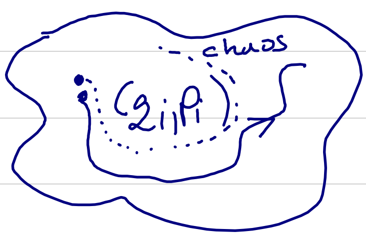
LECTURE 2: Density operator formalism for proper and improper mixed quantum states

1°

Classical Theory:

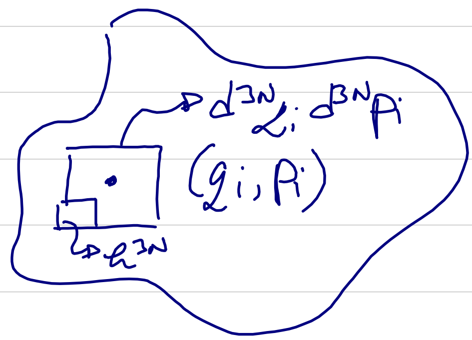
CM → $\vec{F} = m\vec{a}$ for MD

CSM →



$H(q_i, p_i)$

$A(q_i, p_i)$



ANALYTICAL MECHANICS

$$dq_i/dt = \partial H/\partial p_i$$
$$dp_i/dt = -\partial H/\partial q_i$$

or

$$dq_i/dt = \{q_i, H\}$$
$$dp_i/dt = \{p_i, H\}$$

$$\int \rho(q_i, p_i)\, \frac{d^{3N}q_i\, d^{3N}p_i}{h^{3N} N!} = 1$$

→ phase space probability density

$$\langle A \rangle = \int A(q_i, p_i)\, \rho(q_i, p_i)\, \frac{d^{3N}q_i\, d^{3N}p_i}{h^{3N} N!}$$

$$S = -k_B \int \rho(q_i, p_i) \ln \rho(q_i, p_i) \frac{d^{3N}q_i\, d^{3N}p_i}{h^{3N} N!}$$

→ state of the system is specified by values of physical quantities which are directly measurable

$x \cdot p_x - p_x \cdot x = 0$

→ c-numbers, so they commute

Quantum Theory:

QM at $T=0$

QSM for $T \neq 0$, $V_b \neq 0$, $\vec{E}(\omega) \neq 0$

→ equilibrium

→ nonequilibrium

$|\psi\rangle$, $\hat{A}$ ↳ physical quantities represented by operators

↓
PURE STATES → assign ket vector

$|\psi\rangle \in \mathcal{H}$, $\hat{A} : \mathcal{H} \mapsto \mathcal{H}$

$\hat{A}^{+} = \hat{A}$

→ Hilbert space: $\alpha|\psi_1\rangle + \beta|\psi_2\rangle \in \mathcal{H}$

$\lim_{n \to \infty} |\psi_n\rangle \in \mathcal{H}$

operators in general DO NOT commute:

$[\hat{x}, \hat{p}_x] = \hat{x} \cdot \hat{p}_x - \hat{p}_x \cdot \hat{x} = i\hbar$

MIXED STATES

$w_1, |\psi_1\rangle$

$w_2, |\psi_2\rangle$ ... $w_i, |\psi_i\rangle$

instead of $|\psi\rangle$

PROPERLY

$$\hat{\rho} = \sum_i w_i |\psi_i\rangle\langle\psi_i|$$

$$\sum_i w_i = 1 \Rightarrow \mathrm{Tr}\,\hat{\rho} = 1$$

statistical or state or density operator

$$\underbrace{\text{SPECTRAL DECOMPOSITION}}$$

$$\hat{A} = \sum_n a_n \underbrace{|a_n\rangle\langle a_n|}_{\hat{P}_n}$$

$\hat{P}_n = \hat{P}_n^{+}$, $\hat{P}_n \hat{P}_m = \hat{P}_n \delta_{nm}$, $\sum_n \hat{P}_n = \hat{I}$

↳ projection operator

functions of $\hat{A}$

$$\boxed{f(\hat{A}) = \sum_n f(a_n) |a_n\rangle\langle a_n|}$$

$\hat{A}_n |a_n\rangle = a_n |a_n\rangle$

↳ eigenvalues are numbers that can be measured

$\hat{P}_n = |a_n\rangle\langle a_n|$ gives probability of measurement

Measurements in Quantum Theory

contrary to classical physics, variables in quantum theory might not have definite values at a given time

QM

$$\text{prob}(a_n) = \langle\psi|\hat{P}_n|\psi\rangle = \langle\psi|a_n\rangle\langle a_n|\psi\rangle = |\langle\psi|a_n\rangle|^2$$

QSM

$$\text{prob}(a_n) = \text{Tr}(\hat{\rho}\cdot\hat{P}_n) = \sum_m \langle a_m|(\hat{\rho}|a_n\rangle\underbrace{\langle a_n|)|a_m\rangle}_{\delta_{nm}} = \langle a_n|\hat{\rho}|a_n\rangle$$

if a_n is degenerate, then change to $\hat{P}_n = \sum_j |a_n^j\rangle\langle a_n^j|$

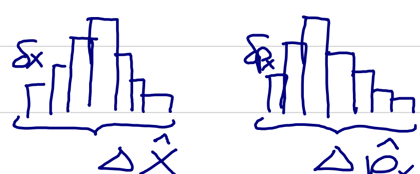
if $\hat{A}$ has continuous spectrum:

$$\hat{A} = \sum_n a_n |a_n\rangle\langle a_n| + \int a\,|a\rangle\langle a|\,da$$

$$\text{prob}([b, b']) = \langle\psi|\int_b^{b'} da\,|a\rangle\langle a|\psi\rangle$$

⇝ connection to experiment: $\Delta\hat{A} = \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2}$

$$\langle\hat{A}\rangle_{QM} = \langle\psi|\hat{A}|\psi\rangle = \sum_n a_n \langle\psi|a_n\rangle\langle a_n|\psi\rangle = \sum_n a_n |\langle\psi|a_n\rangle|^2 \rightsquigarrow \text{prob}(a_n)$$



$$\Delta\hat{x}\cdot\Delta\hat{p}_x \geq \frac{\hbar}{2}$$

MEASUREMENTS: strong (projective) as well as weak and protective

$$|\psi\rangle \mapsto \frac{\hat{P}_n|\psi\rangle}{|\hat{P}_n|\psi\rangle|} \qquad \hat{\rho} \mapsto \frac{\hat{P}_n\hat{\rho}\hat{P}_n}{\text{Tr}(\hat{\rho}\hat{P}_n)}$$

⇝ one role of strong measurement is to obtain information on the values of physical observables; the other role is to generate nonunitary evolution and thereby prepare states

$\mathrm{Tr}(\ldots) = \sum_n \langle b_n | \ldots | b_n \rangle$ where $|b_n\rangle$ is basis in $\mathcal{H}$

choose

$$\langle \hat{A} \rangle_{QSM} = \mathrm{Tr}(\hat{\rho}\cdot\hat{A}) = \sum_{\ell} \langle a_\ell | \sum_i w_i |\psi_i\rangle\langle\psi_i| \sum_n a_n |a_n\rangle \underbrace{\langle a_n | a_\ell\rangle}_{\delta_{n\ell}}$$

$$= \sum_i w_i \sum_n a_n \underbrace{|\langle\psi_i|a_n\rangle|^2}$$

↳ quantum probability

$$= \sum_i w_i \langle\psi_i|\hat{A}|\psi_i\rangle$$

↳ classical probability due to lack of knowledge like in CSM

FUNDAMENTAL PROPERTIES:

i) $\mathrm{Tr}(\hat{\rho}) = \sum_i w_i = 1$ — unit trace

ii) $\hat{\rho} = \hat{\rho}^\dagger$ — Hermitian

iii) $\langle\phi|\hat{\rho}|\phi\rangle \geq 0$ — positive definite

⇒ QM is special case of QSM:

$$\underbrace{\hat{\rho} = |\psi\rangle\langle\psi|}_{\text{density operator of pure state}} \Rightarrow \langle\hat{A}\rangle = \mathrm{Tr}(\hat{\rho}\cdot\hat{A}) =$$

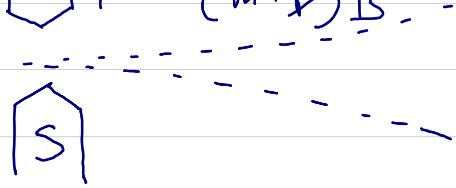
$$= \sum_{\ell} \langle a_\ell|\psi\rangle\langle\psi| a_n \sum_n a_n |a_n\rangle\langle a_n|a_\ell\rangle$$

$$= \sum_n a_n \langle a_n|\psi\rangle\langle\psi|a_n\rangle$$

$$= \langle\psi|\hat{A}|\psi\rangle$$

2° Examples of density operators:

