Emergence of Quantum Mechanics from Classical Statistics

what is an atom ?

- quantum mechanics : isolated object
- quantum field theory : excitation of complicated vacuum
- classical statistics : sub-system of ensemble with infinitely many degrees of freedom

quantum mechanics can be described by classical statistics !

quantum mechanics from classical statistics

- probability amplitude
- entanglement
- interference
- superposition of states
- fermions and bosons
- unitary time evolution
- transition amplitude
- non-commuting operators

probabilistic observables

Holevo; Beltrametti,Bugajski

classical ensemble , discrete observable

- Classical ensemble with probabilities $\hat{p}_\tau$

$$\hat{p}_\tau \geq 0 \quad , \quad \sum_\tau \hat{p}_\tau = 1$$

- one discrete observable A , values +1 or -1

effective micro-states

group states together $\tau = (\sigma, t_\sigma)$

σ labels effective micro-states , t_σ labels sub-states

$$p_\sigma = \sum_{t_\sigma} \hat{p}_{(\sigma,t_\sigma)} \quad , \quad p_\sigma \geq 0 \quad , \quad \sum_\sigma p_\sigma = 1$$

in effective micro-states σ :

probabilities to find A=1 : $w_{\sigma+}$ and A=-1: $w_{\sigma-}$

mean value in micro-state σ :

$$\overline{A}_\sigma = w_{\sigma+} - w_{\sigma-} \quad , \quad \overline{A_\sigma^2} = 1$$

expectation values

$$\langle A \rangle = \sum_\sigma p_\sigma \overline{A}_\sigma \quad , \quad \langle A^2 \rangle = \sum_\sigma p_\sigma \overline{A^2_\sigma} = 1$$

only measurements +1 or -1 possible !

probabilistic observables have a probability distribution of values in a microstate , classical observables a sharp value

deterministic and probabilistic observables

- **classical or deterministic observables** describe atoms and environment
- probabilities for infinitely many sub-states needed for computation of classical correlation functions $\tau = (\sigma, t_\sigma)$

- **probabilistic observables** can describe atom only
- environment is integrated out
- suitable system observables need only state of system for computation of expectation values and correlations

three probabilistic observables

- characterize by vector (e_1, e_2, e_3)

$$A^{(1)} : e = (1,0,0)$$

$$A^{(2)} : e = (0,1,0) \quad , \quad A^{(3)} : e = (0,0,1)$$

- each $A^{(k)}$ can only take values ± 1 ,

  "orthogonal spins"

- expectation values :

$$\langle A^{(k)} \rangle = \rho_k e_k \quad , \quad \rho_k = \sum_\sigma p_\sigma \overline{A}_\sigma^{(k)}$$

density matrix and pure states

elements of density matrix

- probability weighted mean values of basis unit observables are sufficient to characterize the state of the system

$$\rho_k = \sum_\sigma p_\sigma \overline{A}_\sigma^{(k)}$$

- $\varrho_k = \pm 1 \Longleftrightarrow$ sharp value for $A^{(k)}$
- in general: $\rho_k^2 \leq 1$

purity

- How many observables can have sharp values ?
- depends on purity $$P = \rho_k \rho_k$$
- P=1 : one sharp observable ok
- for two observables with sharp values :

$$\rho_1^2 = 1 \quad , \quad \rho_2^2 = 1 \quad \Rightarrow \quad P \geq 2$$

purity

for $\boxed{M \leq P < M+1}$:

at most M discrete observables can be sharp

consider P ≤ 1

“ three spins , at most one sharp “

density matrix

- define hermitean 2x2 matrix :

$$\rho = \frac{1}{2}(1 + \rho_k \tau_k)$$

- properties of density matrix

$$tr\rho = 1 \qquad \rho_{\alpha\alpha} \geq 1 \qquad tr\rho^2 \leq 1$$

M – state quantum mechanics

- density matrix for P ≤ M+1 :

$$\rho = \frac{1}{M}(1 + \rho_k L_k) \quad , \quad tr L_k L_\ell = M\delta_{k\ell}$$

$$tr\rho^2 = \frac{1}{M}(1 + \rho_k \rho_k) = \frac{1}{M}(1 + P)$$

- choice of M depends on observables considered
- restricted by maximal number of "commuting observables"

