

3.5: Thermalization of Quantum Systems

Quantum Dephasing

Thermalization of quantum systems is fundamentally different from that of classical systems. Whereas time evolution in classical mechanics is in general a nonlinear dynamical system, the Schrödinger equation for time evolution in quantum mechanics is linear:

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi, \quad (3.5.1)$$

where \hat{H} is a many-body Hamiltonian. In classical mechanics, the thermal state is constructed by time evolution – this is the content of the ergodic theorem. In quantum mechanics, as we shall see, the thermal distribution must be encoded in the eigenstates themselves.

Let us assume an initial condition at $t = 0$,

$$|\Psi(0)\rangle = \sum_{\alpha} C_{\alpha} |\Psi_{\alpha}\rangle, \quad (3.5.2)$$

where $\{|\Psi_{\alpha}\rangle\}$ is an orthonormal eigenbasis for \hat{H} satisfying $\hat{H}|\Psi_{\alpha}\rangle = E_{\alpha}|\Psi_{\alpha}\rangle$. The expansion coefficients satisfy $C_{\alpha} = \langle \Psi_{\alpha} | \Psi(0) \rangle$ and $\sum_{\alpha} |C_{\alpha}|^2 = 1$. Normalization requires

$$\langle \Psi(0) | \Psi(0) \rangle = \sum_{\alpha} |C_{\alpha}|^2 = 1. \quad (3.5.3)$$

The time evolution of $|\Psi\rangle$ is then given by

$$|\Psi(t)\rangle = \sum_{\alpha} C_{\alpha} e^{-iE_{\alpha}t/\hbar} |\Psi_{\alpha}\rangle. \quad (3.5.4)$$

The energy is distributed according to the time-independent function

$$P(E) = \langle \Psi(t) | \delta(E - \hat{H}) | \Psi(t) \rangle = \sum_{\alpha} |C_{\alpha}|^2 \delta(E - E_{\alpha}). \quad (3.5.5)$$

Thus, the average energy is time-independent and is given by

$$\langle E \rangle = \langle \Psi(t) | \hat{H} | \Psi(t) \rangle = \int_{-\infty}^{\infty} dE P(E) E = \sum_{\alpha} |C_{\alpha}|^2 E_{\alpha}. \quad (3.5.6)$$

The root mean square fluctuations of the energy are given by

$$(\Delta E)_{rms} = \left\langle (E - \langle E \rangle)^2 \right\rangle^{1/2} = \sqrt{\sum_{\alpha} |C_{\alpha}|^2 E_{\alpha}^2 - \left(\sum_{\alpha} |C_{\alpha}|^2 E_{\alpha} \right)^2}. \quad (3.5.7)$$

Typically we assume that the distribution $P(E)$ is narrowly peaked about $\langle E \rangle$, such that $(\Delta E)_{rms} \ll E - E_0$, where E_0 is the ground state energy. Note that $P(E) = 0$ for $E < E_0$, the eigenspectrum of \hat{H} is bounded from below.

Now consider a general quantum observable described by an operator \mathcal{A} . We have

$$\langle \mathcal{A}(t) \rangle = \langle \Psi(t) | \mathcal{A} | \Psi(t) \rangle = \sum_{\alpha, \beta} C_{\alpha}^* C_{\beta} e^{i(E_{\alpha} - E_{\beta})t/\hbar} \mathcal{A}_{\alpha\beta}, \quad (3.5.8)$$

where $\mathcal{A}_{\alpha\beta} = \langle \Psi_{\alpha} | \mathcal{A} | \Psi_{\beta} \rangle$. In the limit of large times, we have

$$\langle \mathcal{A} \rangle_t \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \langle \mathcal{A}(t) \rangle = \sum_{\alpha} |C_{\alpha}|^2 \mathcal{A}_{\alpha\alpha}. \quad (3.5.9)$$

Note that this implies that all coherence between different eigenstates is lost in the long time limit, due to *dephasing*.

