אוניברסיטת בן-גוריון בנגב
Ben-Gurion University of the Negev

Entanglement in nuclear quadrupole resonance

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OUTLINE

1. Some history
2. Definition of entangled state
3. Entanglement of two dipolar coupling spins ½
4. Entanglement of a single spin 3/2
5. Conclusions

- Quantum entanglement is at the heart of the EPR paradox that was developed by Albert Einstein, Boris Podolsky, and Nathan Rosen in 1935.

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Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?

A. Einstein, B. Podolsky and N. Rosen, *Institute for Advanced Study, Princeton, New Jersey*

(Received March 25, 1935)

In a complete theory there is an element corresponding to each element of reality. A sufficient condition for the reality of a physical quantity is the possibility of predicting it with certainty, without disturbing the system. In quantum mechanics in the case of two physical quantities described by non-commuting operators, the knowledge of one precludes the knowledge of the other. Then either (1) the description of reality given by the wave function in quantum mechanics is not complete or (2) these two quantities cannot have simultaneous reality. Consideration of the problem of making predictions concerning a system on the basis of measurements made on another system that had previously interacted with it leads to the result that if (1) is false then (2) is also false. One is thus led to conclude that the description of reality as given by a wave function is not complete.

- In 1964 Bell published what for many has become the single most important theoretical paper in physics to appear since 1945; it was entitled *On the Einstein Podolsky Rosen Paradox*.
- In 1964,John Bell showed that the predictions of quantum mechanics in the EPR thought experiment are significantly different from the predictions of a very broad class of hidden variable theories (the local hidden variable theories).

III.5 ON THE EINSTEIN PODOLSKY ROSEN PARADOX*

JOHN S. BELL†

I. Introduction

THE paradox of Einstein, Podolsky and Rosen [1] was advanced as an argument that quantum mechanics could not be a complete theory but should be supplemented by additional variables. These additional variables were to restore to the theory causality and locality [2]. In this note that idea will be formulated mathematically and shown to be incompatible with the statistical predictions of quantum mechanics. It is the requirement of locality, or more precisely that the result of a measurement on one system be unaffected by operations on a distant system with which it has interacted in the past, that creates the essential difficulty. There have been attempts [3] to show that even without such a separability or locality requirement no "hidden variable" interpretation of quantum mechanics is possible. These attempts have been examined elsewhere [4] and found wanting. Moreover, a hidden variable interpretation of elementary quantum theory [5] has been explicitly constructed. That particular interpretation has indeed a grossly non-local structure. This is characteristic, according to the result to be proved here, of any such theory which reproduces exactly the quantum mechanical predictions.

Originally published in *Physics*, *1*, 195-200 (1964).

Definition of entangled state

A pure state of a pair of quantum systems is called entangled if it is unfactorizable.

Applications :

- Quantum information and quantum computer (entanglement of qubits)
- Condensed matter physics (search for new order parameters)

Divide a given quantum system into two parts A and B.

Then the total Hilbert space becomes factorized

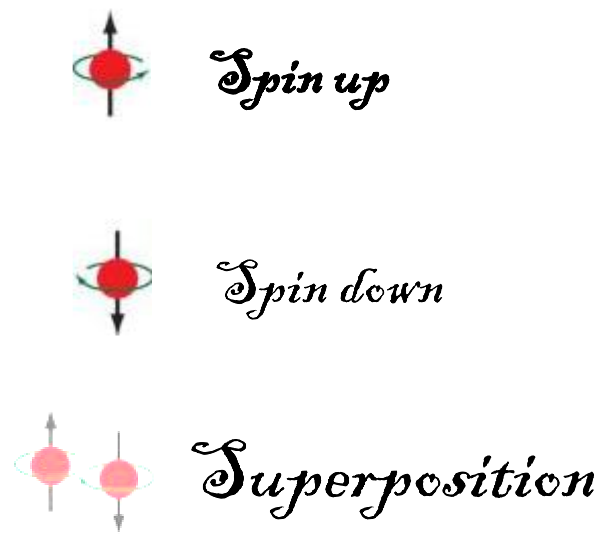
$$H_{total}=H_A \times H_B$$

Entanglement is a property of a state, not of Hamiltonian.