(a) Stern-Gerlach $\boxed{N}$ $\vec{F} = (\vec{m}\cdot\nabla)\vec{B}$



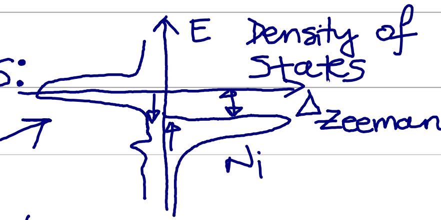
↑ ↑
↓ ↓ Ag
spin-unpolarized beam injected

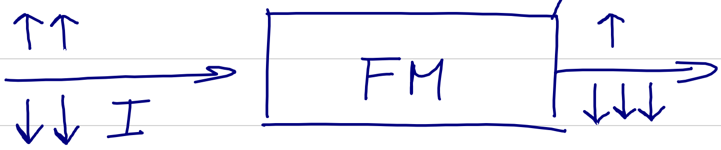
↑ ↑ ↑ $\hat{\rho} = |\uparrow\rangle\langle\uparrow|$

$\hat{\rho}^2 = \hat{\rho}$, $\mathrm{Tr}\hat{\rho}^2 = 1$

purity ← often used in quantum computing

(b) Spin-polarized current generation in spintronics:





$$\hat{\rho}_{out} = \underbrace{\tfrac{1}{4}}_{w_1}|\uparrow\rangle\langle\uparrow| + \underbrace{\tfrac{3}{4}}_{w_2}|\downarrow\rangle\langle\downarrow|$$

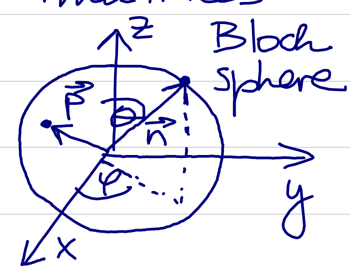
$$\hat{\rho}_{in} = \tfrac{1}{2}|\uparrow\rangle\langle\uparrow| + \tfrac{1}{2}|\downarrow\rangle\langle\downarrow|$$

(c) Density operator for arbitrary state of spin-$\frac{1}{2}$ or qubit:

unit vectors along x, y, z axis

$\hat{\vec{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) = \hat{\sigma}_x \vec{e}_x + \hat{\sigma}_y \vec{e}_y + \hat{\sigma}_z \vec{e}_z$ is the vector operator of Pauli matrices

$\hat{\sigma}_z |\uparrow\rangle = +1\,|\uparrow\rangle, \qquad \hat{\sigma}_z|\downarrow\rangle = -1\,|\downarrow\rangle$



arbitrary pure state

$$\boxed{|S\rangle = \cos\theta/2\,|\uparrow\rangle + \sin\theta/2\; e^{i\varphi}|\downarrow\rangle}$$

$$\hat{\vec{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) \Rightarrow \vec{\sigma}\cdot\vec{n}\,(\pm|S\rangle) = \pm|S\rangle$$

$\vec{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$

more general mixed state — Bloch or polarization vector

$$\hat{\rho} = \begin{pmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix} = \frac{1}{2}\left(\hat{I} + \hat{\vec{P}}\cdot\hat{\vec{\sigma}}\right) \xrightarrow{\text{eigenvalues}} \begin{cases} \frac{1}{2}(1+|\vec{P}|) \\ \frac{1}{2}(1-|\vec{P}|) \end{cases}$$

$\rho_{\uparrow\uparrow} = \langle\uparrow|\hat{\rho}|\uparrow\rangle$ stems from

purity: $\mathrm{Tr}\,\hat{\rho}^2 = \frac{1}{2}(1+|\vec{P}|^2)$

$\mathrm{Tr}\,\hat{\rho}^2 = 1 \Leftrightarrow |\vec{P}| = 1 \Leftrightarrow \hat{\rho} = |S\rangle\langle S|$

$\frac{1}{2}\mathrm{Tr}(\sigma_\alpha \sigma_\beta) = \delta_{\alpha\beta} \Rightarrow \frac{1}{\sqrt{2}}\hat{I}, \frac{1}{\sqrt{2}}\hat{\sigma}_x, \frac{1}{\sqrt{2}}\hat{\sigma}_y, \frac{1}{\sqrt{2}}\hat{\sigma}_z$ is orthonormal basis

$(\hat{A}, \hat{B}) = \mathrm{Tr}(\hat{A}^\dagger \hat{B})$ in the space of 2×2 matrices

↳ inner product of two "vectors" in the vector space of matrices

$\mathrm{Tr}\,\frac{1}{2}(I + \vec{P}\cdot\hat{\vec{\sigma}}) = 1$ because $\mathrm{Tr}(\hat{\sigma}_x) = \mathrm{Tr}(\hat{\sigma}_y) = \mathrm{Tr}(\hat{\sigma}_z)$

$\Rightarrow$ to find the physical meaning of $\vec{P}$ (i.e., its connection to measurable quantities) we compute expectation value of spin operator $\hat{\vec{S}}$ in mixed quantum state $\hat{\rho}$

$$\hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}} \Rightarrow \langle \hat{\vec{S}} \rangle_{QSM} = \mathrm{Tr}\,(\hat{\rho}\,\hat{\vec{S}})$$ instead of $$\langle \hat{\vec{S}} \rangle_{QM} = \langle s | \hat{\vec{S}} | s \rangle$$

I) Compute using abstract operators:

$$\underbrace{\mathrm{Tr}\,(\hat{\rho}\cdot\hat{\sigma}_x)} = \mathrm{Tr}\left[\frac{1}{2}(\hat{I} + \vec{P}\cdot\hat{\vec{\sigma}})\cdot\hat{\sigma}_x\right] = \overbrace{\mathrm{Tr}\,(\tfrac{1}{2}\hat{I}\hat{\sigma}_x)}^{0}$$

$$+ \mathrm{Tr}\,(\tfrac{1}{2}P_x\hat{\sigma}_x\hat{\sigma}_x) + \mathrm{Tr}\,(\tfrac{1}{2}P_y\hat{\sigma}_y\cdot\hat{\sigma}_x) + \mathrm{Tr}\,(\tfrac{1}{2}P_z\hat{\sigma}_z\hat{\sigma}_x)$$

$$= \frac{1}{2}P_x\cdot 2 + 0 + 0 = P_x$$

$$\mathrm{Tr}\,(\hat{\rho}\cdot\hat{\vec{\sigma}}) = \vec{P} \Rightarrow \boxed{\langle \hat{\vec{S}} \rangle = \mathrm{Tr}\,(\hat{\rho}\cdot\frac{\hbar}{2}\hat{\vec{\sigma}}) = \frac{\hbar}{2}\vec{P}}$$

II) Compute using matrix representation of operators:

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

$$|\uparrow\rangle \mapsto \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle \mapsto \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \hat{I} \mapsto \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\mathrm{Tr}\,(\hat{\rho}\hat{\vec{\sigma}}) = \mathrm{Tr}\Bigg[\frac{1}{2}\begin{pmatrix} 1+P_z & P_x - iP_y \\ P_x + iP_y & 1-P_z \end{pmatrix}\cdot\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\vec{e}_x$$

$$+ \frac{1}{2}\begin{pmatrix} 1+P_z & P_x - iP_y \\ P_x + iP_y & 1-P_z \end{pmatrix}\cdot\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\vec{e}_y$$

$$+ \frac{1}{2}\begin{pmatrix} 1+P_z & P_x - iP_y \\ P_x + iP_y & 1-P_z \end{pmatrix}\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\vec{e}_z\Bigg] = P_x\vec{e}_x + P_y\vec{e}_y + P_z\vec{e}_z = \vec{P}$$

(d) Interpretation of density matrix elements:

outer product of two vectors

$\hat{P}_\uparrow = |\uparrow\rangle\langle\uparrow|$ is projector on $|\uparrow\rangle \Rightarrow \hat{P}_\uparrow \mapsto \begin{pmatrix}1\\0\end{pmatrix}(1\ 0) = \begin{pmatrix}1&0\\0&0\end{pmatrix}$

QM: $\text{prob}(\uparrow \parallel \vec{e}_z) = \langle s|\hat{P}_\uparrow|s\rangle = |\langle\uparrow|s\rangle|^2$

