 = p_1 = 1/2$ giving maximum Information. Following Shannon we then define Information S (Shannon entropy of the signal) in terms of the number of possible length N bit signals that can be created subject to the statistics of the signal characterized by $p_{0,1}^i$. The latter

is nothing but the multiplicity,

$$\Omega = \frac{N!}{M_0!M_1!} = \frac{N!}{(p_0N)!(p_1N)!}, \quad (56)$$

$$= \frac{N^N}{(p_0N)^{p_0N}(p_1N)^{p_1N}} \equiv 2^{NS}, \quad (57)$$

$$= p_0^{-p_0N} (1 - p_0)^{-(1-p_0)N}, \quad (58)$$

where in the second line we used Stirling approximation. This then gives Shannon's information per bit, $S = N^{-1} \log_2 \Omega$,

$$S = -p_0 \log_2(p_0) - (1 - p_0) \log_2(1 - p_0), \quad (59)$$

just like the entropy of a Ising magnet at fixed magnetization. In the more general case of m (rather than just 2) letters a_i , with $i = 1, \dots, m$ and corresponding probability for each letter p_i , Shannon's information is given by,

$$S = - \sum_{i=1}^m p_i \log_2 p_i. \quad (60)$$

This and many other aspects of classical and quantum informations are well discussed by J. Preskill in his Caltech notes as well as by Ed Witten in his “mini-review of information theory”, that appeared on the arXiv.

With this lecture discussion, amplified by your detailed homework analysis we are now experts on the role and utility of density matrix in quantum statistical mechanics. In the next lecture we will turn to some important applications.

Appendix A: Path-integrals formulation in quantum mechanics

Inspired by Dirac's beautiful on role of the action in quantum mechanics, Richard Feynman developed a path-integral quantization method[14] complementary to the Schrödinger equation and noncommuting operators Heisenberg formalism.

As a warmup we begin with a phase-space path-integral formulation of a single particle quantum mechanics. We will then generalize it to a many-body system, simplest formulated in terms of a coherent states path-integral.

1. phase-space path-integral

A central object in formulation of quantum mechanics is the unitary time evolution operator $\hat{U}(t)$ that relates a state $|\psi(t)\rangle$ at time t to the $|\psi(0)\rangle$ at time 0,

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle.$$

Given that $|\psi(t)\rangle$ satisfies the Schrödinger's equation, the formal solution is given by $\hat{U}(t) = e^{-\frac{i}{\hbar}Ht}$. In a 1d coordinate representation, we have

$$\langle x_f|\psi(t)\rangle = \int_{-\infty}^{\infty} dx_0 \langle x_f|\hat{U}(t)|x_0\rangle \langle x_0|\psi(0)\rangle, \quad (\text{A1})$$

$$\psi(x_N, t) = \int_{-\infty}^{\infty} dx_0 U(x_N, x_0; t) \psi(x_0, 0), \quad (\text{A2})$$

where we defined $x_f \equiv x_N$, $x_i \equiv x_0$, $t = t_N = N\epsilon$, $t_0 = 0$. Our goal then is to find an explicit expression for the evolution operator, equivalent to a solution of the Schrödinger's.

To this end we employ the so-called Trotter decomposition of the evolution operator $\hat{U}(t_N)$ in terms of the infinitesimal evolution over time $t/N = \epsilon$:

$$\hat{U}(t_N) = e^{-\frac{i}{\hbar}\hat{H}t} = \left(e^{-\frac{i}{\hbar}\hat{H}\frac{t}{N}} \right)^N = \underbrace{\hat{U}(\epsilon)\hat{U}(\epsilon)\dots\hat{U}(\epsilon)}_N. \quad (\text{A3})$$

$$(\text{A4})$$

In coordinate representation, we have

$$U(x_N, x_0; t_N) = \langle x_N | \hat{U}(\epsilon) \hat{U}(\epsilon) \dots \hat{U}(\epsilon) | x_0 \rangle, \quad (\text{A5})$$

$$= \prod_{n=1}^{N-1} \left[\int_{-\infty}^{\infty} dx_n \right] \langle x_N | \hat{U}(\epsilon) | x_{N-1} \rangle \langle x_{N-1} | \hat{U}(\epsilon) | x_{N-2} \rangle \dots \langle x_{n+1} | \hat{U}(\epsilon) | x_n \rangle \dots \langle x_1 | \hat{U}(\epsilon) | x_0 \rangle, \\ = \prod_{n=1}^{N-1} \left[\int_{-\infty}^{\infty} dx_n \langle x_n | \hat{U}(\epsilon) | x_{n-1} \rangle \right] = \prod_{n=1}^{N-1} \left[\int_{-\infty}^{\infty} dx_n \langle x_n | e^{-\frac{i}{\hbar} (\frac{\hat{p}^2}{2m} + V(\hat{x})) \epsilon} | x_{n-1} \rangle \right], \quad (\text{A6})$$