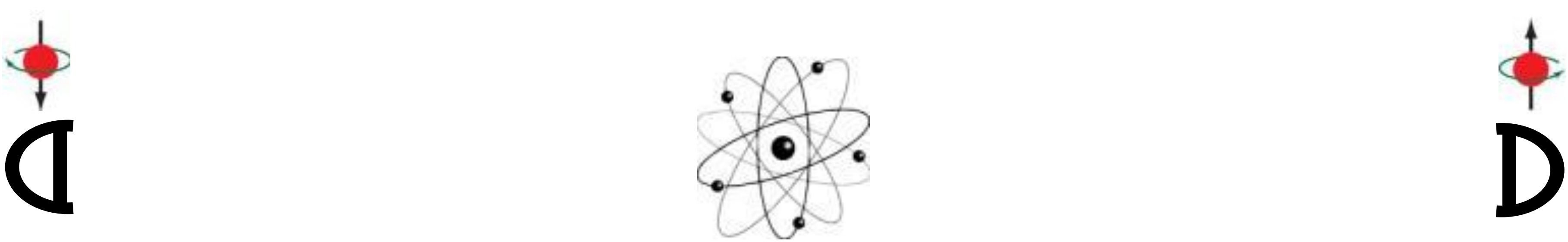
Non-separable quantum state (entangled state):

$$\rho_{total} \neq \rho_A \quad \rho_B$$

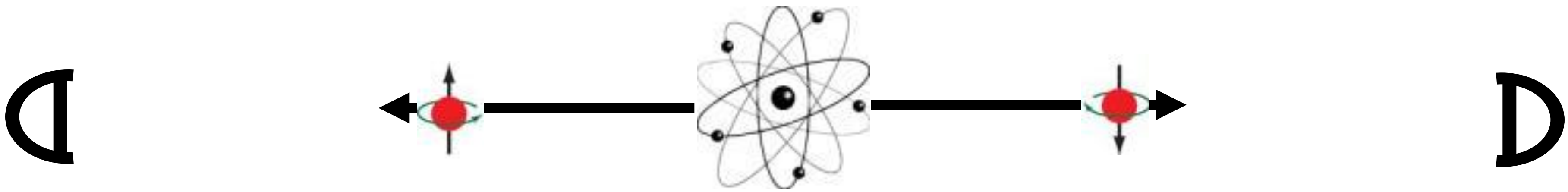
Superposition



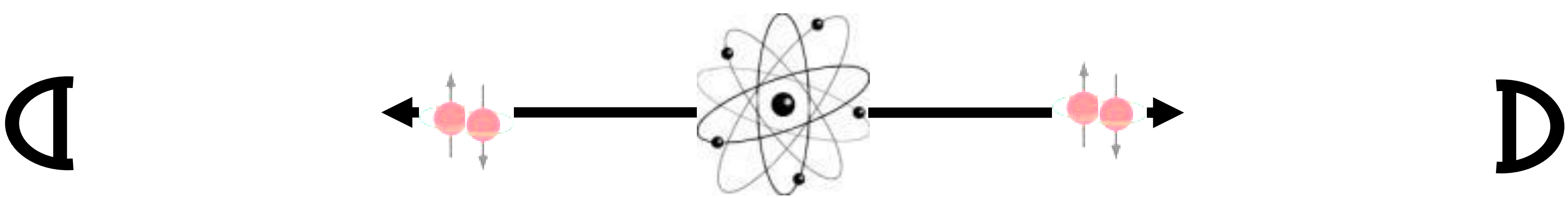
- Superposition = Action at a distance
- Action at a distance   Contradiction with relativity!



If the particles have predefined values – there is no "telepathy" and everything is fine