QSM:

$$\text{prob}(\uparrow \parallel \vec{e}_z) = \text{Tr}(\hat{\rho}\cdot\hat{P}_\uparrow) = \left[\begin{pmatrix}\rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow}\\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow}\end{pmatrix}\cdot\begin{pmatrix}1&0\\0&0\end{pmatrix}\right] = \rho_{\uparrow\uparrow} = \langle\uparrow|\hat{\rho}|\uparrow\rangle$$

$$|\otimes\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + i|\downarrow\rangle) \Rightarrow \hat{\rho} = |\otimes\rangle\langle\otimes|$$ spin-↑ state along y-axis

$$\hat{\rho} = \frac{1}{2}\begin{pmatrix}1\\i\end{pmatrix}\cdot(1\ \ -i) = \frac{1}{2}\begin{pmatrix}1 & -i\\ i & 1\end{pmatrix} \xrightarrow[\text{decoherence}]{e^{-t/T_2}} \hat{\rho}_{\text{incoherent}} = \frac{1}{2}\begin{pmatrix}1&0\\0&1\end{pmatrix}$$

$$\boxed{S = -k_B\,\text{Tr}(\hat{\rho}\ln\hat{\rho})}$$ → 0 for PURE (or fully coherent) state

→ $k_B \ln 2$ for INCOHERENT mixed state

↳ Von Neumann entropy

$T_2 \sim$ ms for superconducting qubit

$T_2 \sim 10^{-13}\,\text{s} - 10^{-20}\,\text{s}$ for human brain

$\begin{pmatrix}\alpha\\\beta\end{pmatrix}(\alpha^*\ \beta^*)$ ← in matrix representation

$$|s\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle \Rightarrow \hat{\rho} = |s\rangle\langle s| = \begin{pmatrix}|\alpha|^2 & \alpha\beta^*\\ \beta\alpha^* & |\beta|^2\end{pmatrix} \xrightarrow{\text{decoherence}} \hat{\rho}_{inc} = \begin{pmatrix}|\alpha|^2 & 0\\ 0 & |\beta|^2\end{pmatrix}$$

$\propto e^{-t/T_2}$

$$\hat{\rho}_{inc} = |\alpha|^2|\uparrow\rangle\langle\uparrow| + |\beta|^2|\downarrow\rangle\langle\downarrow|$$

vs.

$$\hat{\rho}_{pure} = |\alpha|^2|\uparrow\rangle\langle\uparrow| + \alpha\beta^*|\uparrow\rangle\langle\downarrow| + \alpha^*\beta|\downarrow\rangle\langle\uparrow| + |\beta|^2|\downarrow\rangle\langle\downarrow|$$

off-diagonal elements ← give coherence between pure state

for spin-$\frac{1}{2}$ or qubit $\begin{cases} |\vec{P}| = 1 & \text{is fully coherent}\\ 0 < |\vec{P}| < 1 & \text{is partially coherent}\\ |\vec{P}| = 0 & \text{is incoherent}\end{cases}$

T2 IN SPINTRONICS

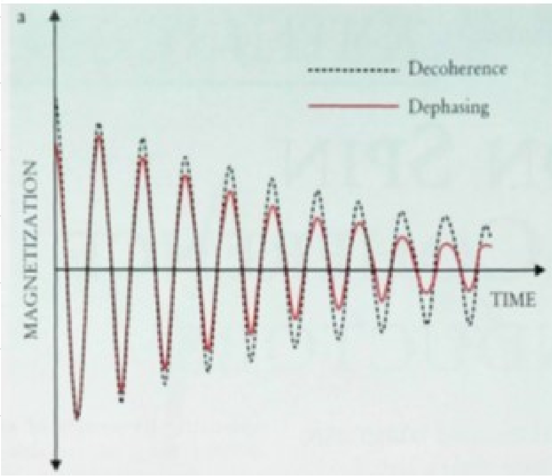
physics today

Electron Spin and Optical Coherence in Semiconductors

David D. Awschalom and James M. Kikkawa

Citation: Phys. Today 52(6), 33 (1999); doi: 10.1063/1.882695

$$M(t) = M(0)\, e^{-t/T_2} \cos(\Delta E t/\hbar)$$



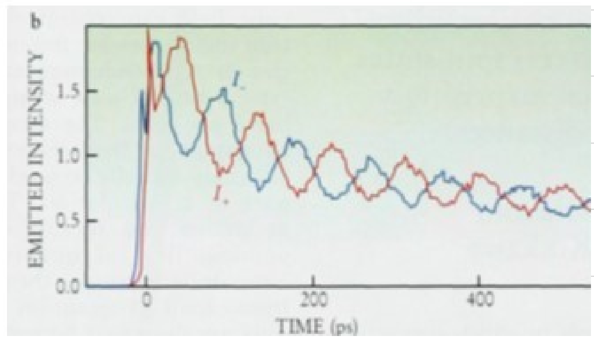


FIGURE 1. PHOTOLUMINESCENCE SPECTROSCOPY in semiconductors reveals the Larmor precession of electrons in an external magnetic field. **(a)** Circularly polarized laser pulses can excite a spin-polarized ensemble of electrons in semiconductors. The resulting net magnetization precesses in a transverse magnetic field. The loss of spin coherence is illustrated by the decay of the magnetization (dotted line). Magnetic field inhomogeneities and other factors can cause additional loss of magnetization, called dephasing, which leads to the experimentally measured evolution (solid line). **(b)** Excited, polarized electrons can give off circularly polarized light when they recombine with holes. The emitted intensities of the positive (I_+) and negative (I_-) circularly polarized light are modulated as the electrons precess. (Adapted from ref. 4.)

T2 IN QUANTUM COMPUTING

Superconducting Qubits: Current State of Play

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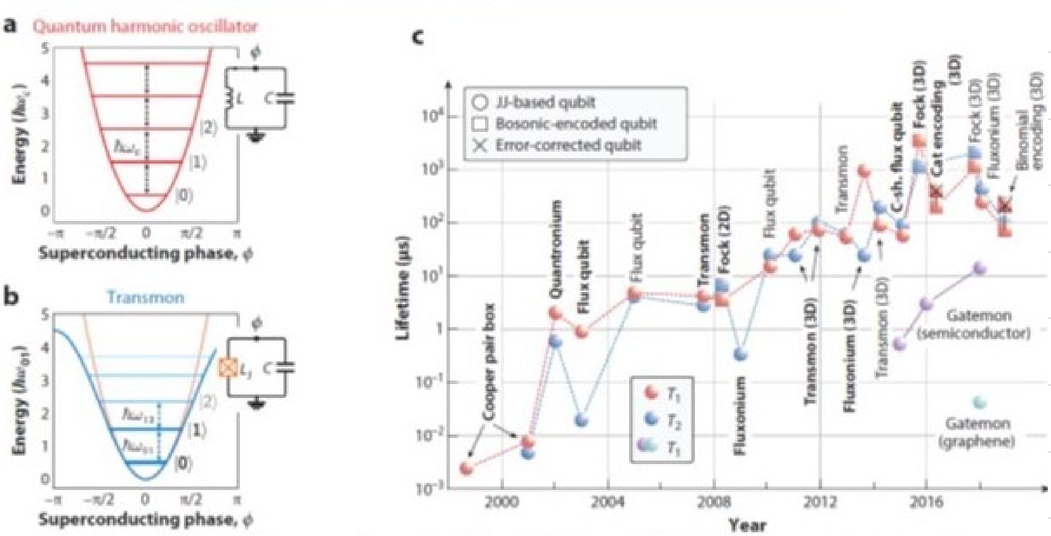
Keywords

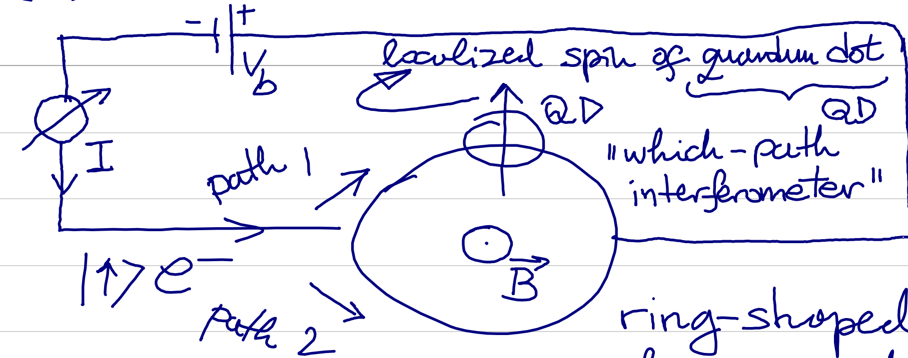


The quantum harmonic oscillator (QHO) shown in **Figure 2a** is a resonant circuit comprising a capacitor and an inductor with resonance frequency $\omega_c = 1/\sqrt{LC}$. For sufficiently low temperature ($k_B T \ll \hbar\omega_c$) and dissipation (level broadening much less than $\hbar\omega_c$), the resulting harmonic potential supports quantized energy levels spaced by $\hbar\omega_c$. However, due to the equidistant level spacing, the QHO by itself cannot be operated as a qubit.