$$M_{\min} = N_{max} + 1$$

quantum mechanics for isolated systems

- classical ensemble admits infinitely many observables (atom and its environment)
- we want to describe isolated subsystem (atom) : finite number of independent observables
- "isolated" situation : subset of the possible probability distributions
- not all observables simultaneously sharp in this subset
- given purity : conserved by time evolution if subsystem is perfectly isolated
- different M describe different subsystems (atom or molecule)

density matrix for two quantum states

hermitean 2x2 matrix :

$$\rho = \frac{1}{2}(1 + \rho_k \tau_k)$$

P $\leq$ 1

“ three spins , at most one sharp “

operators

hermitean operators

$$\hat{A}(e_k) = e_k \tau_k$$

$$\begin{aligned} \langle A(e_k) \rangle &= tr(\hat{A}(e_k)\rho) \\ &= \frac{1}{2}\rho_k e_\ell \{\tau_k, \tau_\ell\} = \rho_k e_k \end{aligned}$$

quantum law for expectation values

$$\langle A \rangle = tr(\hat{A}\rho)$$

operators do not commute

at this stage : convenient way to express expectation values

deeper reasons behind it …

rotated spins

- correspond to rotated unit vector e_k
- new two-level observables
- expectation values given by

$$\langle A(e_k)\rangle = \rho_k e_k \qquad \langle A\rangle = tr(\hat{A}\rho)$$

- only density matrix needed for computation of expectation values , $\rho_k = \sum_\sigma p_\sigma \overline{A}_\sigma^{(k)}$

not full classical probability distribution $\hat{p}_\tau$

pure states

- pure states show no dispersion with respect to one observable A

$$\langle A\rangle^2 = \langle A^2\rangle$$

- recall classical statistics definition

$$\langle A\rangle = \sum_\sigma p_\sigma \overline{A}_\sigma \quad , \quad |\overline{A}_\sigma| \le 1$$

quantum pure states are classical pure states

- probability vanishing except for one micro-state

$$\langle A \rangle = 1 : \begin{cases} p_\sigma = 0 \quad \text{for} \quad \overline{A}_\sigma < 1 \\ p_\sigma = 1 \quad \text{for} \quad \overline{A}_\sigma = 1 \end{cases}$$

pure state density matrix

- elements ϱ_k are vectors on unit sphere
- can be obtained by unitary transformations

$$\rho = U \hat{\rho}_1 U^\dagger \quad , \quad U U^\dagger = U^\dagger U = 1$$

$$\hat{\rho}_1 = \begin{pmatrix} 1 & , & 0 \\ 0 & , & 0 \end{pmatrix}$$

- SO(3) equivalent to SU(2)

wave function

- "root of pure state density matrix "

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

$$\hat{\psi}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad \psi = U \hat{\psi}_1$$

$$\rho_{\alpha\beta} = \psi_\alpha \psi^*_\beta$$

$$tr(\hat{A}\rho) = \hat{A}_{\alpha\beta}\rho_{\beta\alpha} = \hat{A}_{\alpha\beta}\psi_\beta\psi^*_\alpha$$

- quantum law for expectation values

$$\langle A \rangle = \psi^\dagger \hat{A} \psi$$

time evolution

transition probability

time evolution of probabilities

$$\partial_t p_\sigma = F_\sigma(p_{\sigma'})$$

(fixed observables)

induces transition probability matrix

$$p_\sigma(t) = \tilde{S}_{\sigma\tau}(t,t')p_\tau(t')$$

reduced transition probability

- induced evolution

$$\partial_t \rho_k = \sum_\sigma \partial_t p_\sigma \overline{A}_\sigma^{(k)} = \sum_\sigma F_\sigma(p_{\sigma'}) \overline{A}_\sigma^{(k)}$$

- reduced transition probability matrix

$$\rho_k(t) = S_{k\ell}(t,t')\rho_\ell(t')$$

$$S_{k\ell}(t,t') = \frac{\sum_{\sigma\tau\rho} \tilde{S}_{\sigma\tau}(t,t') p_\tau(t') p_\rho(t') \overline{A}_\sigma^{(k)} \overline{A}_\rho^{(\ell)}}{\rho_m(t')\rho_m(t')}$$

evolution of elements of density matrix

- infinitesimal time variation

$$\partial_t \rho_k(t) = \partial_t S_{k\ell}(t,t') S^{-1}_{\ell m}(t,t') \rho_m(t)$$