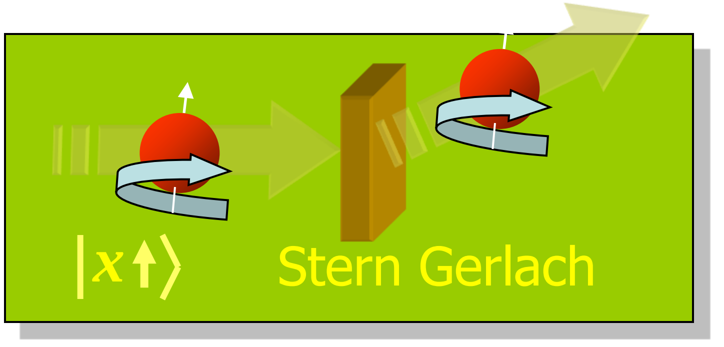


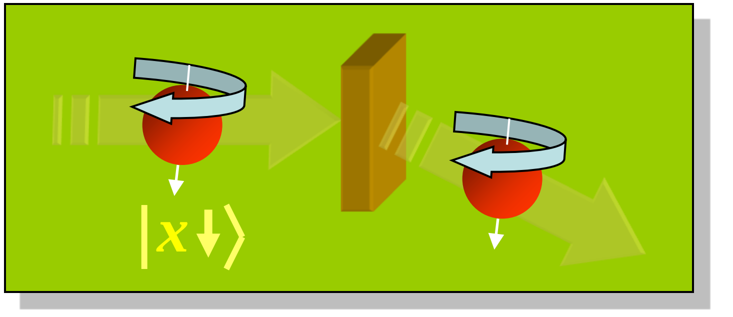
If the particles go off in superposition - has "telepathy" in conflict with relativity