$$= \prod_{n=1}^{N-1} \left[\int_{-\infty}^{\infty} dx_n \langle x_n | e^{-\frac{i}{\hbar} \frac{\hat{p}^2}{2m}} | x_{n-1} \rangle e^{-\frac{i}{\hbar} V(x_{n-1}) \epsilon} \right], \quad (\text{A7})$$

$$= \prod_{n=1}^{N-1} \left[\int_{-\infty}^{\infty} dx_n dp_n \langle x_n | e^{-\frac{i}{\hbar} \frac{\hat{p}^2}{2m}} | p_n \rangle \langle p_n | x_{n-1} \rangle e^{-\frac{i}{\hbar} V(x_{n-1}) \epsilon} \right], \quad (\text{A8})$$

$$= \prod_{n=1}^{N-1} \left[\int_{-\infty}^{\infty} dx_n dp_n e^{\frac{i}{\hbar} \left[p_n(x_n - x_{n-1}) - \frac{p_n^2}{2m} - V(x_{n-1}) \right] \epsilon} \right], \quad (\text{A9})$$

$$\equiv \int \int \mathcal{D}x(t) \mathcal{D}p(t) e^{\frac{i}{\hbar} S[x(t), p(t)]}, \quad (\text{A10})$$

$$\equiv \int_{x(0)=x_i}^{x(t)=x_f} \mathcal{D}x(t) e^{\frac{i}{\hbar} S[x(t)]}, \quad (\text{A11})$$

where we took the continuum limit $\epsilon \rightarrow 0$, defined a functional integral $\int \mathcal{D}x(t) \dots \equiv \prod_{n=1}^{N-1} \left[\int_{-\infty}^{\infty} dx_n \right] \dots$, and the phase-space and coordinate actions are given by

$$S[x(t), p(t)] = \int_0^t dt \left[p\dot{x} - \frac{p^2}{2m} - V(x) \right], \quad (\text{A12})$$

$$S[x(t)] = \int_0^t dt \left[\frac{1}{2} m \dot{x}^2 - V(x) \right]. \quad (\text{A13})$$

In going from phase-space to coordinate space path-integral, (A11), we performed the Gaussian integrals over the momenta $p_n = p(t_n)$. The a graphical visualization of the path-integral is given in Fig.2.

The advantage of the path integral formulation is that it allows us to work with commuting functions rather than noncommuting operators. It also very powerful for semi-classical analysis with classical $\hbar \rightarrow 0$ limit emerges as its saddle point that extremizes the action. As discussed in great detail in Feynman and Hibbs[14] and references therein, most problems in quantum mechanics and field theory can be reproduced using this approach, often much more efficiently. However, some problems are much more amenable to treatment through

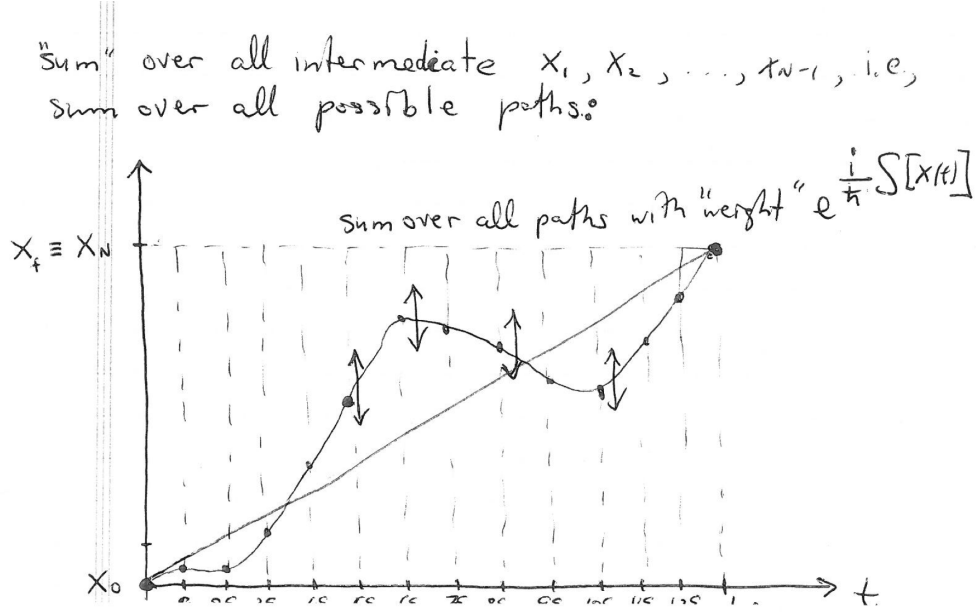


FIG. 2: A graphical illustration of a coordinate path integral for an evolution operator in one dimension.

the operator formalism (e.g., spin quantization).