- scaling + rotation

$$S_{k\ell} = \hat{S}_{k\ell}\, d$$

$$\hat{S}^{-1}_{k\ell} = \hat{S}_{\ell k}$$

$$\partial_t S S^{-1} = \partial_t \hat{S} \hat{S}^T + \partial_t \ln d$$

time evolution of density matrix

- Hamilton operator and scaling factor

$$\hat{H} = -\frac{1}{4}(\partial_t \hat{S}\hat{S}^T)_{\ell m}\,\varepsilon_{\ell m k}\tau_k$$

$$\lambda = \partial_t \ln d$$

- Quantum evolution and the rest ?

$$\partial_t \rho = -i[\hat{H},\rho] + \lambda(\rho - \frac{1}{2})$$

λ=0 and pure state :

$$i\partial_t \psi = \hat{H}\psi$$

quantum time evolution

It is easy to construct explicit ensembles where

$$\lambda = 0$$

⇒ quantum time evolution

evolution of purity

change of purity

$$\begin{aligned} \partial_t P &= \partial_t(\rho_k \rho_k) = \partial_t(2tr\,\rho^2 - 1) \\ \partial_t P &= 2\lambda P \end{aligned}$$

$$P = \rho_k \rho_k$$

attraction to randomness :
decoherence

$$\lambda < 0 \quad : \quad P \to 0$$

attraction to purity :
syncoherence

$$\lambda > 0 \quad : \quad P \to 1$$

classical statistics can describe
decoherence and syncoherence !
unitary quantum evolution : special case

pure state fixed point

pure states are special :

“ no state can be purer than pure “

fixed point of evolution for $$P = 1 \quad , \quad \lambda = 0$$

approach to fixed point $$\partial_t \lambda = \beta_\lambda(\lambda, P, \rho_k/\sqrt{P}, \ldots)$$

$$\beta_\lambda = -a\lambda + b(1-P)$$

approach to pure state fixed point

solution : $$1 - P = x_1 e^{-\varepsilon_1 t} + x_2 e^{-\varepsilon_2 t}$$ $$\lambda = \varepsilon_1 x_1 e^{-\varepsilon_1 t} + \varepsilon_2 x_2 e^{-\varepsilon_2 t}$$

$$\varepsilon_{1,2} = \frac{1}{2}(a \pm \sqrt{a^2 - 4b}$$

- syncoherence describes exponential approach to pure state if $$a > 0 \quad , \quad a < b < \frac{1}{4}a^2$$

- decay of mixed atom state to ground state *purity conserving evolution : subsystem is well isolated*

two bit system and entanglement

ensembles with P=3

non-commuting operators

15 spin observables labeled by $e_k \quad , \quad k = 1 \ldots 15$

$$\rho_k = \sum_\sigma p_\sigma \overline{A}_\sigma^{(k)} \quad , \quad \langle A(e_k) \rangle = \sum_k \rho_k e_k \quad , \quad -1 \le \rho_k \le 1$$

density matrix $\rho = \frac{1}{4}(1 + \rho_k L_k)$

$$L_k^2 = 1 \quad , \quad tr L_k = 0 \quad , \quad tr(L_k L_\ell) = 4\delta_{k\ell}$$

SU(4) - generators

$$L_k^2 = 1\ ,\ \ \mathrm{tr} L_k = 0\ ,\ \ \mathrm{tr}(L_k L_l) = 4\delta_{kl}.$$

$$L_1 \ = \ \mathrm{diag}(1,1,-1,-1)\ ,\ L_2 = \mathrm{diag}(1,-1,1,-1)$$

$$L_3 \ = \ \mathrm{diag}(1,-1,-1,1)$$

$$L_4 = \begin{pmatrix} \tau_1, & 0 \\ 0, & \tau_1 \end{pmatrix} \quad L_5 \ = \ \begin{pmatrix} \tau_2, & 0 \\ 0, & \tau_2 \end{pmatrix}$$

$$L_6 = \begin{pmatrix} \tau_1, & 0 \\ 0, & -\tau_1 \end{pmatrix}, L_7 = \begin{pmatrix} \tau_2, & 0 \\ 0, & -\tau_2 \end{pmatrix}$$

density matrix

- pure states : P=3

$$tr\rho^2 = \frac{1}{4}(1+\rho_k\rho_k) = \frac{1}{4}(1+P)$$

$$P \leq 3 \quad : \quad tr\rho^2 \leq 1$$

$$\hat{A}(e_k) = e_k L_k \quad , \quad e_k e_k = 1 \quad \text{for} \quad \hat{A}^2(e_k) = 1$$

entanglement

- three commuting observables

$$L_1 = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}, \quad L_2 = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}, \quad L_3 = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}$$