EPR experiment

Spin



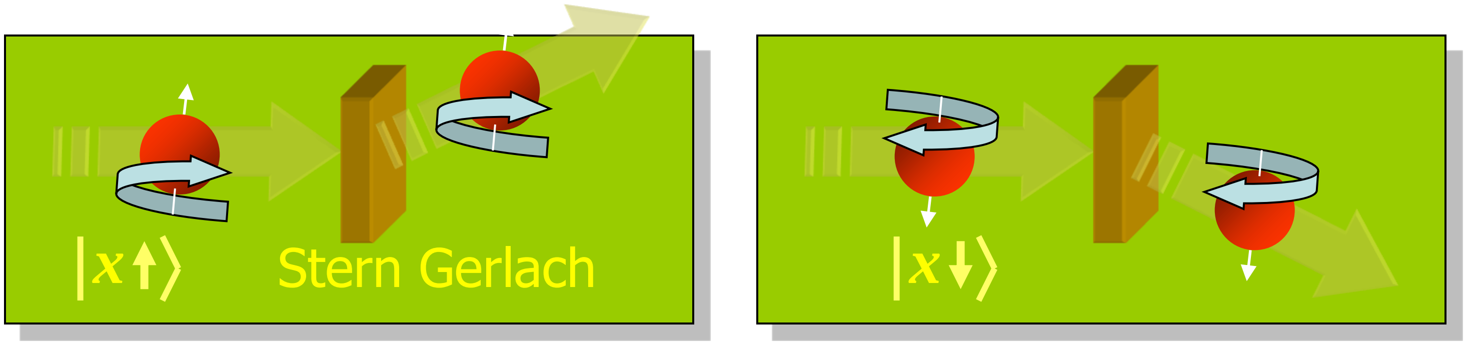


P_{up}=1/2

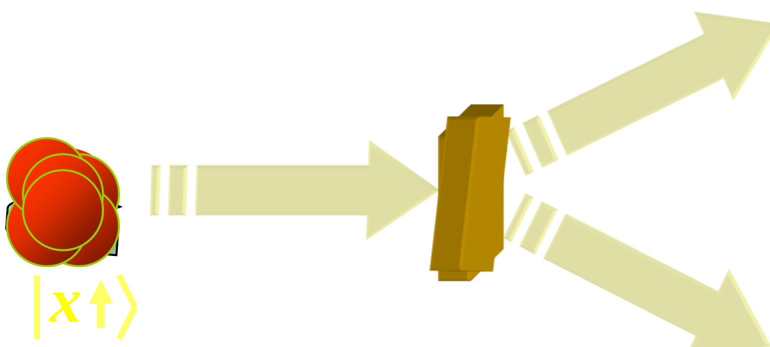
P_{donw}=1/2

EPR experiment

Spin



Turning the magnets by an angle α

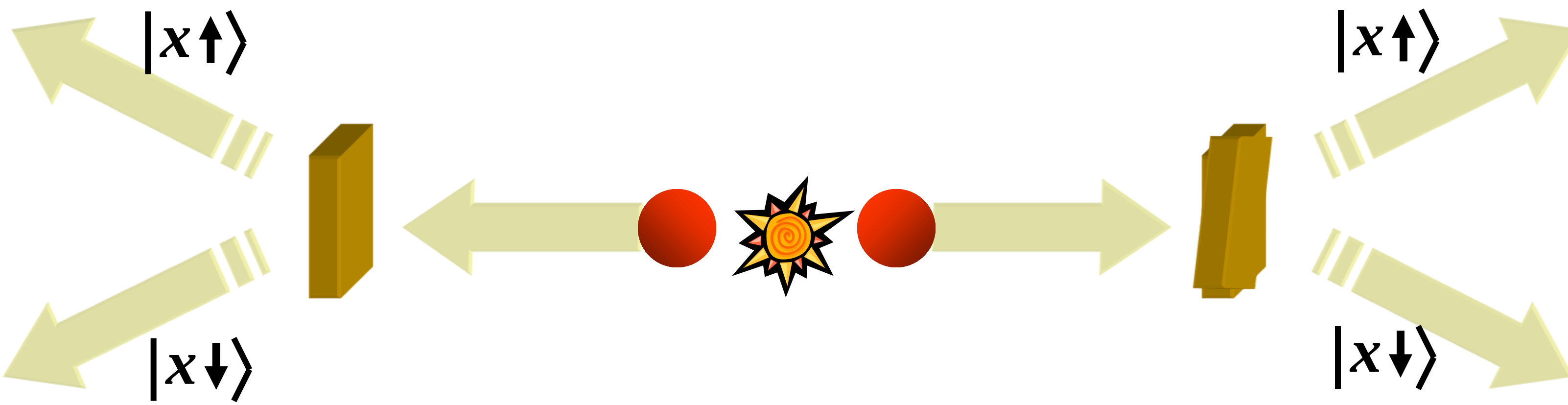


$\boldsymbol{P} = \mathrm{Cos}^2(2\alpha)$

$\boldsymbol{P} = 1-\mathrm{Cos}^2(2\alpha)$

EPR experiment

EPR system



- The two particles' spin is **always** correlated (opposite)

Measure of Entanglement

- Two particles of spin 1/2

Density matrix ρ_{AB}

$$\tilde{\rho}_{AB} = (\sigma_y \otimes \sigma_y)\rho^*_{AB}(\sigma_y \otimes \sigma_y)$$

$$M = \rho_{AB}\tilde{\rho}_{AB}$$

$$M\lambda'_j = m\lambda'_j \qquad \lambda_i = \lambda'^{\,2}_i$$

- Pauli matrix

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

- Concurrence – measure of entanglement

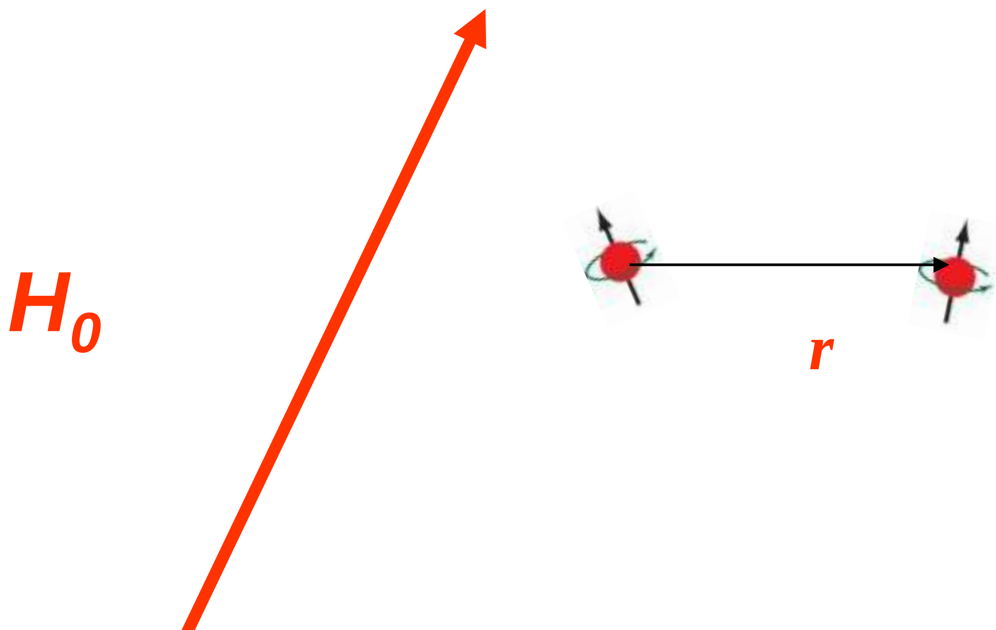
$$C_{AB} = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}$$

W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998)

Measure of Entanglement

For the maximally entangled states, the concurrence is C=1, while for the separable states C=0.