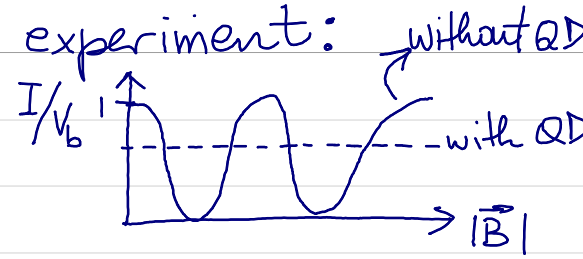
To remedy this situation, the circuit potential is made anharmonic by introducing a nonlinear inductor—the Josephson junction. The imparted anharmonicity leads to a nonequidistant spacing of the energy levels, enabling one to uniquely address each transition (see **Figure 2b**). Typically, the two lowest levels are used to define a qubit, with $|0\rangle$ corresponding to the ground state and $|1\rangle$ corresponding to the excited state. Large anharmonicity is generally favorable to suppress unwanted excitations to higher levels.

Josephson junction: two superconducting electrodes that are separated by a thin insulating barrier, allowing for the coherent tunneling of Cooper pairs

(e) IMPROPER mixtures and true DECOHERENCE



experiment:



ring-shaped nanostructure of size ≪ dephasing length (~1nm at T=1K)

$|\Psi\rangle \in \mathcal{H}_e^o \otimes \mathcal{H}_e^s \otimes \mathcal{H}_{QD}$ Hilbert space of composite quantum system

$|1\rangle \otimes |e_1\rangle$ is pure & SEPARABLE

$|1\rangle \otimes |e_1\rangle + |2\rangle \otimes |e_2\rangle$ is pure & ENTANGLED

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\Big[\overbrace{|1\rangle_e}^{|1\rangle} \otimes \overbrace{|\downarrow\rangle_e \otimes |\downarrow\rangle_{QD}}^{|e_1\rangle} + \overbrace{|2\rangle_e}^{|2\rangle} \otimes \overbrace{|\uparrow\rangle_e \otimes |\uparrow\rangle_{QD}}^{|e_2\rangle}\Big]$$

$$\langle e_1|e_2\rangle = 0, \quad \langle e_1|e_1\rangle = 1, \quad \langle e_2|e_2\rangle = 1$$

$$\hat{\rho}_{tot} = |\Psi\rangle\langle\Psi| = \frac{1}{2}\Big[\big(|1\rangle\otimes|e_1\rangle + |2\rangle\otimes|e_2\rangle\big)\big(\langle 1|\otimes\langle e_1| + \langle 2|\otimes\langle e_2|\big)\Big]$$

$$= \frac{1}{2}\Big(|1\rangle\langle 1|\otimes|e_1\rangle\langle e_1| + |1\rangle\langle 2|\otimes|e_1\rangle\langle e_2| + |2\rangle\langle 1|\otimes|e_2\rangle\langle e_1| + |2\rangle\langle 2|\otimes|e_2\rangle\langle e_2|\Big)$$

$$\hat{\rho}_{electron} = \mathrm{Tr}_{QD}|\Psi\rangle\langle\Psi| = \langle e_1|\hat{\rho}_{tot}|e_1\rangle + \langle e_2|\hat{\rho}_{tot}|e_2\rangle$$

↳ partial trace over QD states

reduced density operator of subsystem

$$= \frac{1}{2}\Big(|1\rangle\langle 1|\otimes\underbrace{\langle e_1|e_1\rangle\langle e_1|e_1\rangle}_{1} + |1\rangle\langle 2|\otimes\langle e_1|e_1\rangle\cancel{\langle e_2|e_1\rangle}^{0}$$
$$+ |2\rangle\langle 1|\otimes\cancel{\langle e_1|e_2\rangle}^{0}\langle e_1|e_1\rangle + |2\rangle\langle 2|\otimes\cancel{\langle e_1|e_2\rangle}^{0}\langle e_2|e_1\rangle$$
$$+ |1\rangle\langle 1|\otimes\cancel{\langle e_2|e_1\rangle}^{0}\langle e_1|e_2\rangle + |1\rangle\langle 2|\otimes\cancel{\langle e_2|e_1\rangle}^{0}\langle e_2|e_1\rangle$$
$$+ |1\rangle\langle 2|\otimes\cancel{\langle e_2|e_1\rangle}^{0}\langle e_2|e_2\rangle + |2\rangle\langle 2|\otimes\underbrace{\langle e_2|e_2\rangle\langle e_2|e_2\rangle}_{1}\Big)$$

$$\hat{\rho}_{\text{electron}} = \frac{1}{2}\left(|1\rangle\langle 1| + |2\rangle\langle 2|\right)$$

$$= \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \text{ in matrix representation } \quad |1\rangle \mapsto \begin{pmatrix}1\\0\end{pmatrix}, \quad |2\rangle \mapsto \begin{pmatrix}0\\1\end{pmatrix}$$

$\Rightarrow$ without QD acting as which path nonhuman observer:

$$|\phi\rangle_e = \frac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right) \Leftrightarrow \hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2}\begin{pmatrix}1\\1\end{pmatrix}\begin{pmatrix}1 & 1\end{pmatrix} =$$

($|\phi\rangle_e \in \mathcal{H}_e$)

so, entanglement with environment leads to DECAY of off-diagonal elements $= \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}$

SUMMARY of TERMINOLOGY:

Quantum States

PURE (state vector): $|\psi\rangle$ or $\underbrace{\hat{\rho} = |\psi\rangle\langle\psi| = \hat{\rho}^2}_{\text{pure state density operator}}$

- single: $|\phi\rangle_1 \in \mathcal{H}_1$
- composite: $\underbrace{|\phi\rangle_1 \otimes |\chi\rangle_2}_{\text{separable or unentangled}} \in \mathcal{H}_1 \otimes \mathcal{H}_2$

$$\underbrace{|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\phi\rangle_1 \otimes |\chi\rangle_2 + |\chi\rangle_1 \otimes |\phi\rangle_2\right)}_{\text{pure entangled}} \in \mathcal{H}_1 \otimes \mathcal{H}_2$$

$$\hat{\rho}_1 = \mathrm{Tr}_2 |\psi\rangle\langle\psi| \quad \Rightarrow \quad \mathrm{Tr}\,\hat{\rho}_1^2 < 1, \quad S > 0$$

$\hat{\rho}_1$: reduced density operator describes quantum state of subsystem!

MIXED: $\hat{\rho} = \sum_i w_i |\psi_i\rangle\langle\psi_i| \neq \hat{\rho}^2$

- single: $\hat{\rho}_1 : \mathcal{H}_1 \mapsto \mathcal{H}_1$
- composite: $\hat{\rho} : \mathcal{H}_1 \otimes \mathcal{H}_2 \mapsto \mathcal{H}_1 \otimes \mathcal{H}_2$

$$\underbrace{\hat{\rho} = \hat{\rho}_1' \otimes \hat{\rho}_2'}_{\text{mixed unentangled}} \Rightarrow \hat{\rho}_1 = \mathrm{Tr}_2 \hat{\rho} = \hat{\rho}_1'$$

$$\underbrace{\hat{\rho} \neq \sum_i w_i \hat{\rho}_1^{(i)} \otimes \hat{\rho}_2^{(i)}}_{\text{mixed entangled}}$$

(f) Mixtures of states expressing density operator are never uniquely defined

I) $\hat{\rho}_z = \frac{1}{2}\left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| \right)$

$|\rightarrow\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle \right)$ is spin-↑ state along x-axis

$$\hat{\rho}_x = \frac{1}{2}\left(|\rightarrow\rangle\langle\rightarrow| + |\leftarrow\rangle\langle\leftarrow| \right) =$$

$$= \frac{1}{2}\cdot\frac{1}{2}\left[\left(|\uparrow\rangle + |\downarrow\rangle \right)\left(\langle\uparrow| + \langle\downarrow| \right) + \left(|\uparrow\rangle - |\downarrow\rangle \right)\left(\langle\uparrow| - \langle\downarrow| \right) \right]$$

$$= \frac{1}{4}\Big(|\uparrow\rangle\langle\uparrow| + \cancel{|\uparrow\rangle\langle\downarrow|} + \cancel{|\downarrow\rangle\langle\uparrow|} + |\downarrow\rangle\langle\downarrow|$$

