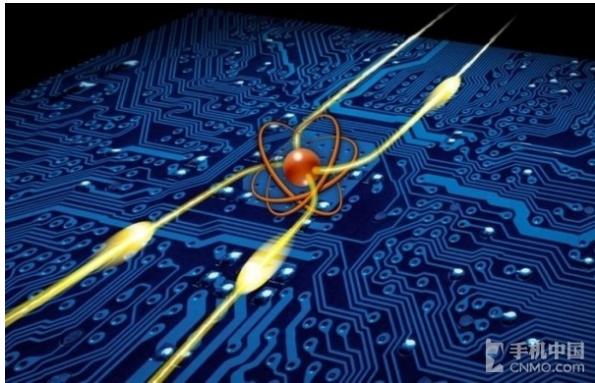
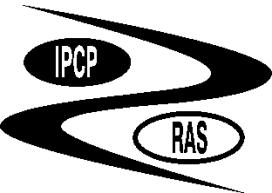


Quantum correlations in bipartite systems

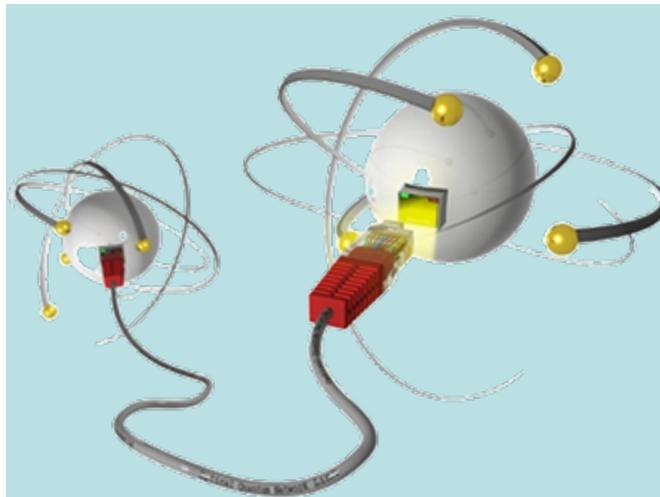
Edward Fel'dman

Institute of Problems of Chemical Physics of Russian Academy of Sciences

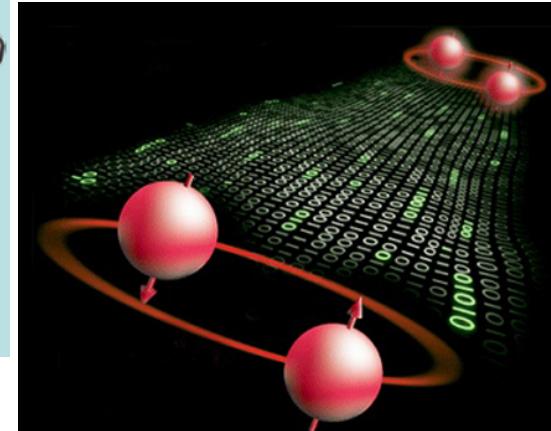




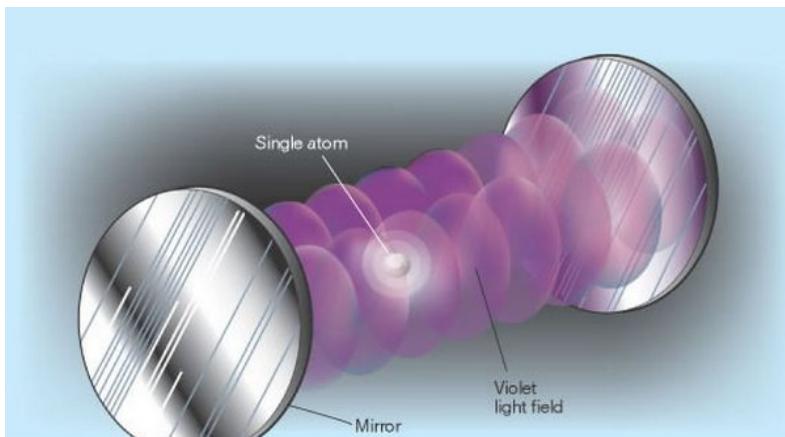
Quantum calculations



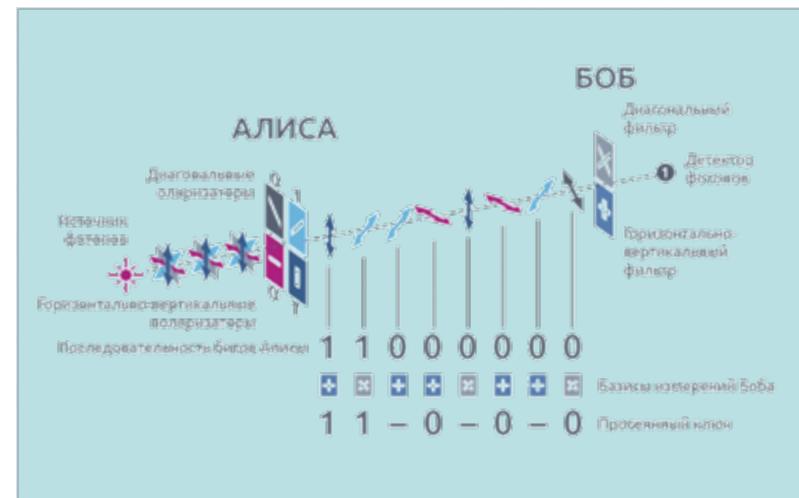
Quantum networks



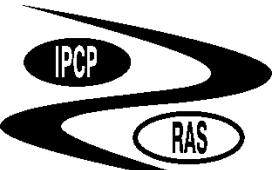
Quantum teleportation



Quantum metrology

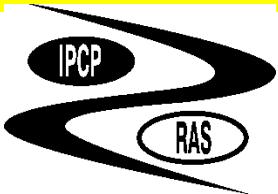


Quantum cryptography

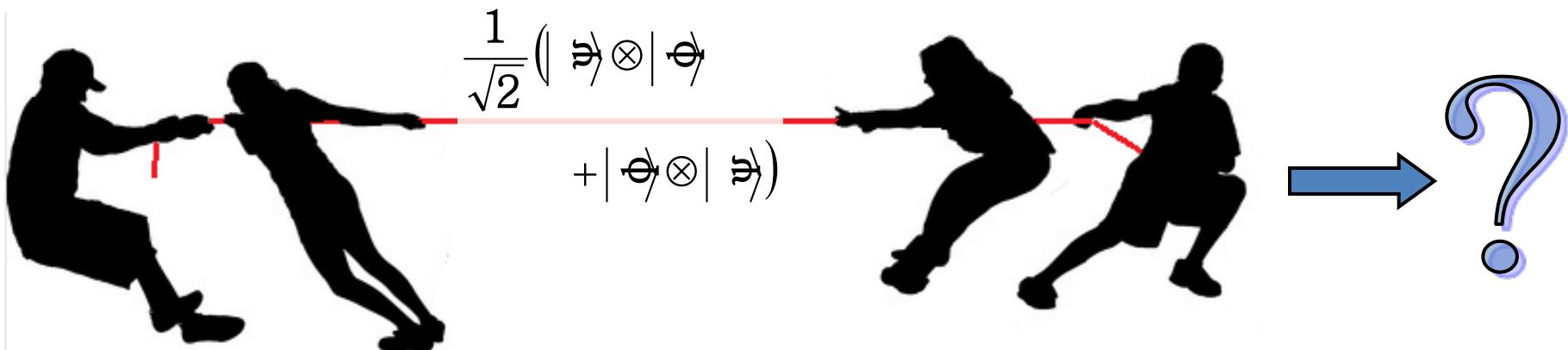
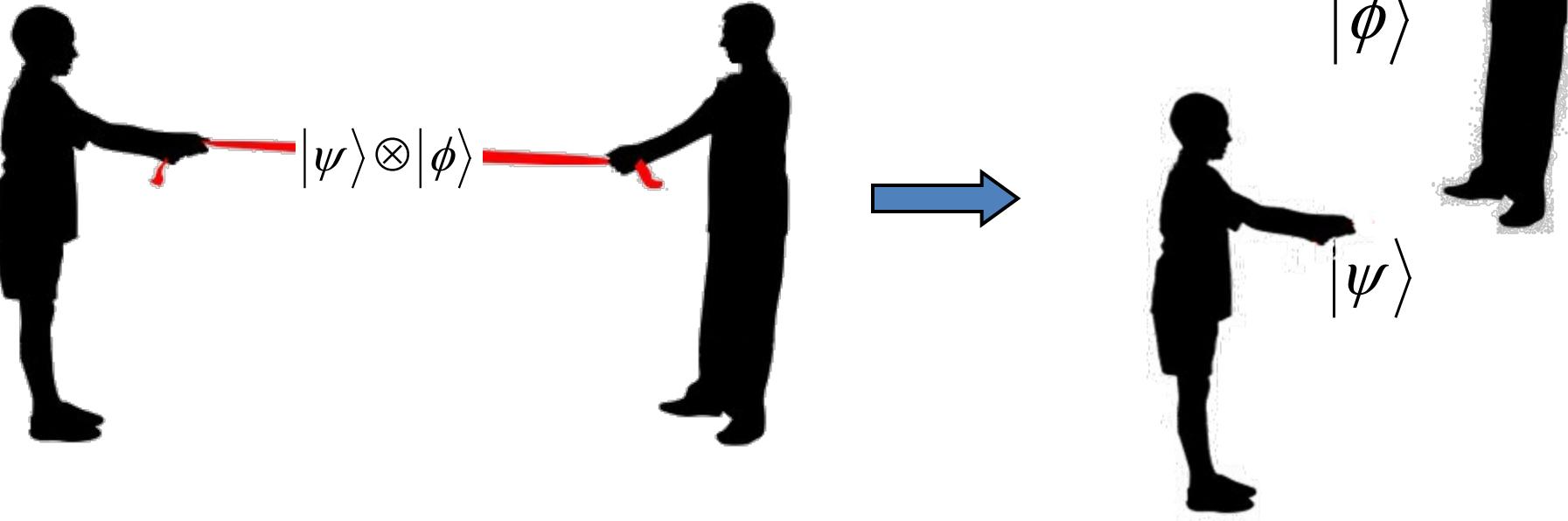