Eigenstate Thermalization Hypothesis

The essential ideas behind the *eigenstate thermalization hypothesis* (ETH) were described independently by J. Deutsch (1991) and by M. Srednicki (1994). The argument goes as follows. If the total energy is the only conserved quantity, and if \mathcal{A} is a local, translationally-invariant, few-body operator, then the time average $\langle \mathcal{A} \rangle$ is given by its microcanonical value,

$$\langle \mathcal{A} \rangle_t = \sum_{\alpha} |C_{\alpha}|^2 \mathcal{A}_{\alpha\alpha} = \frac{\sum_{\alpha} \mathcal{A}_{\alpha\alpha} \Theta(E_{\alpha} \in I)}{\sum_{\alpha} \Theta(E_{\alpha} \in I)} \equiv \langle \mathcal{A} \rangle_E, \quad (3.5.10)$$

where $I = [E, E + \Delta E]$ is an energy interval of width ΔE . So once again, time averages are micro canonical averages.

But how is it that this is the case? The hypothesis of Deutsch and of Srednicki is that thermalization in isolated and bounded quantum systems occurs *at the level of individual eigenstates*. That is, for all eigenstates $|\Psi_{\alpha}\rangle$ with $E_{\alpha} \in I$, one has

$$\mathcal{A}_{\alpha\alpha} = \langle \mathcal{A} \rangle_{E_{\alpha}}. \quad (3.5.11)$$

This means that *thermal information is encoded in each eigenstate*. This is called the *eigenstate thermalization hypothesis* (ETH).

An equivalent version of the ETH is the following scenario. Suppose we have an infinite or extremely large quantum system U (the ‘universe’) fixed in an eigenstate $|\Psi_{\alpha}\rangle$. Then form the projection operator $P_{\alpha} = |\Psi_{\alpha}\rangle\langle\Psi_{\alpha}|$. Projection operators satisfy $P^2 = P$ and their eigenspectrum consists of one eigenvalue 1 and the rest of the eigenvalues are zero¹¹. Now consider a partition of $U = W \cup S$, where $W \gg S$. We imagine S to be the ‘system’ and W the ‘world’. We can always decompose the state $|\Psi_{\alpha}\rangle$ in a complete product basis for W and S , viz.

$$|\Psi_{\alpha}\rangle = \sum_{p=1}^{N_W} \sum_{j=1}^{N_S} \mathcal{Q}_{pj}^{\alpha} |\psi_p^W\rangle \otimes |\psi_j^S\rangle. \quad (3.5.12)$$

Here $N_{W/S}$ is the size of the basis for W/S . The *reduced density matrix* for S is defined as

$$\rho_S = \text{Tr}_W P_{\alpha} = \sum_{j,j'=1}^{N_S} \left(\sum_{p=1}^{N_W} \mathcal{Q}_{pj}^{\alpha} \mathcal{Q}_{pj'}^{\alpha*} \right) |\psi_j^S\rangle\langle\psi_{j'}^S|. \quad (3.5.13)$$

The claim is that ρ_S approximates a *thermal density matrix* on S ,

$$\rho_S \approx \frac{1}{Z_S} e^{-\beta \hat{H}_S}, \quad (3.5.14)$$

where \hat{H}_S is some Hamiltonian on S , and $Z_S = \text{Tr} e^{-\beta \hat{H}_S}$, so that $\text{Tr} \rho_S = 1$ and ρ_S is properly normalized. A number of issues remain to be clarified:

- What do we mean by “approximates”?
- What do we mean by \hat{H}_S ?
- What do we mean by the temperature T ?