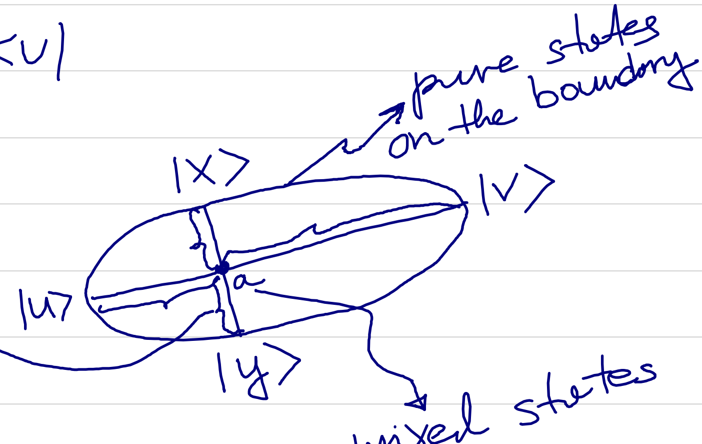
$$+ |\uparrow\rangle\langle\uparrow| - \cancel{|\uparrow\rangle\langle\downarrow|} - \cancel{|\downarrow\rangle\langle\uparrow|} - |\downarrow\rangle\langle\downarrow| \Big)$$

$$= \frac{1}{2}\left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| \right) \Rightarrow \hat{\rho}_x \equiv \hat{\rho}_z \equiv \hat{\rho}_y \equiv \frac{1}{2}\hat{I} \text{ as } \vec{P} = 0$$

II $\hat{\rho}_a = a|u\rangle\langle u| + (1-a)|v\rangle\langle v|$

$|x\rangle = \sqrt{a}\,|u\rangle + \sqrt{1-a}\,|v\rangle$

$|y\rangle = \sqrt{a}\,|u\rangle - \sqrt{1-a}\,|v\rangle$



$\hat{\rho}_a = \frac{1}{2}|x\rangle\langle x| + \frac{1}{2}|y\rangle\langle y|$

weights are inversely proportional to distance

$\Rightarrow$ mixed states can be written as a CONVEX combination $\rightarrow \hat{\rho} = \sum_i a_i \hat{\rho}^{(i)}$, $0 \leq a_i \leq 1$, $\sum_i a_i = 1 \leftarrow$ of density operators of pure states, but there are ∞ many combinations

(g) REDUCED density operators of (un)correlated states

→ bipartite system requires $\mathcal{H}_1 \otimes \mathcal{H}_2$ spanned by $\overbrace{|a_m\rangle \otimes |b_n\rangle}^{|a_m b_n\rangle}$

$$\langle \hat{A} \rangle = Tr\,(\hat{\rho} \cdot \hat{A}) = \sum_{m,n,m',n'} \langle a_m b_n | \hat{\rho} | a_{m'} b_{n'} \rangle \langle a_{m'} b_{n'} | \hat{A} | a_m b_n \rangle$$

$$\langle \hat{A}_1 \rangle = \sum_{m,n,m',n'} \langle a_m b_n | \hat{\rho} | a_{m'} b_{n'} \rangle \langle a_{m'} | \hat{A}_1 | a_m \rangle \underbrace{\langle b_{n'} | b_n \rangle}_{\delta_{nn'}}$$

$$= \sum_{m,m'} \sum_{n} \langle a_m b_n | \hat{\rho} | a_{m'} b_n \rangle \langle a_{m'} | \hat{A}_1 | a_m \rangle$$

$$= Tr_1\,(\hat{\rho}_1\, \hat{A}_1) \; ; \; \hat{\rho}_1^{\dagger} = \hat{\rho}_1 \; ; \; \langle \phi | \hat{\rho}_1 | \phi \rangle \geq 0$$

$$\hat{\rho}_1 = Tr_2\, \hat{\rho} \iff \begin{cases} \langle a_m | \hat{\rho}_1 | a_{m'} \rangle = \sum_n \langle a_m b_n | \hat{\rho} | a_{m'} b_n \rangle \\ \text{or} \\ \hat{\rho}_1 = \sum_n \langle b_n | \hat{\rho} | b_n \rangle \end{cases}$$

$$Tr_1\, \hat{\rho}_1 = \sum_m \langle a_m | \hat{\rho}_1 | a_m \rangle = \sum_m \sum_n \langle a_m b_n | \hat{\rho} | a_m b_n \rangle = Tr\, \hat{\rho} = 1$$

$\langle \hat{A}_1 \cdot \hat{A}_2 \rangle = \langle \hat{A}_1 \rangle \cdot \langle \hat{A}_2 \rangle$ UNCORRELATED state

the only case for which $\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2$

the total state is obtained from the tensor product of the reduced density operators of two subsystems

$\hat{\rho}_1$	$\hat{\rho}_2$	$\hat{\rho}$	correlated	uncorrelated
pure	pure	pure	N	Y
pure	mixed	mixed	N	Y
mixed	mixed	pure	Y	N
mixed	mixed	mixed	Y	Y

→ show that YES is possible via examples:

1) $\hat{\rho}_1$ is pure ; $\hat{\rho}_2$ is pure ; $\hat{\rho}$ is pure uncorr.

$\Downarrow$ $\hat{\rho}_1 = |\phi\rangle\langle\phi|$; $\hat{\rho}_2 = |\omega\rangle\langle\omega|$; $\hat{\rho} = |\psi\rangle\langle\psi|$

$|\psi\rangle = |\phi\rangle \otimes |\omega\rangle$

2) $\hat{\rho}_1$ is pure ; $\hat{\rho}_2$ is mixed ; $\hat{\rho}$ is mixed uncorr.

$\mathrm{Tr}\,\hat{\rho}_1^2 = 1$ $\quad$ $\mathrm{Tr}\,\hat{\rho}_2^2 < 1$ $\quad$ $\hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2$

$\boxed{\mathrm{T}(\hat{\rho}_1 \otimes \hat{\rho}_2) = \mathrm{Tr}\,\hat{\rho}_1 \cdot \mathrm{Tr}\,\hat{\rho}_2}$ theorem $\quad$ $\mathrm{Tr}\,\hat{\rho}^2 = \mathrm{Tr}\,\hat{\rho}_1^2 \cdot \mathrm{Tr}\,\hat{\rho}_2^2 < 1$

3) $\hat{\rho}_1$ is mixed ; $\hat{\rho}_2$ is mixed ; $\hat{\rho}$ is pure corr.

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle\right)$$

$\hat{\rho} = |\psi\rangle\langle\psi|$ is pure $\quad$ → for any chosen direction prob $= 0.5$ for $\uparrow, \downarrow$

$$\hat{\rho}_1 = \mathrm{Tr}_2\,\hat{\rho} \equiv \hat{\rho}_2 = \mathrm{Tr}_1\,\hat{\rho} = \frac{1}{2}\left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\right)$$

→ Einstein's spooky action at distance

→ spin-$\uparrow$ for particle 1 means spin-$\downarrow$ for particle 2

4) $\hat{\rho}_1$ is mixed ; $\hat{\rho}_2$ is mixed ; $\hat{\rho}$ is mixed uncorr.

$\Downarrow$ $\mathrm{Tr}\,\hat{\rho}_1^2 < 1$ $\quad$ $\mathrm{Tr}\,\hat{\rho}_2^2 < 1 \Rightarrow \hat{\rho} = \hat{\rho}_1 \otimes \hat{\rho}_2$, $\mathrm{Tr}(\hat{\rho}^2) < 1$

5) $\hat{\rho}_1$ is mixed ; $\hat{\rho}_2$ is mixed ; $\hat{\rho}$ is mixed corr.

$$\hat{\rho} = \frac{1}{2}\left(|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|\right) \Rightarrow \hat{\rho}_1 = \hat{\rho}_2 = \frac{1}{2}\left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\right)$$

but z components of the spins are correlated

(h) Einstein-Podolsky-Rosen (EPR) "paradox": instantaneous nonclassical correlations between subsystems at $\boxed{\text{arbitrary separation}}$

1200 km in Chinese satellite exp.