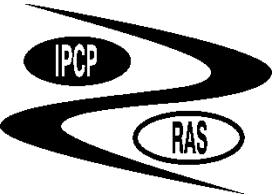
Outline

- Quantum correlations in pure states . Entanglement as a measure of these correlations .
- Multiple quantum (MQ) NMR spectroscopy in solids. Emergence of entangled states in MQ NMR spectroscopy.
- The quantum discord as a measure of quantum correlations in pure and mixed states.
- A comparison of the quantum discord with entanglement in the nitrosyl iron complexes.
- The ring model of interacting spins for an investigation of quantum correlations.
- Contributions of different parts of spin-spin interactions to quantum correlations in a spin ring model in an external magnetic field.
- Quantum correlations in the multi-pulse spin locking



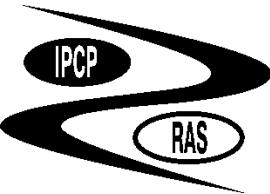
Entanglement



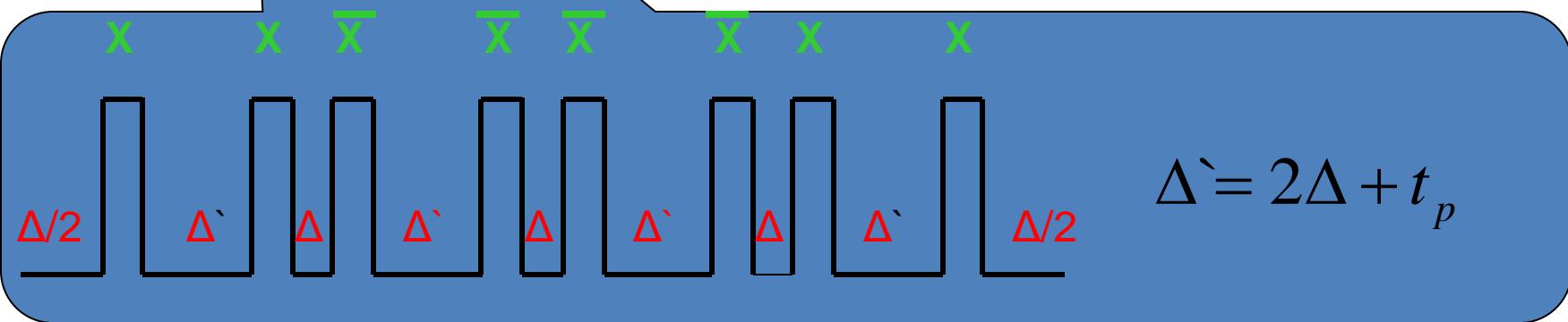
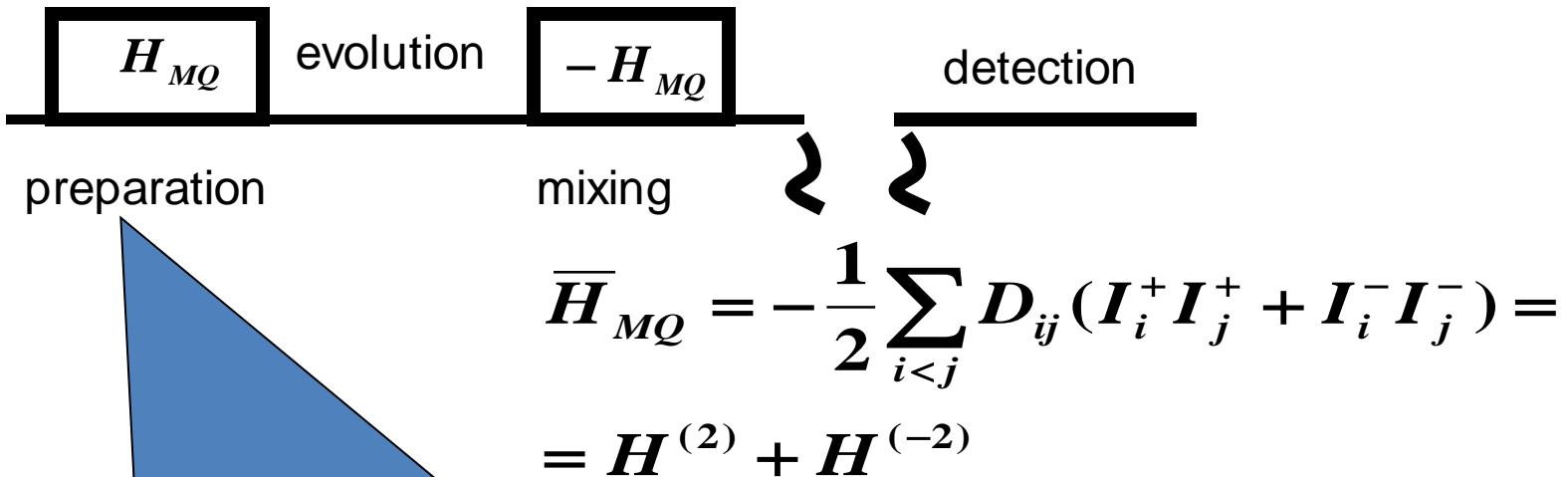


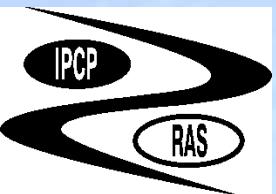
Classical and quantum correlations at measurements

$$\begin{aligned} |\psi\rangle &= |\uparrow\uparrow\rangle \xrightarrow{\text{measurement}} |\uparrow\uparrow\rangle \\ |\psi\rangle &= \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \xrightarrow{\text{measurement}} |\uparrow\downarrow\rangle \end{aligned}$$



Multiple quantum NMR in solids



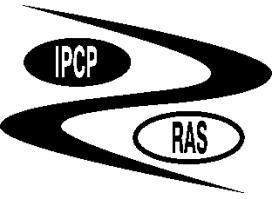


Emergence of entanglement

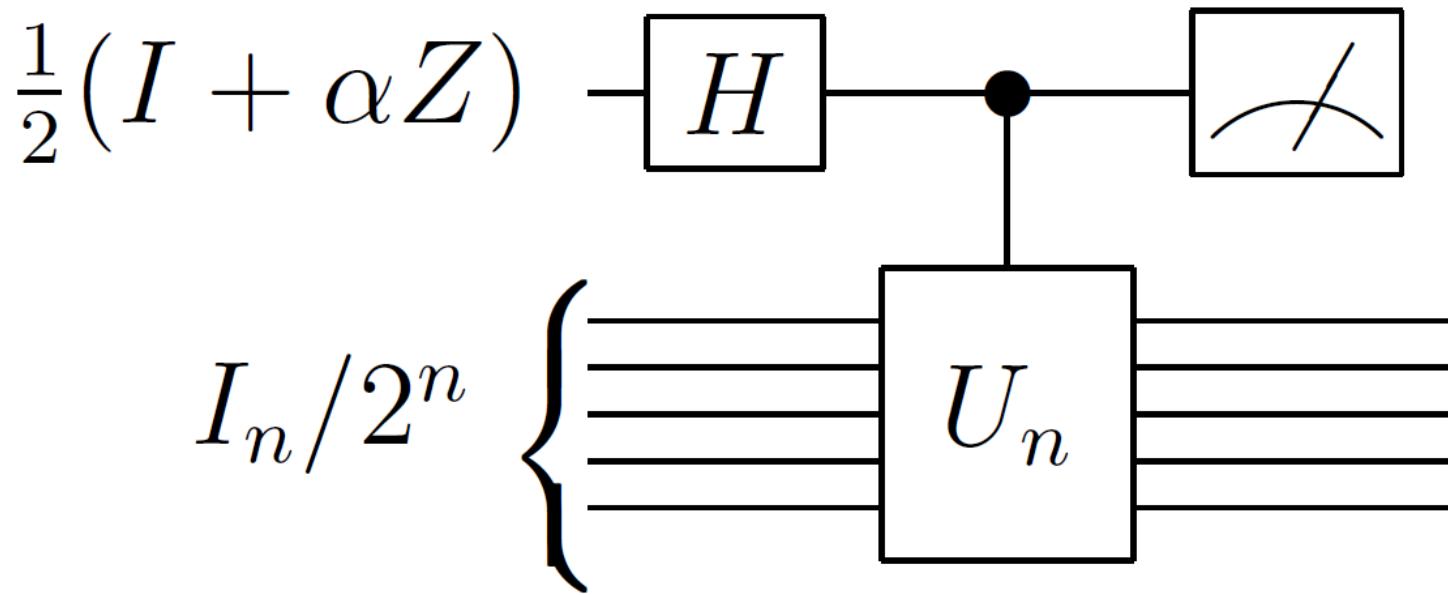
$$T \leq T_E = \frac{\hbar\omega_0}{k \ln(1 + \sqrt{2})}$$