L_1 : bit 1 , L_2 : bit 2 L_3 : product of two bits

- expectation values of associated observables related to probabilities to measure the combinations (++) , etc.

$$\begin{aligned} \langle T_1 \rangle &= W_{++} + W_{+-} - W_{-+} - W_{--} \\ \langle T_2 \rangle &= W_{++} - W_{+-} + W_{-+} - W_{--} \\ \langle T_3 \rangle &= W_{++} - W_{+-} - W_{-+} + W_{--} \end{aligned}$$

“classical” entangled state

- pure state with maximal anti-correlation of two bits

$$W_{++} = W_{--} = 0 \quad , \quad W_{+-} = W_{-+} = \frac{1}{2}$$

- bit 1: random , bit 2: random
- **if bit 1 = 1 necessarily bit 2 = -1 , and vice versa**

$$\langle L_1 \rangle = \langle L_2 \rangle = 0 \quad , \quad \langle L_3 \rangle = -1$$

classical state described by entangled density matrix

$$\rho = \frac{1}{2}\begin{pmatrix} 0, & 0, & 0, & 0 \\ 0, & 1, & \pm 1, & 0 \\ 0, & \pm 1, & 1, & 0 \\ 0, & 0, & 0, & 0 \end{pmatrix} \quad , \quad tr\rho^2 = 1$$

$$\rho = \frac{1}{4}(1 - L_3 \pm (L_{12} - L_{14}))$$

$$\rho_1 = \rho_2 = 0 \quad \Rightarrow \quad \langle T_1 \rangle = \langle T_2 \rangle = 0$$

$$\rho_3 = -1 \quad \Rightarrow \quad \langle T_3 \rangle = -1$$

entangled quantum state

$$\psi_{\pm} = \frac{1}{\sqrt{2}}(\psi_2 \pm \psi_3) = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ \pm 1 \\ 0 \end{pmatrix}$$

conditional correlations

classical correlation

- pointwise multiplication of classical observables on the level of sub-states
- not available on level of probabilistic observables

- definition depends on details of classical observables , while many different classical observables correspond to the same probabilistic observable
- classical correlation depends on probability distribution for the atom and its environment

needed : correlation that can be formulated in terms of probabilistic observables and density matrix !

pointwise or conditional correlation ?

- Pointwise correlation appropriate if two measurements do not influence each other.

- Conditional correlation takes into account that system has been changed after first measurement.

  Two measurements of same observable immediately after each other should yield the same value !

pointwise correlation

pointwise product of observables $(\overline{A \cdot B})_\alpha = \bar{A}_\alpha \bar{B}_\alpha$

$$(\overline{A \cdot B})_\alpha = w_{+,\alpha}^{AB} - w_{-,\alpha}^{AB}$$

α=σ

$$w_{+,\alpha}^{AB} = w_{+,\alpha}^{A} w_{+,\alpha}^{B} + w_{-,\alpha}^{A} w_{-,\alpha}^{B}$$
$$w_{-,\alpha}^{AB} = w_{+,\alpha}^{A} w_{-,\alpha}^{B} + w_{-,\alpha}^{A} w_{+,\alpha}^{B}$$

does not describe $A^2 = 1$:

$$\langle A \cdot A \rangle = \sum_\alpha p_\alpha \bar{A}_\alpha^2 \leq 1$$

conditional correlations

$w^{AB}_{+,\alpha}$ probability to find value +1 for product of measurements of A and B

$$\begin{aligned} w^{AB}_{+,\alpha} &= (w^A_+)^B_+ w^B_{+,\alpha} + (w^A_-)^B_- w^B_{-,\alpha} \\ w^{AB}_{-,\alpha} &= (w^A_+)^B_- w^B_{-,\alpha} + (w^A_-)^B_+ w^B_{+,\alpha} \end{aligned}$$