For a vanishing potential, the path integral becomes Gaussian and the evolution operator is easily computed[14] by a number of methods (for example via a direct Gaussian integration of (A9), a saddle-point solution, exact in this case, or by a solution of the Schrödinger's equation), giving

$$U_0(x_f, x_i; t) = \left(\frac{m}{2\pi i \hbar t} \right)^{1/2} e^{\frac{i}{\hbar} \frac{m}{2} (x_f - x_i)^2 / t}.$$

This is why Gaussian integrals play such a crucial role in theoretical physics.

We now turn to a seemingly distinct problem of a quantum partition function for this system given by a trace of the density matrix $\hat{\rho}(\beta) = e^{-\beta \hat{H}}$

$$Z = \text{Tr} e^{-\beta \hat{H}} = \int_{-\infty}^{\infty} dx_0 \langle x_0 | e^{-\beta \hat{H}} | x_0 \rangle = \int_{x(0)=x(\beta\hbar)} \mathcal{D}x(\tau) e^{-\frac{1}{\hbar} S_E[x(\tau)]}, \quad (\text{A14})$$

where

$$S_E[x(\tau)] = \int_0^{\beta\hbar} d\tau \left[\frac{1}{2} m \dot{x}^2 + V(x) \right],$$

obtained by repeating Trotter decomposition of the previous analysis, but here applying it to imaginary time $0 \leq \tau = it < \beta\hbar$, with the maximum imaginary time given by $\tau = \beta\hbar$. The saddle-point Euler-Lagrange equation for S_E corresponds to a particle moving in an inverted

potential $-V(x)$. We note that this Euclidean action can also be obtained directly from the real action (A13) by replacement $it = \tau$ with compact imaginary time $\beta\hbar$. Immediately, we can also obtain an analog of the Schrödinger's equation in imaginary time, satisfied by the density matrix

$$\partial_\beta \hat{\rho}(\beta) = -\hat{H} \hat{\rho}(\beta).$$

We note that correlation functions computed with a path integral automatically give time-ordered ones (operators are arranged in later ones appearing to the left),

$$\text{Tr} [T(x(\tau_1) \dots x(\tau_n) \hat{\rho}(\beta))] = \int \mathcal{D}x(\tau) x(\tau_1) \dots x(\tau_n) e^{-\frac{1}{\hbar} S_E[x(\tau)]} \quad (\text{A15})$$

as it is only these time-ordered operators are arranged in the necessary order to apply the Trotter decomposition to a correlation function.

Finally, generalizing this single variable coordinate path-integral to many variables, its formulation for quantum field theory is straightforward. For example, a quantum partition function for a phonon field $\mathbf{u}(\mathbf{r})$ in a continuum of an isotropic model is given by

$$Z = \int_{\mathbf{u}(\mathbf{r},0)=\mathbf{u}(\mathbf{r},\beta\hbar)} \mathcal{D}\mathbf{u}(\mathbf{r},\tau) e^{-\frac{1}{\hbar} S_E[\mathbf{u}(\mathbf{r},\tau)]}, \quad (\text{A16})$$

where

$$S_E[\mathbf{u}(\mathbf{r},\tau)] = \int_0^{\beta\hbar} d\tau d^d r \left[\frac{1}{2} \rho (\partial_\tau \mathbf{u})^2 + \frac{1}{2} \mu (\nabla \mathbf{u})^2 \right].$$

We observe that in a path-integral formulation a d -dimensional quantum field theory looks like a path integral of an effective “classical” theory in $d+1$ dimensions with the extra imaginary time dimension confined to a slab $0 \leq \tau < \beta\hbar$.