$$\omega_0 = 2\pi \cdot 500 \times 10^6 \text{ s}^{-1}, \quad T_E = 27 \text{ mK.}$$

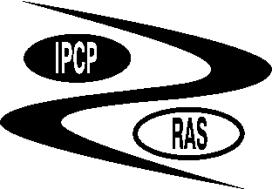
$$T < T_E = \frac{\hbar\omega_0}{k \ln\left(\frac{\sqrt{2+a}}{2-\sqrt{2+a}}\right)} \quad a = e^{\tau/T_{MQ}} - 1$$



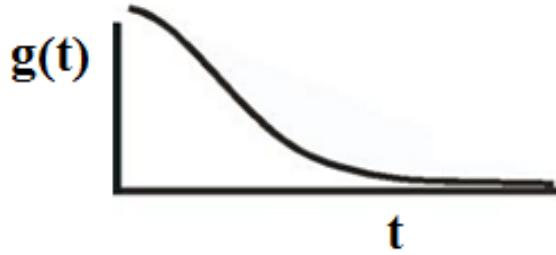
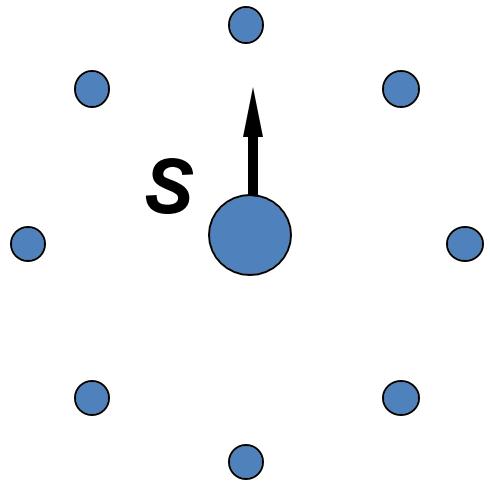
The DQC1 algorithm for computing the trace of a unitary operator



Datta et al., Phys. Rev. Lett. 100, 050502 (2008)



Quantum calculations with a free induction decay in electron-nuclear system

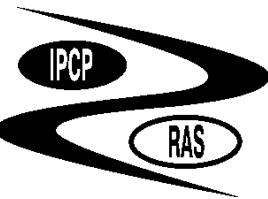


$$H = \hat{S}_z \hat{B} + \omega_0 \hat{S}_z$$

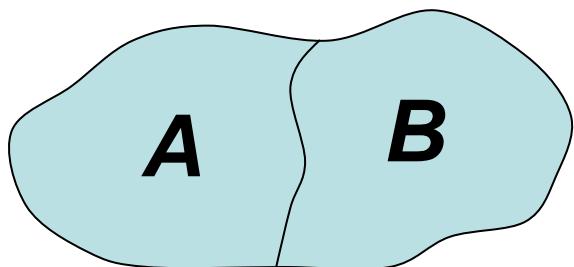
$$\hat{B} = \sum \left(A_{jz} \hat{I}_{jz} + A_{jy} \hat{I}_{jy} + A_{jx} \hat{I}_{jx} \right)$$

$$U(t) = \exp \left\{ -i \hat{B} t \right\}$$

$$g(t) = \frac{\text{Tr} \left\{ U(t) S^+ U^+(t) S^- \right\}}{\text{Tr} \left\{ S^+ S^- \right\}} = \text{Tr} \left\{ U(t) \right\} = \sum_{k=1}^{2^N} e^{-i \lambda_k t}$$

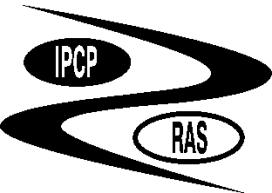


Mutual information and correlations



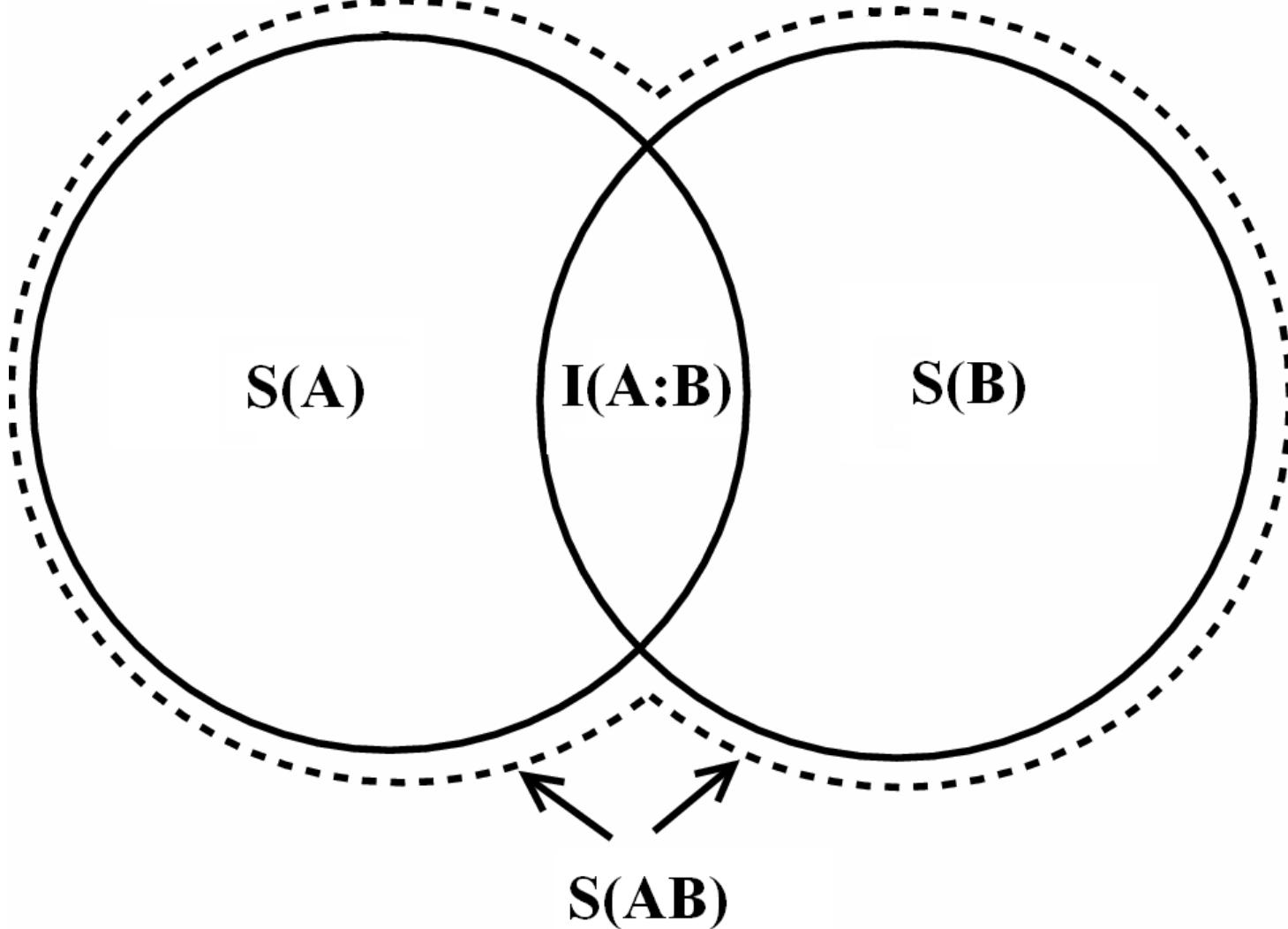
$$I(A : B) = S(A) + S(B) - S(AB)$$

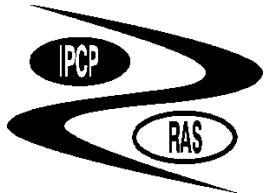
**Mutual information is a measure of total correlations
in the system**