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_A|\uparrow\rangle_B + |\downarrow\rangle_A|\downarrow\rangle_B\right)$$

→ before Alice measures $\langle\hat{\sigma}_A^z\rangle$, Bob can obtain $\langle\hat{\sigma}_z^B\rangle = \pm 1$, but after Alice completes the measurement the state B collapses, so Bob gets with certainty $\langle\hat{\sigma}_z^B\rangle = 1$

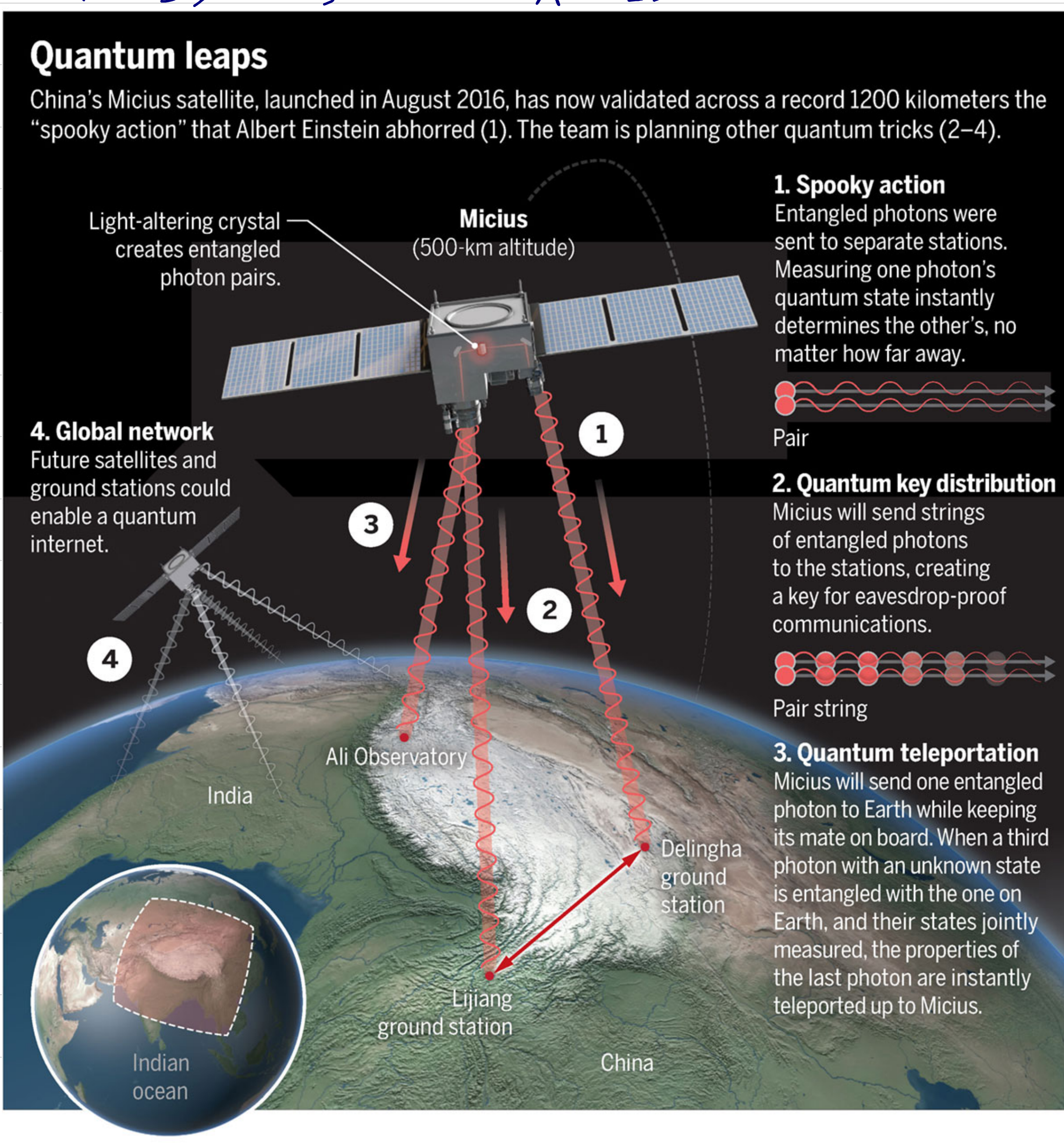
$$\langle\hat{\sigma}_A^z\cdot\hat{\sigma}_B^z\rangle = 1 \neq \langle\hat{\sigma}_A^z\rangle\cdot\langle\hat{\sigma}_B^z\rangle$$

$$\langle\hat{\sigma}_A^x\cdot\hat{\sigma}_B^x\rangle = 1 \neq \langle\hat{\sigma}_A^x\rangle\cdot\langle\hat{\sigma}_B^x\rangle$$

→ compare with classically correlated state:

$$\hat{\rho} = \frac{1}{2}|\uparrow\rangle_A|\uparrow\rangle_B\langle\uparrow|_A\langle\uparrow|_B + \frac{1}{2}|\downarrow\rangle_A|\downarrow\rangle_B\langle\downarrow|_A\langle\downarrow|_B$$

↳ $\langle\hat{\sigma}_A^z\cdot\hat{\sigma}_B^z\rangle = 1$, but $\langle\hat{\sigma}_A^x\cdot\hat{\sigma}_B^x\rangle = 0$



(i) Schmidt decomposition for quantum systems

bipartite composite $|\Psi\rangle \in \mathcal{H} = \mathcal{H}_u \otimes \mathcal{H}_v$

$$|\Psi\rangle = \sum_{ij} c_{ij} \, |a_i\rangle \otimes |b_j\rangle \; ; \quad |a_i\rangle \in \mathcal{H}_u , \; |b_j\rangle \in \mathcal{H}_v$$

$\Updownarrow$ $\quad$ $\sum_{ij} \to$ in general, sum over two indices

$$\hat{\rho} = |\Psi\rangle\langle\Psi| = \sum_{i,j,k,l} c_{ij} \, c^*_{kl} \, |a_i\rangle\langle a_k| \otimes |b_j\rangle\langle b_l|$$

$$= \sum_{i,j,k,l} \rho_{ij,kl} \, |a_i\rangle\langle a_k| \otimes |b_j\rangle\langle b_l|$$

$\Rightarrow$ $|\Psi\rangle$ can be recast into a sum of biorthogonal terms:

SCHMIDT
$$\begin{cases} |\Psi\rangle_S = \sum_i g_i \, |u_i\rangle \otimes |v_i\rangle \\ \Updownarrow \\ \hat{\rho}_S = \sum_{i,k} g_i g_k^* \, |u_i\rangle\langle u_k| \otimes |v_i\rangle\langle v_k| \, , \quad \sum_i |g_i|^2 = 1 \end{cases}$$

$\sum_i \to$ sum over only one index

1) two different states $|\Psi\rangle_S$ & $|\Psi'\rangle_S$ have two different Schmidt decompositions
2) Summation over i in $|\Psi\rangle$ goes over the smaller in dimensionality $\mathcal{H}_u$ or $\mathcal{H}_v$
3) It is not unique $\to$ maximally entangled EPR state
$\frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle) = \frac{1}{\sqrt{2}}(|\leftarrow\rangle \otimes |\rightarrow\rangle - |\rightarrow\rangle \otimes \langle\leftarrow|) =$
$\frac{1}{\sqrt{2}}(|\nearrow\rangle \otimes |\swarrow\rangle - |\swarrow\rangle \otimes |\nearrow\rangle)$
4) in general, it cannot be extended to more than two systems
5) both $\hat{\rho}_u = \mathrm{Tr}_v \hat{\rho}_S$ & $\hat{\rho}_v = \mathrm{Tr}_u \hat{\rho}_S$ are diagonal and have the same positive eigenspectrum
6) observables $\hat{U} = \sum_i \mu_i |u_i\rangle\langle u_i|$ and $\hat{V} = \sum_i \nu_i |v_i\rangle\langle v_i|$ are perfectly correlated $\Rightarrow$ whenever $\hat{U}$ is measured on the first subsystem with result μ_k, subsequent measurement of $\hat{V}$ yields ν_k

■ perfect correlation from 6) when measuring on EPR states is used to demonstrate violation of Bell inequality which means quantum mechanics DISOBEYS:

LOCAL = any change at point A CANNOT have effect on measurement at point B before time $\frac{d_{AB}}{c}$ elapses

REALISM = measurements reveal preexisting properties

LETTER

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Loophole-free Bell inequality violation using electron spins separated by 1.3 kilometres

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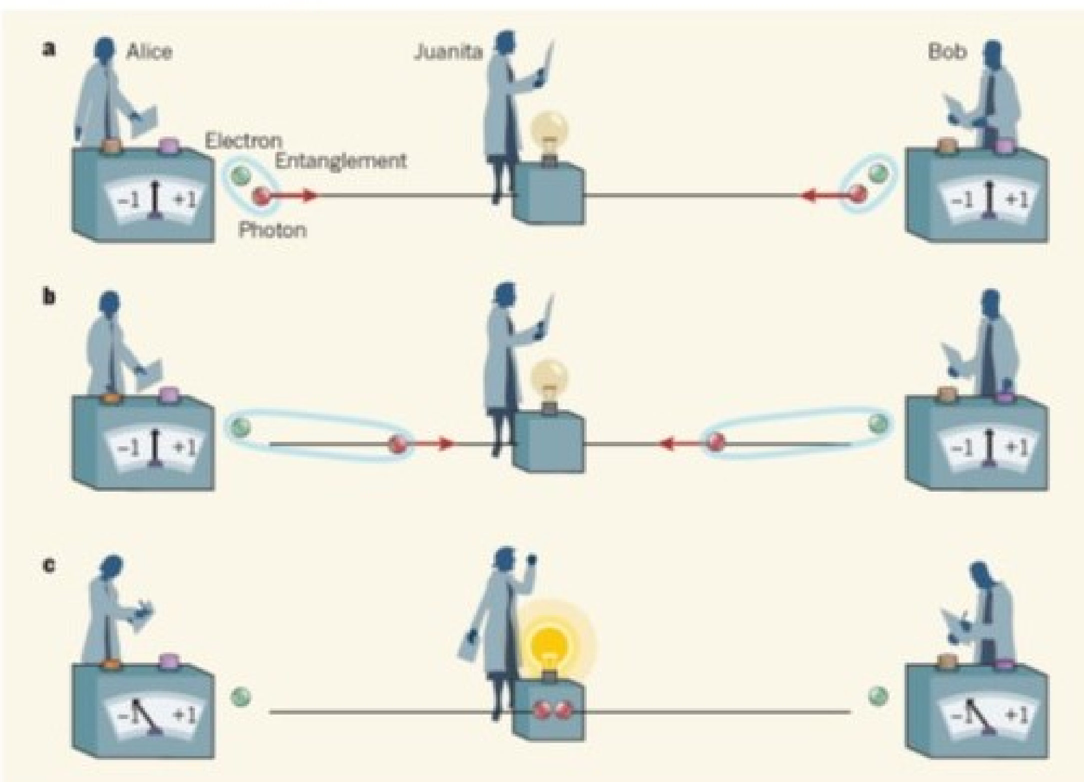