At zero temperature $\beta\hbar \rightarrow \infty$, leading to a classical like path-integral in all $d+1$ dimensions. In contrast, at high temperature, $\beta\hbar \rightarrow 0$, the field $\mathbf{u}$ becomes τ independent (otherwise the time-derivatives cost too much action and are suppressed) and the partition function reduces to that of a d -dimensional classical one

$$Z \rightarrow Z_{cl} = \int \mathcal{D}\mathbf{u}(\mathbf{r}) e^{-\beta \int d^d r \frac{1}{2} \mu (\nabla \mathbf{u})^2}$$

over time-independent classical phonon field $\mathbf{u}(\mathbf{r})$ with a Boltzmann weight controlled by the elastic energy. This is indeed as expected, as quantum fluctuations are insignificant at

high temperature.

2. coherent states path-integral

From the derivation of the coordinate path-integral above, it is quite clear that other equivalent representations are possible, determined by the basis set of the resolution of identity in the Trotter decomposition. One particularly convenient representation is that of coherent states $|z\rangle$

$$|z\rangle = e^{-\frac{1}{2}|z|^2} e^{za^\dagger} |0\rangle = e^{-\frac{1}{2}|z|^2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle \quad (\text{A17})$$

labelled by a complex number z . From the canonical commutation relation $[a, a^\dagger] = 1$ it is clear that $e^{za^\dagger}$ is an operator (analogously to $e^{\frac{i}{\hbar}cp}$ for x) that shifts a 's eigenvalue of the vacuum state $|0\rangle$ by z , leading to coherent state's key property

$$a|z\rangle = z|z\rangle.$$

These states are overcomplete with nontrivial overlap given by

$$\langle z_1 | z_2 \rangle = e^{-\frac{1}{2}|z_1|^2} e^{-\frac{1}{2}|z_2|^2} e^{\bar{z}_1 z_2}$$

and resolution of identity

$$\hat{1} = \int \frac{d^2 z}{2\pi i} |z\rangle \langle z| \quad (\text{A18})$$

where $\frac{d^2 z}{2\pi i} \equiv \frac{d\text{Re}z d\text{Im}z}{\pi}$.

Armed with these properties, we derive a very useful coherent-state path-integral. Using the resolution of identity, (A18), we deduce Trotter decomposition of the density matrix,

$$\langle z_f | e^{-\beta \hat{H}} | z_i \rangle = \langle z_N | e^{-\frac{\epsilon}{\hbar} \hat{H}} | z_{N-1} \rangle \langle z_{N-1} | e^{-\frac{\epsilon}{\hbar} \hat{H}} | z_{N-1} \rangle \dots \langle z_j | e^{-\frac{\epsilon}{\hbar} \hat{H}} | z_{j-1} \rangle \dots \langle z_1 | e^{-\frac{\epsilon}{\hbar} \hat{H}} | z_0 \rangle. \quad (\text{A19})$$

where $\epsilon = \beta\hbar/N$. The matrix element can be evaluated for $\epsilon \ll 1$, given by

$$\langle z_j | e^{-\frac{\epsilon}{\hbar} \hat{H}} | z_{j-1} \rangle = \langle z_j | z_{j-1} \rangle \left(1 - \frac{\epsilon}{\hbar} \frac{\langle z_j | \hat{H} | z_{j-1} \rangle}{\langle z_j | z_{j-1} \rangle} \right), \quad (\text{A20})$$

$$= \langle z_j | z_{j-1} \rangle e^{-\frac{\epsilon}{\hbar} \frac{\langle z_j | \hat{H} | z_{j-1} \rangle}{\langle z_j | z_{j-1} \rangle}} = \langle z_j | z_{j-1} \rangle e^{-\frac{\epsilon}{\hbar} H(\bar{z}_j, z_{j-1})}, \quad (\text{A21})$$

$$= e^{-\frac{1}{2}[\bar{z}_j(z_j - z_{j-1}) - z_{j-1}(\bar{z}_j - \bar{z}_{j-1})]} e^{-\frac{\epsilon}{\hbar} H(\bar{z}_j, z_{j-1})}. \quad (\text{A22})$$

where in the last line we simplified expression by taking the Hamiltonian $H[a^\dagger, a]$ to be normal-ordered (all $a^\dagger$ s are to the left of a 's).