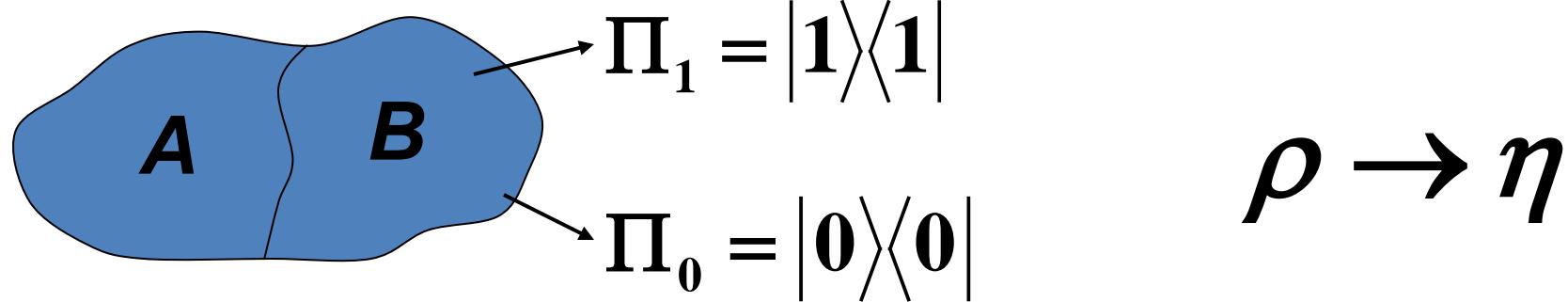
Mutual information

$$I(A : B) = S(A) + S(B) - S(AB)$$





Quantum and classical correlations, quantum discord



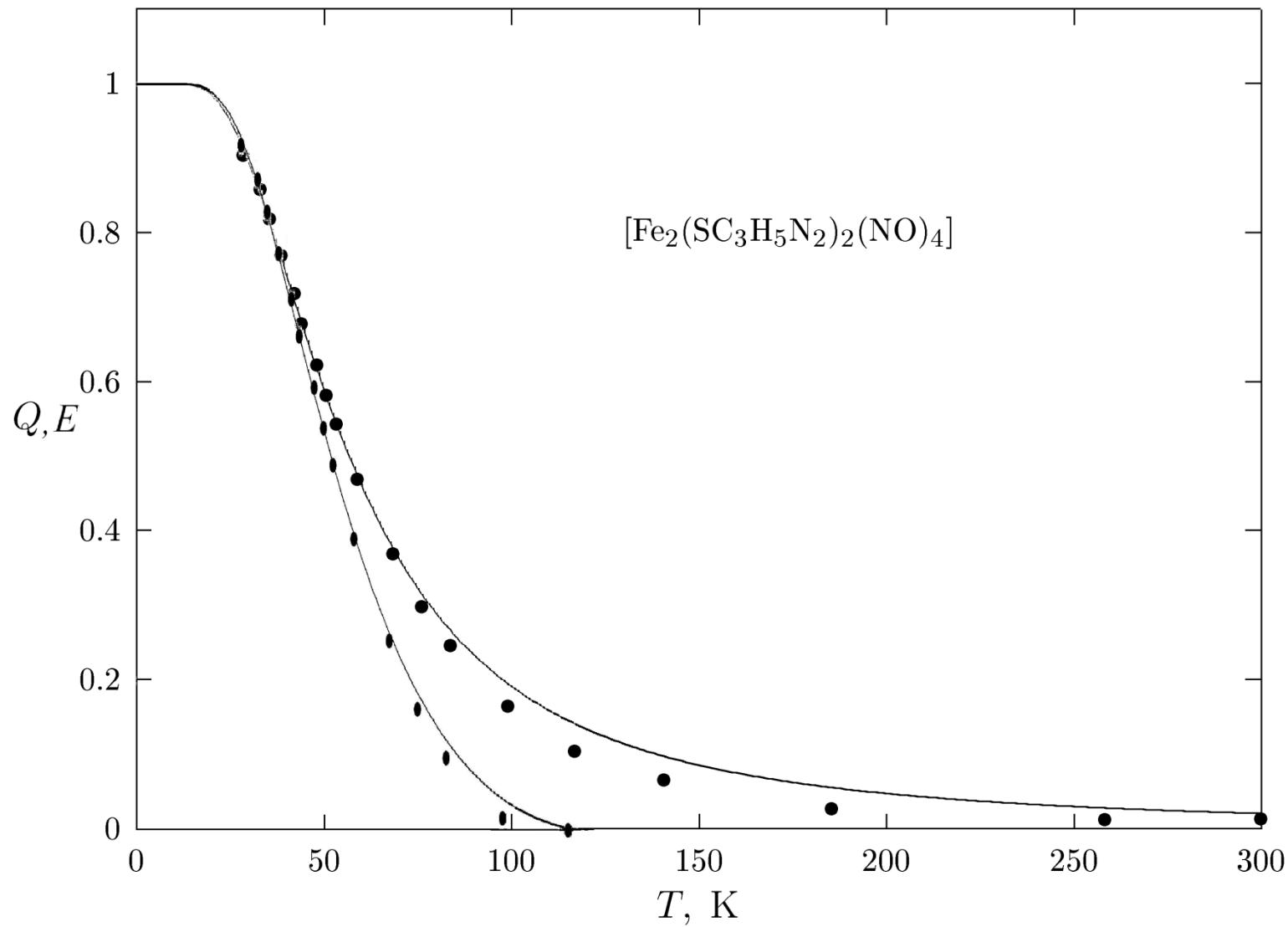
$$K(\rho) = \max_{\{\Pi_j^B\}} I(\eta)$$

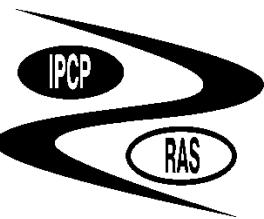
Quantum discord:

$$D(\rho) = I(\rho) - K(\rho)$$

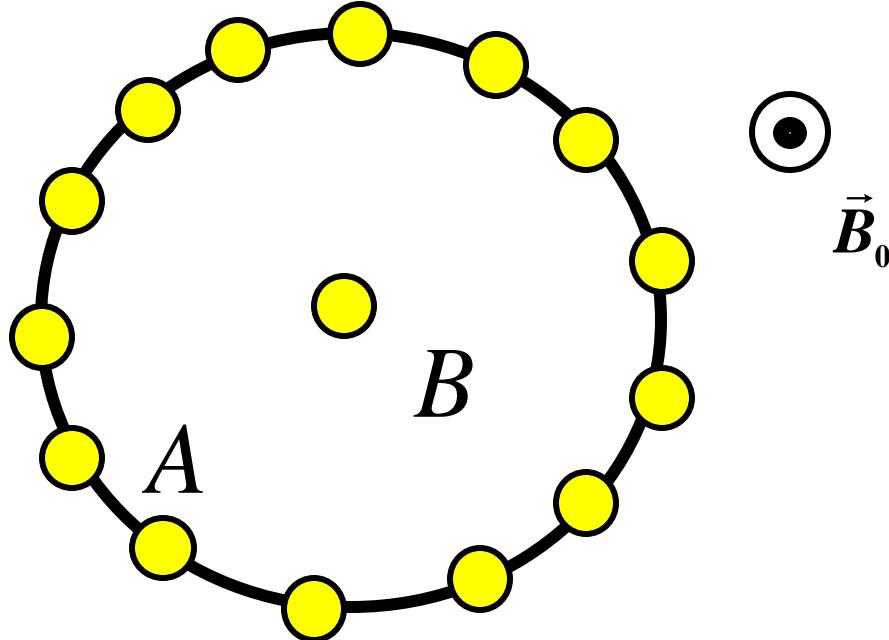


Entanglement and quantum discord in nitrosyl iron complexes





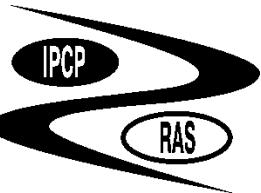
The spin model for an investigation of the quantum correlation (ring model)



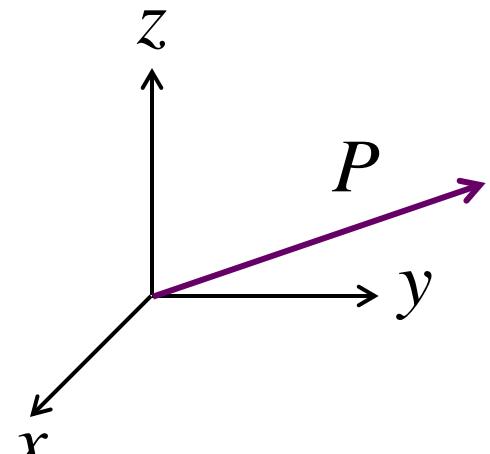
$$H_{dz} = \sum_{i < j} d_{ij} \left(3I_{iz}I_{jz} - \vec{I}_i \cdot \vec{I}_j \right)$$

$$H_{zz} = g \sum_i I_{iz} S_z = g I_z S_z \quad [H_{dz}, H_{zz}] = 0$$

S.I. Doronin, E.B. Fel'dman, E.I. Kuznetsova,
Physica Scripta **90**, 074016 (2015)