Figure 1 | Violation of a three-party Bell inequality. A Bell inequality is a mathematical relationship regarding the statistics of measurement outcomes obtained by two or more parties. Under certain physical conditions relating to the timing of events, a violation of a Bell inequality proves that local realism — a hypothesis satisfied in all of science except quantum mechanics — is false. Hensen *et al.*[4] have violated a Bell inequality in such a way that the requisite physical conditions were satisfied for the first time, using the scheme shown in this cartoon. **a**, At separate locations, Alice and Bob create entangled states of an electron and a photon, then send the photons to Juanita's laboratory. **b**, Alice and Bob randomly choose a setting for measurements of their respective electrons. **c**, They obtain their measurement outcomes, and Juanita performs a joint measurement of the photons. Alice's and Bob's outcomes are purely random unless Juanita gets a rare successful outcome (as shown here) that indicates entanglement between Alice's and Bob's electrons. By collating the results over many runs, Hensen *et al.* showed that a Bell inequality had been violated by a statistically significant amount.

3° Time evolution of density operator

$i\hbar \frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$ ⟶ Schrödinger equation

$$\hat{\rho} = \sum_i w_i |\psi_i\rangle\langle\psi_i| \Rightarrow \frac{\partial\hat{\rho}}{\partial t} = \sum_i w_i\left(\frac{\partial|\psi_i\rangle}{\partial t}\langle\psi_i| + |\psi_i\rangle\frac{\partial}{\partial t}\langle\psi_i|\right)$$

$$= \sum_i w_i \left(\frac{1}{i\hbar}\hat{H}|\psi_i\rangle + |\psi_i\rangle\left(\frac{1}{-i\hbar}\right)\langle\psi_i|\hat{H}\right)$$

$[\alpha\hat{A}|\psi\rangle]^\dagger = \langle\psi|\hat{A}^\dagger\alpha^*$ using nonrigorous $(|\psi\rangle)^\dagger = \langle\psi|$

$i\hbar\,\partial\hat{\rho}/\partial t = [\hat{H},\hat{\rho}]$ ⟶ von Neumann equation

$\Updownarrow$ quantum-classical correspondence

Liouville equation: $\frac{\partial\rho}{\partial t} = \{H,\rho\} \Leftrightarrow \partial\rho/\partial t + \{\rho, H\} = d\rho/dt = 0$

$$\frac{1}{i\hbar}[\hat{A},\hat{B}] \longleftrightarrow \{A,B\} = \sum_{\alpha=1}^{3N}\left\{\frac{\partial A}{\partial q_\alpha}\frac{\partial B}{\partial p_\alpha} - \frac{\partial A}{\partial p_\alpha}\frac{\partial B}{\partial q_\alpha}\right\}$$

$$S = -k_B\int \rho \ln\rho \frac{d^{3N}q\, d^{3N}p}{h^{3N}N!} \mapsto S = -k_B \operatorname{Tr}\hat{\rho}\ln\hat{\rho}$$

→ equilibrium:

$$\text{CSM}\left\{\begin{matrix}\{H,\rho\}=0 \\ \Downarrow \\ \rho = f(H)\end{matrix}\right. \quad \text{or} \quad \left.\begin{matrix}[\hat{H},\hat{\rho}]=0 \\ \Downarrow \\ \hat{\rho} = f(\hat{H})\end{matrix}\right\}\text{QSM}$$

or steady-state nonequilibrium where $\hat{\rho}$ does not change in time

$i \longrightarrow f$

nonzero flux, but no change in time $\quad \hat{\rho} = \frac{e^{-\beta(\hat{H}-\hat{Y})}}{Z}$

ANSATZ

4° Properly mixed states due to $T \neq 0$

i) MICROCANONICAL ENSEMBLE: $\hat{H}|E_n\rangle = E_n|E_n\rangle$

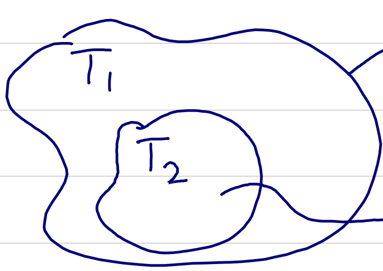
$$\varrho = \frac{\delta(E-H)}{\Omega(E)} \Rightarrow \langle E_n|\hat{\varrho}|E_m\rangle = \begin{cases} 1/\Omega, & \text{if } E_n \in [E, \Delta E] \text{ or } m=n \\ 0, & \text{if } E_n \notin [E, \Delta E] \text{ or } m \neq n \end{cases}$$

$$\hat{\varrho} = \delta(E-\hat{H})/\Omega(E), \quad \mathrm{Tr}\,\hat{\varrho} = 1 \Rightarrow \Omega(E) = \sum_n \delta(E-E_n)$$

$$\hat{\varrho} = \sum_n \frac{1}{\Omega} |E_n\rangle\langle E_n|, \quad E \leq E_n \leq E + \Delta E$$

$\hookrightarrow$ $|E_n\rangle$ are superimposed into a density matrix with random phases $\Leftrightarrow$ incoherent superposition

ii) CANONICAL ENSEMBLE:



$\hat{\varrho}_{micro}$ $\quad T_1 = T_2$ in equilibrium

$$\hat{\varrho} = \mathrm{Tr}_{env}\,\hat{\varrho}_{micro} = \frac{e^{-\beta\hat{H}}}{Z} \leftarrow \varrho = \frac{e^{-\beta H}}{Z}$$

system and environment are exchanging energy microscopically

$$\mathrm{Tr}\,\hat{\varrho} = 1 \Rightarrow Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right) = \sum_n e^{-\beta E_n}$$

$E_n \hookrightarrow$ many body eigenenergies

$$E = \langle\hat{H}\rangle = \frac{\mathrm{Tr}\left(e^{-\beta\hat{H}}\cdot\hat{H}\right)}{\mathrm{Tr}\,e^{-\beta\hat{H}}} = -\frac{\partial}{\partial\beta}\ln\left[\mathrm{Tr}\,e^{-\beta\hat{H}}\right] = -\frac{\partial}{\partial\beta}\ln Z$$

$$S = -k_B\,\mathrm{Tr}(\hat{\varrho}\ln\hat{\varrho}) = -k_B\,\mathrm{Tr}\left[\hat{\varrho}\left(-\beta\hat{H} - \ln Z\,\hat{I}\right)\right] = k_B\beta\underbrace{\langle\hat{H}\rangle}_{E} + k_B\ln Z$$

$F = E - TS = -k_B T \ln Z \rightsquigarrow$ free energy from thermodynamics

iii) GRAND CANONICAL ENSEMBLE

$$\hat{\rho} = e^{-\beta(\hat{H}-\mu\hat{N})}/Z_G, \quad Z_G = \mathrm{Tr}\left[e^{-\beta\hat{H}+\beta\mu\hat{N}}\right] = \sum_{N=0}^{\infty} e^{\beta\mu N} Z_N$$