Putting this matrix element into the (A23), we find

$$\langle z_f | e^{-\beta \hat{H}} | z_i \rangle = \int \prod_{j=1}^{N-1} \frac{d^2 z_j}{2\pi i} e^{-\frac{1}{\hbar} S_E[\{\bar{z}_j, z_j\}]} = \int_{\bar{z}(\beta\hbar)=\bar{z}_f}^{z(0)=z_i} \mathcal{D}\bar{z}(\tau) \mathcal{D}z(\tau) e^{-\frac{1}{\hbar} S_E[\bar{z}(\tau), z(\tau)]}, \quad (\text{A23})$$

in the second equality we took the continuum limit $N \rightarrow \infty$, and the Euclidean action in discrete and continuous forms is respectively given by

$$S_E[\{\bar{z}_j, z_j\}] = \sum_{j=1}^{N-1} \left[\frac{1}{2} \bar{z}_j (z_j - z_{j-1}) - \frac{1}{2} z_j (\bar{z}_{j+1} - \bar{z}_j) + \frac{\epsilon}{\hbar} H(\bar{z}_j, z_{j-1}) \right] \\ + \frac{1}{2} \bar{z}_f (z_f - z_{N-1}) - \frac{1}{2} z_i (\bar{z}_1 - \bar{z}_i), \quad (\text{A24})$$

$$S_E[\bar{z}(\tau), z(\tau)] = \int_0^{\beta\hbar} d\tau \left[\frac{1}{2} (\bar{z} \partial_\tau z - z \partial_\tau \bar{z}) + \frac{\epsilon}{\hbar} H[\bar{z}(\tau), z(\tau)] \right] \\ + \frac{1}{2} \bar{z}_f (z_f - z(\beta\hbar)) - \frac{1}{2} z_i (\bar{z}(0) - \bar{z}_i), \quad (\text{A25})$$

where the last terms involving $\bar{z}_f, z_i$ are boundary terms that can be important in some situations but not in the cases that we will consider.

With this single-particle formulation in place, it is straightforward to generalize it to many variables, and then by extension to a coherent-state path-integral formulation of a quantum field theory. Applying this to bosonic matter, with identification $a^\dagger, a \rightarrow \psi^\dagger, \psi$ and $\bar{z}(\tau), z(\tau) \rightarrow \bar{\psi}(\tau, \mathbf{r}), \psi(\tau, \mathbf{r})$

$$Z = \int \mathcal{D}\bar{\psi}(\tau, \mathbf{r}) \mathcal{D}\psi(\tau, \mathbf{r}) e^{-\frac{1}{\hbar} S_E[\bar{\psi}(\tau, \mathbf{r}), \psi(\tau, \mathbf{r})]}, \quad (\text{A26})$$

where the Euclidean bosonic action is given by

$$S_E[\bar{\psi}(\tau, \mathbf{r}), \psi(\tau, \mathbf{r})] = \int_0^{\beta\hbar} d\tau d^d r \left[\frac{1}{2} \hbar (\bar{\psi} \partial_\tau \psi - \psi \partial_\tau \bar{\psi}) - \bar{\psi} \frac{\hbar^2 \nabla^2}{2m} \psi \right], \quad (\text{A27})$$

$$= \int_0^{\beta\hbar} d\tau d^d r \bar{\psi} (\hbar \partial_\tau - \frac{\hbar^2 \nabla^2}{2m}) \psi, \quad (\text{A28})$$

with periodic boundary conditions on the bosonic field $\psi(0, \mathbf{r}) = \psi(\beta\hbar, \mathbf{r})$ and its conjugate, allowing us to integrate by parts to obtain the second form above. The action can also be immediately obtained from the real-time action S , (??) by replacing $it \rightarrow \tau$. A huge advantage of this formulation is that it now allows us to calculation bosonic (time-ordered) correlation functions using simple Gaussian integrals over commuting “classical” $d + 1$ -dimensional fields, with the only price the extra imaginary time dimension, as compared to the classical d -dimensional statistical field theory.

Fourier transforming the coherent bosonic fields,

$$\psi(\tau, \mathbf{r}) = \frac{1}{\sqrt{\beta\hbar}} \sum_{\omega_n} \int \frac{d^d k}{(2\pi)^d} \psi(\omega_n, \mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_n \tau}, \quad \bar{\psi}(\tau, \mathbf{r}) = \frac{1}{\sqrt{\beta\hbar}} \sum_{\omega_n} \int \frac{d^d k}{(2\pi)^d} \bar{\psi}(\omega_n, \mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r} + i\omega_n \tau},$$

we obtain

$$S_E[\bar{\psi}(\omega_n, \mathbf{k}), \psi(\omega_n, \mathbf{k})] = \sum_{\omega_n} \int \frac{d^d k}{(2\pi)^d} \bar{\psi}(-i\hbar\omega_n + \epsilon_k) \psi, \quad (\text{A29})$$

where $\omega_n = \frac{2\pi}{\beta\hbar} n$ is the bosonic Matsubara frequency.

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