A spin approach to calculations of the quantum discord

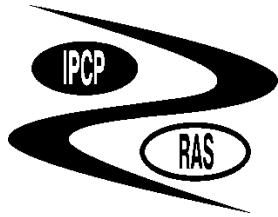


$$P_0 = \frac{1}{2} + (n_x S_x + n_y S_y + n_z S_z)$$

$$P_1 = \frac{1}{2} - (n_x S_x + n_y S_y + n_z S_z)$$

$$P_k^2 = P_k, \quad k = 0,1.$$

$$P_k S_\alpha P_k = \frac{(-1)^k}{2} n_\alpha P_k, \quad \alpha = x, y, z; \quad k = 0,1.$$

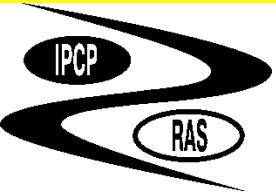


Conditional entropy and discord

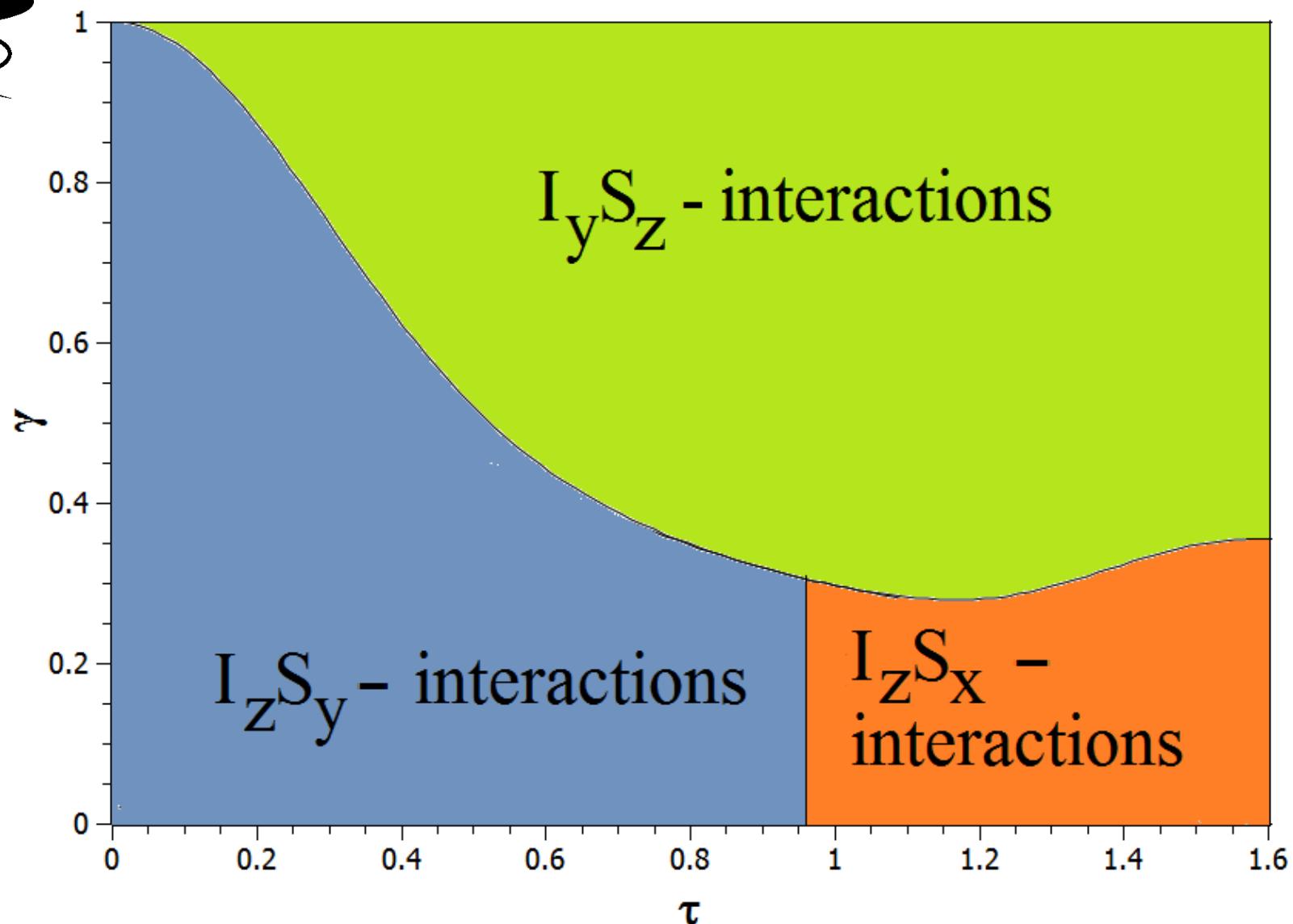
$$\begin{aligned}
 S_{cond} = & -\frac{1}{2 \ln 2} \left\{ n_x^2 \left[u^2 \frac{1+\cos^{N-1}(2\tau)-2\cos^{2(N-1)}(\tau)}{2} \right. \right. \\
 & - (N-1)v^2 \sin^2(\tau) \Big] + n_y^2 \left[u^2 \frac{1-\cos^{N-1}(2\tau)}{2} \right. \\
 & \left. \left. - (N-1)v^2 \sin^2(\tau) \right] + a(u, v) \right\}
 \end{aligned}$$

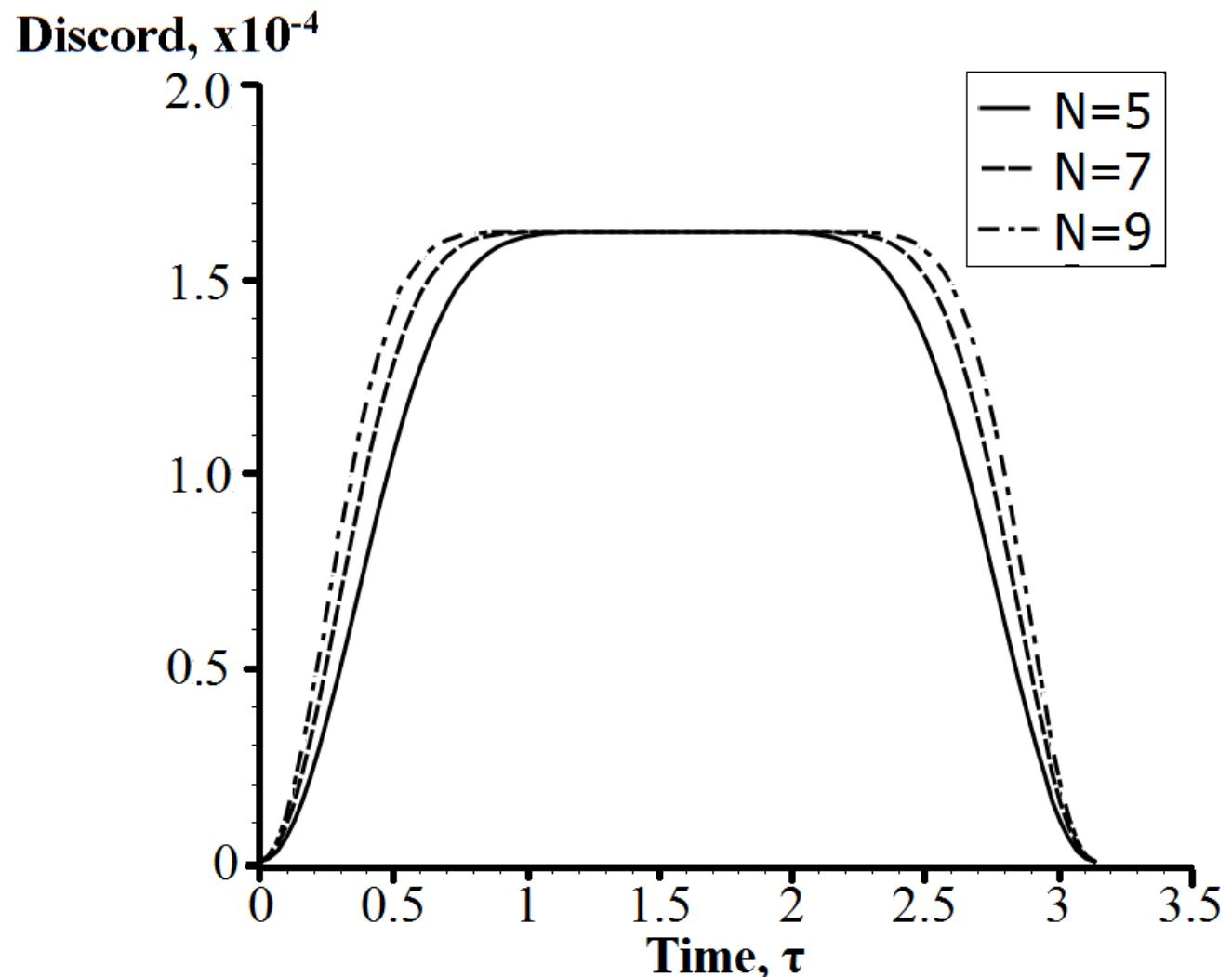
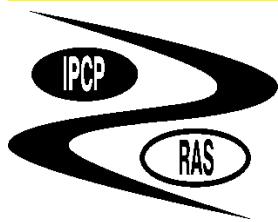
$$u = \frac{1}{2}(N-1)\beta\omega_B < 1, \quad v = \frac{1}{2}(N-1)\beta\omega_A < 1 \quad n_{x,y} \in [-1,1]$$

$$\frac{v}{u} = \frac{\omega_A}{\omega_B} > 1 : \quad D = \frac{\beta^2 \omega_B^2}{8 \ln 2} \left(1 - \cos^{2(N-1)}(\tau) \right)$$