We address these in reverse order. The temperature T of an eigenstate $|\Psi_{\alpha}\rangle$ of a Hamiltonian \hat{H} is defined by setting its energy density E_{α}/V_U to the thermal energy density,

$$\frac{E_{\alpha}}{V} = \frac{1}{V} \frac{\text{Tr} \hat{H} e^{-\beta \hat{H}}}{\text{Tr} e^{-\beta \hat{H}}}. \quad (3.5.15)$$

Here, $\hat{H} = \hat{H}_U$ is the full Hamiltonian of the universe $U = W \cup S$. Our intuition is that \hat{H}_S should reflect a restriction of the original Hamiltonian \hat{H}_U to the system S . What should be done, though, about the interface parts of \hat{H}_U which link S and W ? For lattice Hamiltonians, we can simply but somewhat arbitrarily cut all the bonds coupling S and W . But we could easily imagine some other prescription, such as halving the coupling strength along all such interface bonds. Indeed, the definition of H_S is somewhat arbitrary. However, so long as we use ρ_S to compute averages of *local operators* which lie sufficiently far from the boundary of S , the precise details of how we truncate \hat{H}_U to \hat{H}_S are unimportant. This brings us to the first issue: the approximation of ρ_S by its Gibbs form in Equation 3.5.14 is only valid when we consider averages of local operators lying within the bulk of S . This means that we must only examine operators whose support is confined to regions greater than some distance ξ_T

from ∂S , where ξ_T is a *thermal correlation length*. This, in turn, requires that $L_S \gg \xi_T$, the region S is very large on the scale of ξ_T . How do we define ξ_T ? For a model such as the Ising model, it can be taken to be the usual correlation length obtained from the spin-spin correlation function $\langle \sigma_{\mathbf{r}} \sigma_{\mathbf{r}'} \rangle_T$. More generally, we may choose the largest correlation length from among the correlators of all the independent local operators in our system. Again, the requirement is that $\exp(-d_{\partial}(\mathbf{r})/\xi_T) \ll 1$, where $d_{\partial}(\mathbf{r})$ is the shortest distance from the location of our local operator $\mathcal{O}_{\mathbf{r}}$ to the boundary of S . At criticality, the exponential is replaced by a power law $(d_{\partial}(\mathbf{r})/\xi_T)^{-p}$, where p is a critical exponent. Another implicit assumption here is that $V_S \ll V_W$.

When is the ETH true?

There is no rigorous proof of the ETH. Deutsch showed that the ETH holds for the case of an integrable Hamiltonian weakly perturbed by a single Gaussian random matrix. Horoi (1995) showed that nuclear shell model wavefunctions reproduce thermodynamic predictions. Recent numerical work by M. Rigol and collaborators has verified the applicability of the ETH in small interacting boson systems. ETH fails for so-called integrable models, where there are a large number of conserved quantities, which commute with the Hamiltonian. Integrable models are, however, quite special, and as Deutsch showed, integrability is spoiled by weak perturbations, in which case ETH then applies.

ETH also fails in the case of noninteracting disordered systems which exhibit *Anderson localization*. Single particle energy eigenstates ψ_j whose energies ε_j the localized portion of the eigenspectrum decay exponentially, as $|\psi_j(\mathbf{r})|^2 \sim \exp(-|\mathbf{r} - \mathbf{r}_j|/\xi(\varepsilon_j))$, where \mathbf{r}_j is some position in space associated with ψ_j and $\xi(\varepsilon_j)$ is the *localization length*. Within the localized portion of the spectrum, $\xi(\varepsilon)$ is finite. As ε approaches a *mobility edge*, $\xi(\varepsilon)$ diverges as a power law¹². Exponentially localized states are unable to thermalize with other distantly removed localized states. Of course, all noninteracting systems will violate ETH, because they are integrable. The interacting version of this phenomenon, *many-body localization* (MBL), is a topic of intense current interest in condensed matter and statistical physics. MBL systems also exhibit a large number of conserved quantities, but in contrast to the case of integrable systems, where each conserved quantity is in general expressed in terms of an integral of a local density, in MBL systems the conserved quantities are themselves local, although *emergent*. The emergent nature of locally conserved quantities in MBL systems means that they are not simply expressed in terms of the original local operators of the system, but rather are arrived at via a sequence of local unitary transformations.

Note again that in contrast to the classical case, time evolution of a quantum state does not create the thermal state. Rather, it *reveals* the thermal distribution which is encoded in all eigenstates after sufficient time for dephasing to occur, so that correlations between all the wavefunction expansion coefficients $\{C_{\alpha}\}$ for $\alpha \neq \alpha'$ are all lost.

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