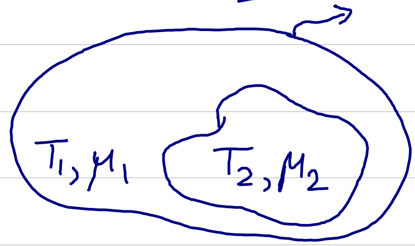
$$\longrightarrow \sum_{n_i;N} \langle n_i;N|\ldots|n_i;N\rangle \quad |n_i;N\rangle \in \text{Fock space } \mathbb{C}\oplus\mathcal{H}\oplus(\mathcal{H}\otimes\mathcal{H})\oplus\ldots$$

$$S = -k_B \mathrm{Tr}\,\hat{\rho}\ln\hat{\rho} = -k_B \mathrm{Tr}\left[\hat{\rho}\left(-\beta\hat{H}+\beta\mu\hat{N}-\ln Z_G\right)\right]$$

$$= k_B\beta\underbrace{\langle\hat{H}\rangle}_{E} - k_B\beta\mu\underbrace{\langle\hat{N}\rangle}_{N} + k_B\ln Z_G$$

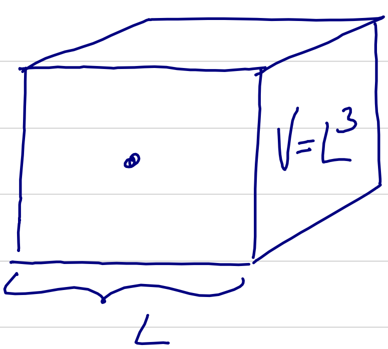
$$\Phi = E - TS - \mu N = -k_B T\ln Z_G$$

$\hat{\rho}_{micro}$



$T_1 = T_2$, $\mu_1 = \mu_2$ in equilibrium

5° EXAMPLE: Single spinless particle in a box via canonical ensembe



$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} = -\frac{\hbar^2\nabla^2}{2m}$$

$$\hat{H}|\vec{k}\rangle = \varepsilon_{\vec{k}}|\vec{k}\rangle, \quad \varepsilon_{\vec{k}} = \frac{\hbar^2k^2}{2m}$$

$$\langle\vec{r}|\vec{k}\rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} \longrightarrow \langle\vec{k}|\vec{k}'\rangle = \delta(\vec{k}-\vec{k}')$$

→ use periodic B.C. to switch to discrete spectrum:

$$\underbrace{\psi(x,y,z) = \psi(x+L,y,z) = \psi(x,y+L,z) = \psi(x,y,z+L)}$$

$$e^{i\vec{k}\cdot\vec{L}} = 1 \Rightarrow \vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z) \qquad n_{x,y,z} = 0, 1, 2, \ldots$$

$$\langle\vec{r}|\vec{k}\rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}, \quad \langle\vec{k}|\vec{k}'\rangle = \delta_{\vec{k}\vec{k}'}$$

$$\int d^3\vec{r}\,\langle\vec{r}|\vec{k}\rangle = 1$$

→ space of quantum microstates is much larger than 6-dim phase space

$$Z = \mathrm{Tr}(\hat{\rho}) = \sum_{\vec{k}} e^{-\beta \hbar^2 k^2/2m}$$

$$\overset{L\to\infty}{=} \frac{V}{(2\pi)^3} \int d^3\vec{k}\, e^{-\beta \hbar^2 k^2/2m} = \frac{V}{(2\pi)^3} \int_0^\infty dk \int_0^\pi d\theta \int_0^{2\pi} d\varphi$$

$$\times\, k^2 \sin\theta\, e^{-\beta \hbar^2 k^2/2m}$$

$$= \cancel{4}\pi \frac{V}{(2\pi)^3} \cdot \frac{1}{\cancel{4}} \sqrt{\frac{\pi}{(\beta \hbar^2/2m)^3}} = \frac{V}{(2\pi)^3}\left(\sqrt{\frac{2m\pi k_B T}{\hbar^2}}\right)^3 = \frac{V}{\lambda^3}$$

$$\boxed{\int_0^\infty x^2 e^{-ax^2} dx = \frac{1}{4}\sqrt{\pi/a^3}}$$

same as classical result which justifies using $d^3\vec{q}\, d^3\vec{p}/h^3$ as dimensionless measure in phase space

$$\lambda = \frac{h}{\sqrt{2\pi m k_B T}}$$

$\to$ de Broglie thermal wavelength for $E = \pi k_B T$ instead of $E = \frac{3}{2} k_B T$

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z} = \frac{1}{Z} \cdot \sum_{\vec{k}} e^{-\beta \varepsilon_{\vec{k}}} |\vec{k}\rangle\langle\vec{k}|$$

$$\langle \vec{k}' | \hat{\rho} | \vec{k} \rangle = \frac{\lambda^3}{V} e^{-\beta \hbar^2 k^2/2m} \delta_{\vec{k}\vec{k}'},$$ is diagonal and its nonzero matrix elements look exactly the same as classical momentum distribution

$$\langle \vec{r}' | \hat{\rho} | \vec{r} \rangle = \sum_{\vec{k}} \langle \vec{r}' | \vec{k} \rangle \frac{e^{-\beta \varepsilon_{\vec{k}}}}{Z} \langle \vec{k} | \vec{r} \rangle$$

$$= \frac{\lambda^3}{V} \int \frac{V}{(2\pi)^3} d^3\vec{k}\, \frac{e^{-i\vec{k}(\vec{r}-\vec{r}')}}{V} e^{-\beta \hbar^2 k^2/2m}$$

Gaussian integral by completing the square:

$$-\beta\frac{\hbar^2k^2}{2m}+i\vec{k}(\vec{r}\,'-\vec{r})=-\beta\frac{\hbar^2}{2m}\Big\{\vec{k}^2-\frac{2mi}{\beta\hbar^2}(\vec{r}\,'-\vec{r})\cdot\vec{k}$$

$$+\left(\frac{mi}{\beta\hbar^2}\right)^2(\vec{r}\,'-\vec{r})^2\Big\}-\frac{m}{2\beta\hbar^2}(\vec{r}\,'-\vec{r})^2=$$

$$=-\beta\hbar^2/2m\,(\vec{k}-\vec{k}_0)^2-\frac{m}{2\beta\hbar^2}(\vec{r}\,'-\vec{r})^2$$

$\vec{k}_0=\frac{mi}{\beta\hbar^2}(\vec{r}\,'-\vec{r})$ is an abbreviation

$$\langle\vec{r}\,'|\hat{\rho}|\vec{r}\rangle=\frac{1}{V}e^{-m(\vec{r}-\vec{r}\,')^2/2\beta\hbar^2}=\frac{1}{V}e^{-\frac{\pi(\vec{r}-\vec{r}\,')^2}{\lambda^2}}$$

→ diagonal elements are $1/V$, which is probability to find particle at position $\vec{r}$

→ off-diagonal elements suggest that we should think of a particle as a wave packet of size $\lambda=h/\sqrt{2\pi mk_BT}$

$T\to\infty\Rightarrow\lambda\to0$ and CM is valid

$T\to0\Rightarrow\lambda\to\infty$ and QM takes over when $\lambda\sim L$

→ energy in thermodynamics ⇔ expectation value of Hamiltonian

$$E=\langle\hat{H}\rangle=-\frac{\partial}{\partial\beta}\ln Z=\frac{3}{2}k_BT \text{ using } \boxed{\frac{\partial}{\partial\beta}=-(k_BT)^2\frac{\partial}{\partial T}}$$

$\Rightarrow$ pedestrian (and longer) version:

$$E = \langle \hat{H} \rangle = \mathrm{Tr}\,(\hat{\rho} \cdot \hat{H}) = \sum_{\vec{k}} \langle \vec{k} | \hat{\rho} \hat{H} | \vec{k} \rangle$$

$$= \sum_{\vec{k}} \sum_{\vec{k}'} \underbrace{\langle \vec{k} | \hat{\rho} | \vec{k}' \rangle}_{\lambda^3/V\, e^{-\beta \hbar^2 k^2/2m}\, \delta_{\vec{k}\vec{k}'}} \underbrace{\langle \vec{k}' | \hat{H} | \vec{k} \rangle}_{\frac{\hbar^2 k^2}{2m} \delta_{\vec{k}\vec{k}'}}$$

$$= \frac{\hbar^2}{2m} \frac{\lambda^3}{V} \frac{V}{(2\pi)^3} \int d^3\vec{k}\; k^2 e^{-\beta \hbar^2 k^2/2m}$$

$$= \frac{\hbar^2}{2m} \cdot \lambda^3 \cdot \frac{2}{(2\pi)^2} \int_0^\infty dk\; k^4 e^{-\beta \hbar^2 k^2/2m}$$

$$x = \beta \hbar^2 k^2/2m \Rightarrow \langle \hat{H} \rangle = \frac{\hbar^2 \lambda^3}{m} \cdot \frac{1}{(2\pi)^2} \frac{1}{2} \left(\frac{2m}{\beta \hbar^2} \right)^{5/2}$$

$$\times \underbrace{\int_0^\infty dx\; x^{3/2} e^{-x}}_{\Gamma(5/2) = 3\sqrt{\pi}/4} = \frac{3}{2} k_B T$$