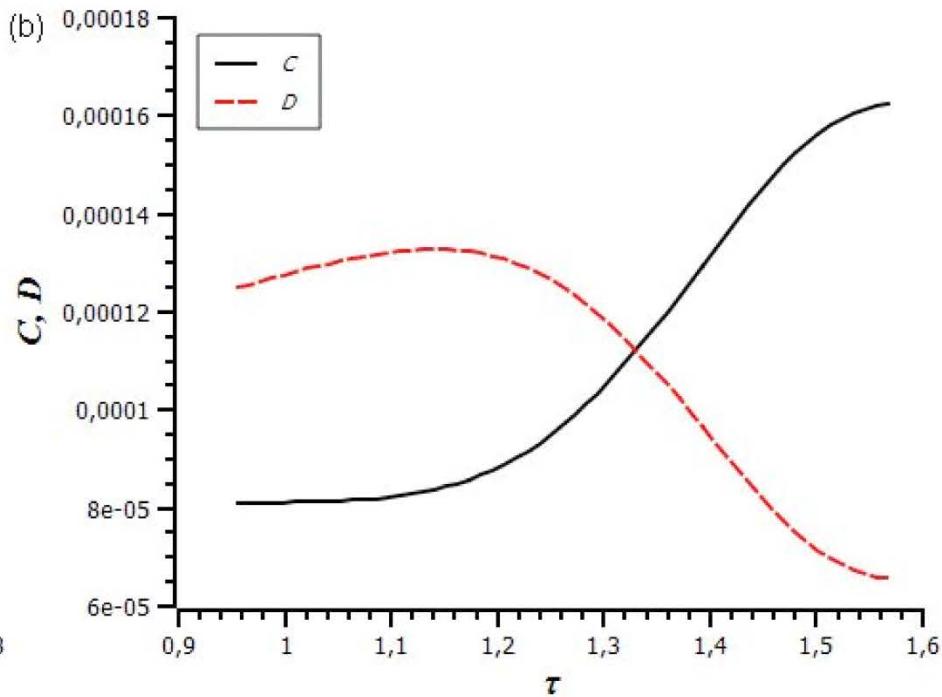
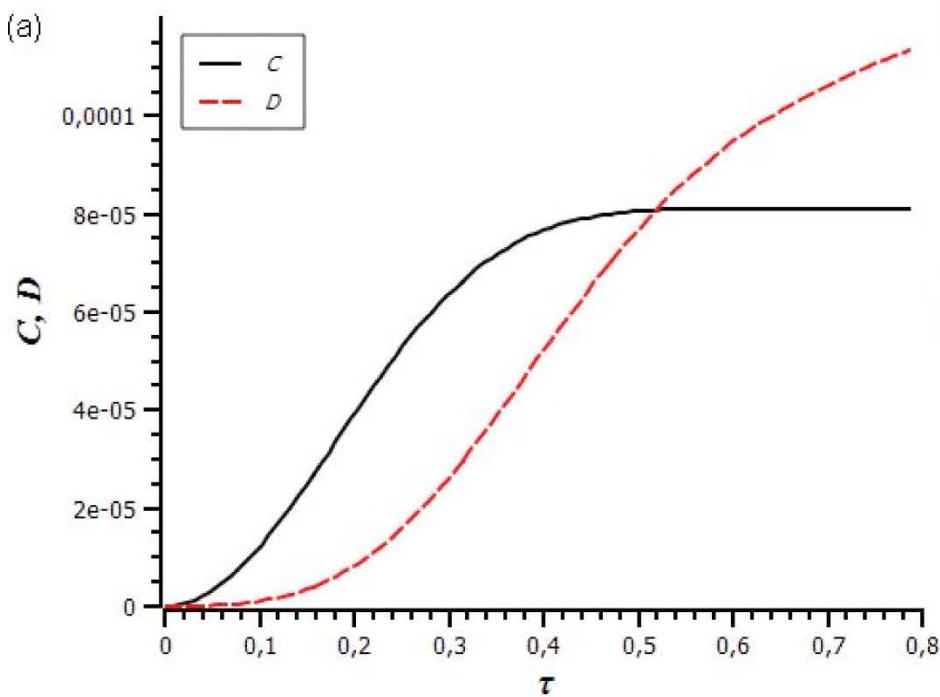
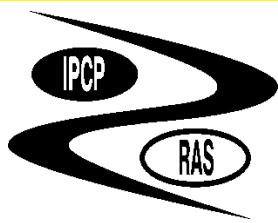


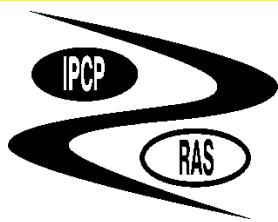
N=9





$$u = 0.015, \quad n_x = n_y = 0, \quad |n_z| = 1.$$





Entanglement in a two-spin system in the multi-pulse spin locking

The initial density matrix:

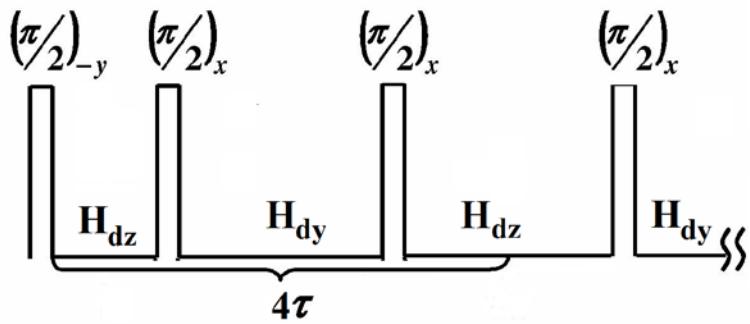
$$\rho = \frac{1}{Z} e^{\beta I_x}, \quad \beta = \frac{\hbar \omega_0}{kT}, \quad Z = 4 \cos^2 \frac{\beta}{2}.$$

$$U(4\tau) = e^{-i\tau H_{dz}} e^{-i2\tau H_{dy}} e^{-i\tau H_{dz}}$$

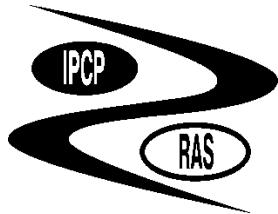
$$U(4\tau) = \frac{1}{2} \begin{pmatrix} e^{-2it} + e^{it} & 0 & 0 & -e^{-2it} + e^{it} \\ 0 & 1 + e^{it} & e^{it} - 1 & 0 \\ 0 & e^{it} - 1 & 1 + e^{it} & 0 \\ -e^{-2it} + e^{it} & 0 & 0 & e^{-2it} + e^{it} \end{pmatrix}$$