$(w^A_+)^B_+$ probability to find A=1 after measurement of B=1

… can be expressed in terms of expectation value of A in eigenstate of B

$$\begin{aligned} (w^A_\pm)^B_+ &= \frac{1}{2}(1 \pm \langle A\rangle_{+B}) \\ (w^A_\pm)^B_- &= \frac{1}{2}(1 \pm \langle A\rangle_{-B}) \end{aligned}$$

conditional product

- conditional product of observables

$$
\begin{aligned}
(\overline{A \circ B})_\alpha &= w^{AB}_{+,\alpha} - w^{AB}_{-,\alpha} = \langle A \rangle_{+B} w^{B}_{+,\alpha} - \langle A \rangle_{-B} w^{B}_{-,\alpha} \\
&= \frac{1}{2}(1 + \bar{B}_\alpha) \langle A \rangle_{+B} - \frac{1}{2}(1 - \bar{B}_\alpha) \langle A \rangle_{-B}.
\end{aligned}
$$

- conditional correlation

$$
\begin{aligned}
\langle A \circ B \rangle = \sum_\alpha p_\alpha (\overline{A \circ B})_\alpha &= \langle A \rangle_{+B} w^{B}_{+,s} - \langle A \rangle_{-B} w^{B}_{-,s} \\
&= \frac{1}{2}(1 + \langle B \rangle) \langle A \rangle_{+B} - \frac{1}{2}(1 - \langle B \rangle) \langle A \rangle_{-B},
\end{aligned}
$$

- does it commute ?

conditional product and anticommutators

- conditional two point correlation commutes

$$\langle A \circ B \rangle = \langle B \circ A \rangle$$

=

$$Re(\langle AB \rangle) \;=\; Re(\mathrm{tr}(\hat{A}\hat{B}\rho)) = \frac{1}{2}\mathrm{tr}(\{\hat{A},\hat{B}\}\rho)$$

quantum correlation

- conditional correlation in classical statistics equals quantum correlation !
- no contradiction to Bell's inequalities or to Kochen-Specker Theorem

conditional three point correlation

$$\langle A \circ B \circ C \rangle$$

$$\begin{aligned}
&= (w_+^A)_+^B (w_+^B)_+^C w_{+,s}^C - (w_+^A)_+^B (w_+^B)_-^C w_{-,s}^C \\
&- (w_+^A)_-^B (w_-^B)_+^C w_{+,s}^C + (w_+^A)_-^B (w_-^B)_-^C w_{-,s}^C \\
&- (w_-^A)_+^B (w_+^B)_+^C w_{+,s}^C + (w_-^A)_+^B (w_+^B)_-^C w_{-,s}^C \\
&+ (w_-^A)_-^B (w_-^B)_+^C w_{+,s}^C - (w_-^A)_-^B (w_-^B)_-^C w_{-,s}^C .
\end{aligned}$$

conditional three point correlation in quantum language

- conditional three point correlation is not commuting !

$$\langle A \circ B \circ C \rangle = \frac{1}{4} \mathrm{tr} \Big(\{\{\hat{A}, \hat{B}\}, \hat{C}\} \rho \Big).$$

$$\langle A^{(k)} \circ A^{(l)} \circ A^{(m)} \rangle = \delta^{kl} \langle A^{(m)} \rangle.$$

conditional correlations and quantum operators

- conditional correlations in classical statistics can be expressed in terms of operator products in quantum mechanics

$$
\begin{aligned}
Re(\langle AB\rangle) &= Re(\mathrm{tr}(\hat{A}\hat{B}\rho)) = \frac{1}{2}\mathrm{tr}(\{\hat{A},\hat{B}\}\rho),\\
Re(\langle ABC\rangle) &= Re(\mathrm{tr}(\hat{A}\hat{B}\hat{C}\rho)) = \frac{1}{2}\mathrm{tr}((\hat{A}\hat{B}\hat{C}+\hat{C}\hat{B}\hat{A})\rho)\\
&= \frac{1}{4}\mathrm{tr}\Big((\{\{\hat{A},\hat{B}\},\hat{C}\}+[[\hat{A},\hat{B}],\hat{C}])\Big)\\
&= \frac{1}{4}\mathrm{tr}\Big((\{\{\hat{A},\hat{B}\},\hat{C}\}+\{\hat{A},\{\hat{B},\hat{C}\}\}\\
&\quad -\{\hat{B},\{\hat{A},\hat{C}\}\})\rho\Big).
\end{aligned}
$$

non – commutativity
of operator product
is closely related to
conditional correlations !

conclusion

- quantum statistics arises from classical statistics

  states, superposition , interference , entanglement , probability amplitudes

- quantum evolution embedded in classical evolution
- conditional correlations describe measurements both in quantum theory and classical statistics

end