$(U(4\tau))$ – centrosymmetric matrix

$t = \tau d_{12}$, dimensionless time)



$$G = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 \end{pmatrix}$$



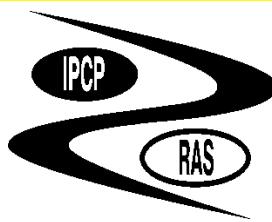
Entanglement is absent in the multi-pulse spin-locking at $\varphi=\pi/2$

$$\rho(4M\tau) = U(4M\tau)\rho_0U(4M\tau)$$

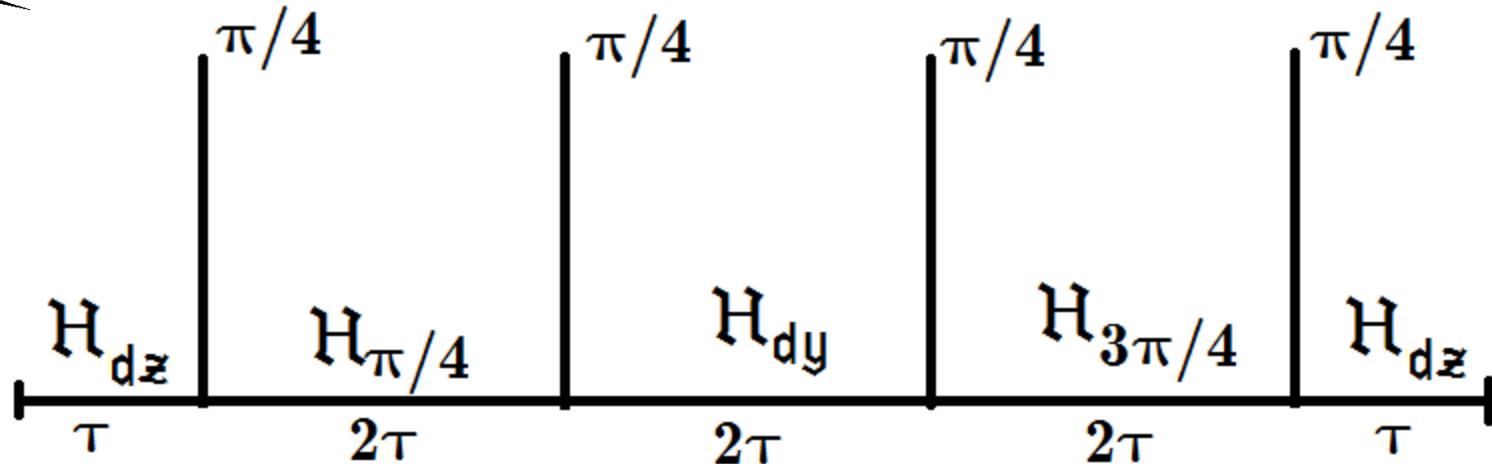
$(M$ is integer)

$$= \frac{1}{8\operatorname{ch}^2 \frac{\beta}{2}} \begin{pmatrix} 2\operatorname{ch}^2 \frac{\beta}{2} & \operatorname{sh} \frac{\beta}{2} & \operatorname{sh} \frac{\beta}{2} & 2\operatorname{sh}^2 \frac{\beta}{2} \\ \operatorname{sh} \frac{\beta}{2} & 2\operatorname{ch}^2 \frac{\beta}{2} & 2\operatorname{sh}^2 \frac{\beta}{2} & \operatorname{sh} \frac{\beta}{2} \\ \operatorname{sh} \frac{\beta}{2} & 2\operatorname{sh}^2 \frac{\beta}{2} & 2\operatorname{ch}^2 \frac{\beta}{2} & \operatorname{sh} \frac{\beta}{2} \\ 2\operatorname{sh}^2 \frac{\beta}{2} & \operatorname{sh} \frac{\beta}{2} & \operatorname{sh} \frac{\beta}{2} & 2\operatorname{ch}^2 \frac{\beta}{2} \end{pmatrix} = \rho_0$$

$$H = -\frac{1}{2} H_{dx}$$

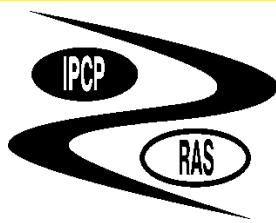


Entanglement in the multi-pulse locking at $\varphi=\pi/4$

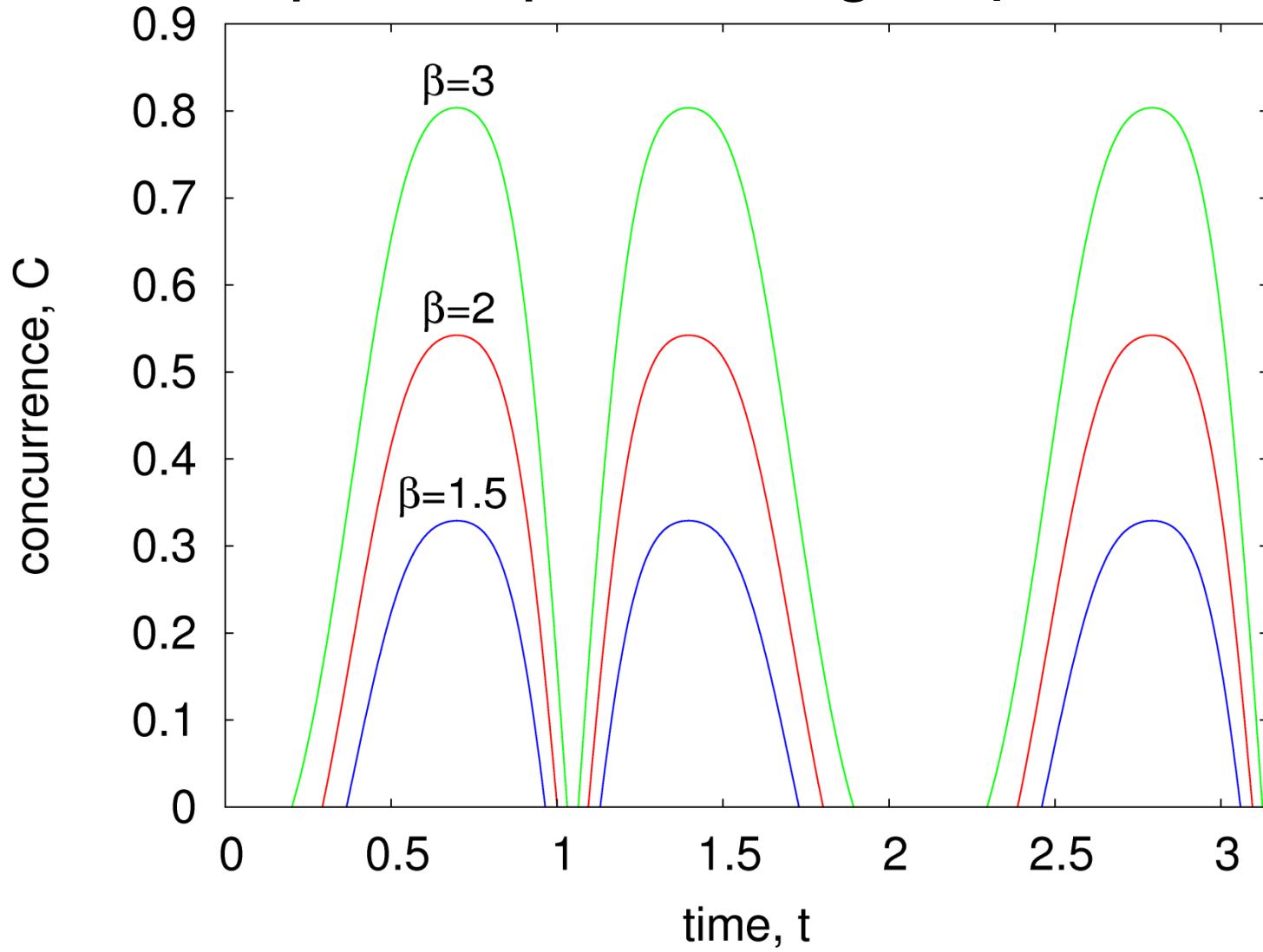


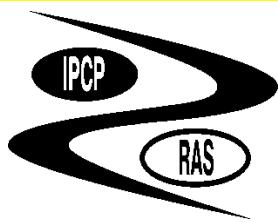
$$H_{\pi/4} = d_{12} e^{i\pi I_x/4} \left(3I_{1z}I_{2z} - \vec{I}_1 \vec{I}_2 \right) e^{-i\pi I_x/4} = \frac{d_{12}}{8} \begin{pmatrix} 1 & -3i & -3i & -3 \\ 3i & -1 & -1 & 3i \\ 3i & -1 & -1 & 3i \\ -3 & -3i & -3i & 1 \end{pmatrix}, \quad [H_{dz}, H_{\pi/4}] \neq 0,$$

$$H_{3\pi/4} = d_{12} e^{i3\pi I_x/4} \left(3I_{1z}I_{2z} - \vec{I}_1 \vec{I}_2 \right) e^{-i3\pi I_x/4} = \frac{d_{12}}{8} \begin{pmatrix} 1 & 3i & 3i & -3 \\ -3i & -1 & -1 & -3i \\ -3i & -1 & -1 & -3i \\ -3 & 3i & 3i & 1 \end{pmatrix} \quad [H_{dz}, H_{3\pi/4}] \neq 0.$$

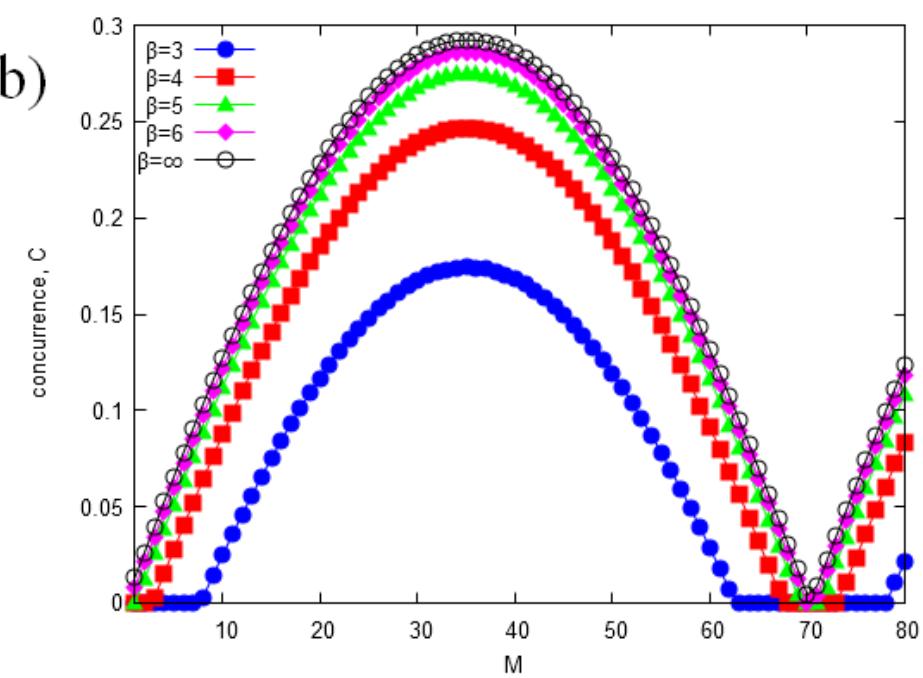
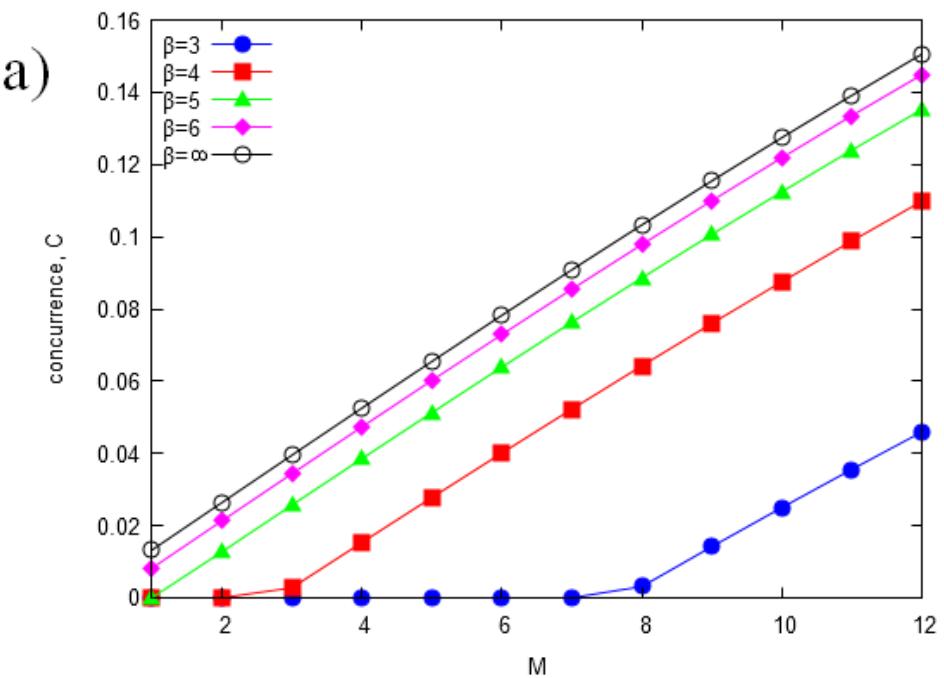


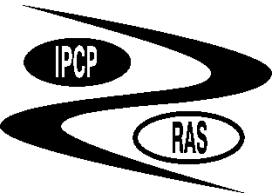
Entanglement in a two-spin system in the multi-pulse spin locking at $\varphi=\pi/4$





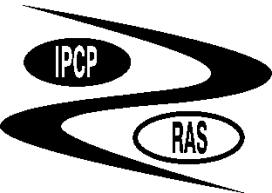
The dependence of entanglement on time in the multi-pulse spin locking





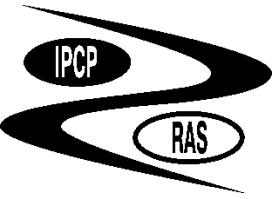
CONCLUSIONS

- 1. Entanglement and the quantum discord are considered as the measures of quantum correlations.**
- 2. Quantum calculations in electron-nuclear systems are discussed.**
- 3. A comparison of the quantum discord and entanglement in the nitrosyl iron complexes is given.**
- 4. The ring spin model for an investigation of quantum correlations is supposed.**
- 5. The contributions of different parts of spin-spin interactions to quantum correlations are considered in the ring spin model.**
- 6. Quantum correlations are considered in multi-pulse spin locking experiments.**

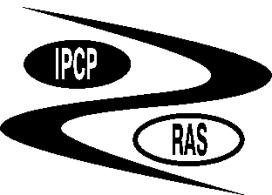


Laboratory of spin dynamics and spin computing





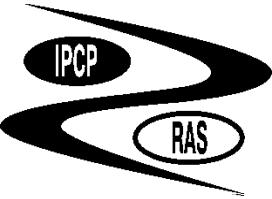
Thank you for
attention!



Entanglement

A two-qubit state is described by four complex numbers. A three-qubit state is described by eight complex numbers. An N qubit-state is described by 2^N complex numbers. A register, consisting of N qubits, is described by $2^{N+1} - 2$ real parameters.

If entanglement would not be in Nature then $2N$ real numbers were sufficient to describe a quantum register. For example, without entanglement, only 2000 parameters would be enough for a 1000 qubit register. However, the actual number of such parameters is more than 10^{300} when entanglement is taken into account. (We note for comparison that the number of protons and neutrons in the Universe is only of order 10^{78}).



Speedup of quantum algorithms and entanglement in pure states

$$|\alpha\rangle = \sum_{i_1, i_2, \dots, i_n} a_{i_1, i_2, \dots, i_n} |i_1\rangle |i_2\rangle \dots |i_n\rangle$$

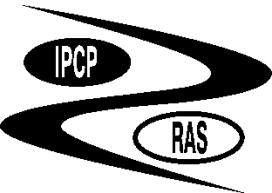
One-qubit gate U:

$$|\alpha\rangle \rightarrow |\alpha'\rangle = \sum_{i_1, i_2, \dots, i_n} a'_{i_1, i_2, \dots, i_n} |i_1\rangle |i_2\rangle \dots |i_n\rangle$$

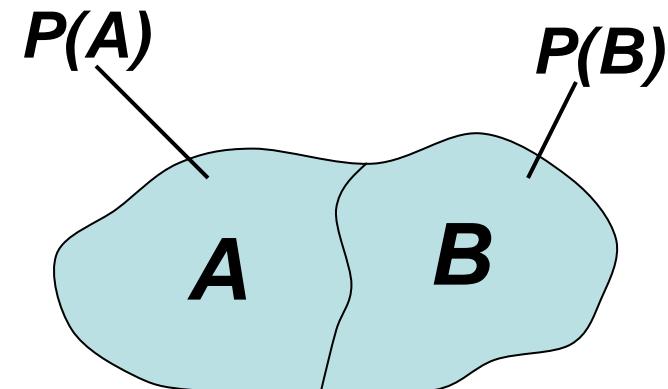
$$a'_{i_1, i_2, \dots, i_n} = \sum_{j_1} U_{i_1 j_1} a_{j_1, i_2, \dots, i_n}$$

Unentangled (separable) states:

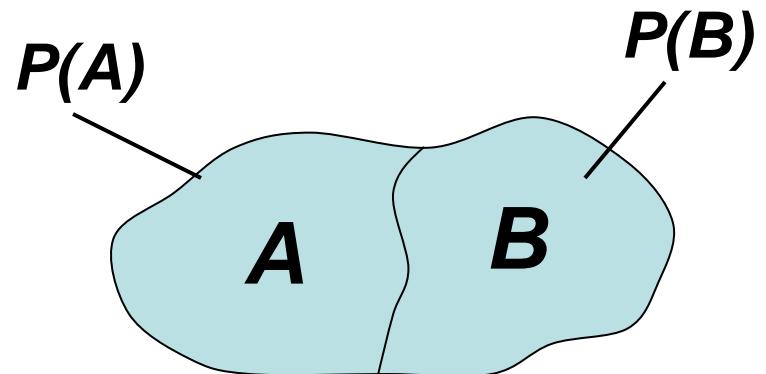
$$a_{j_1, i_2, \dots, i_n} = \alpha_{j_1} \alpha_{i_2} \dots \alpha_{i_n}$$



Correlations in two-partite systems



$$P(A, B) = P(A)P(B)$$



$$P(A, B) \neq P(A)P(B)$$

Correlation coefficient:

$$\rho_{A,B} = \frac{E[AB]}{\sqrt{E[A^2] \cdot E[B^2]}} \quad (E[A] = E[B] = 0)$$

If $P(A, B) = P(A)P(B)$ then $\rho_{A,B} = 0$. If $\rho_{A,B} = 0$, then the condition $P(A, B) = P(A)P(B)$ may not be satisfied.