Dipolar coupling spin system and concurrence between nuclear spins 1/2



θ and φ are the spherical coordinates of the vector ***r*** connecting the nuclei in a coordinate system with the ***z***-axis along the external magnetic field, H_0

Hamiltonian of dipolar coupling spin system

$$H=H_z+H_{dd}$$

where the Hamiltonian H_z *describes the Zeeman interaction between the nuclear spins and external magnetic field and* H_{dd} *is the Hamiltonian of dipolar interactions*

In the thermodynamic equilibrium the considered system is described by the density matrix

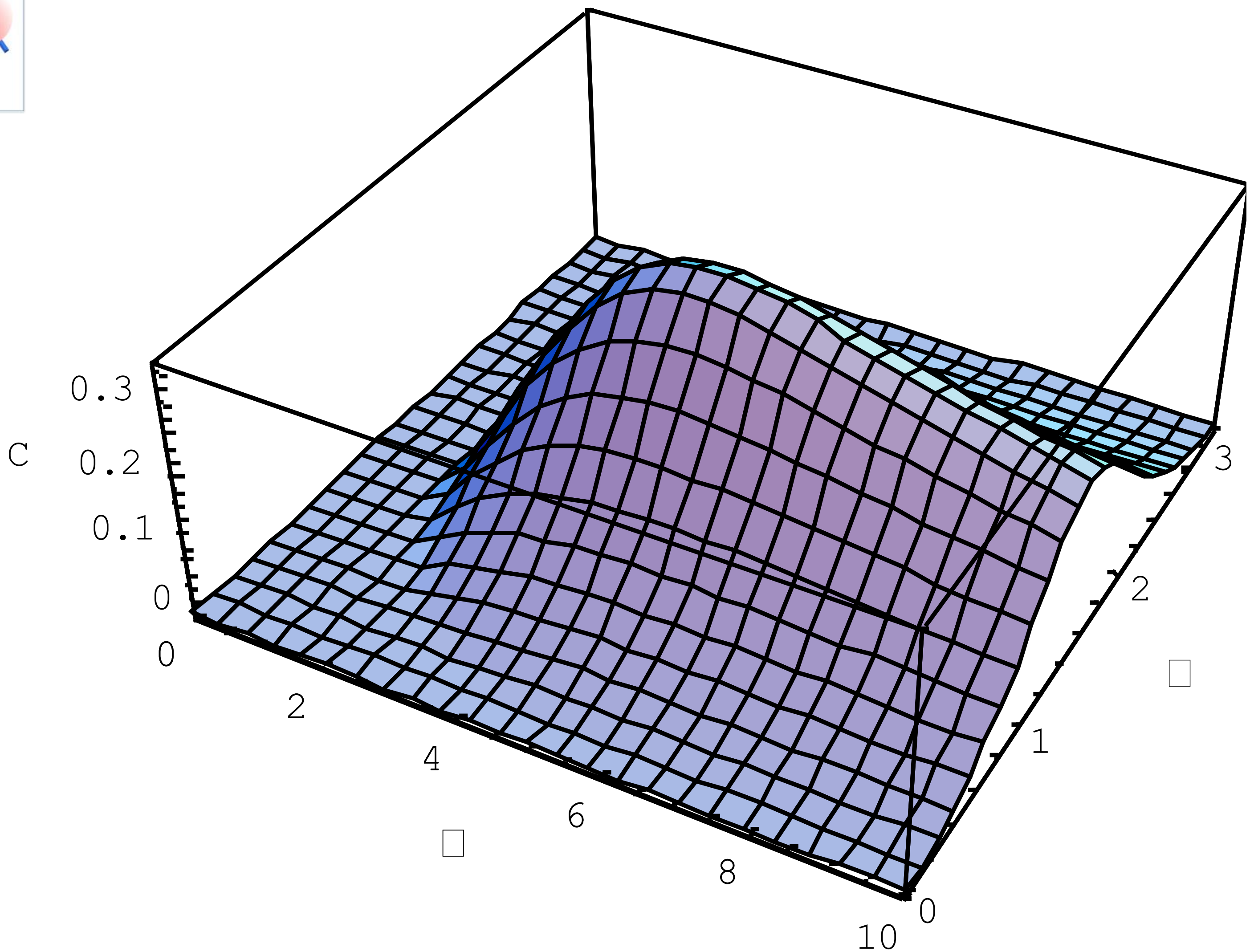
$$\rho = \exp(-H/k_B T)/Z$$

where Z is the partial function, k_B is the Boltzmann constant, and T is the temperature.

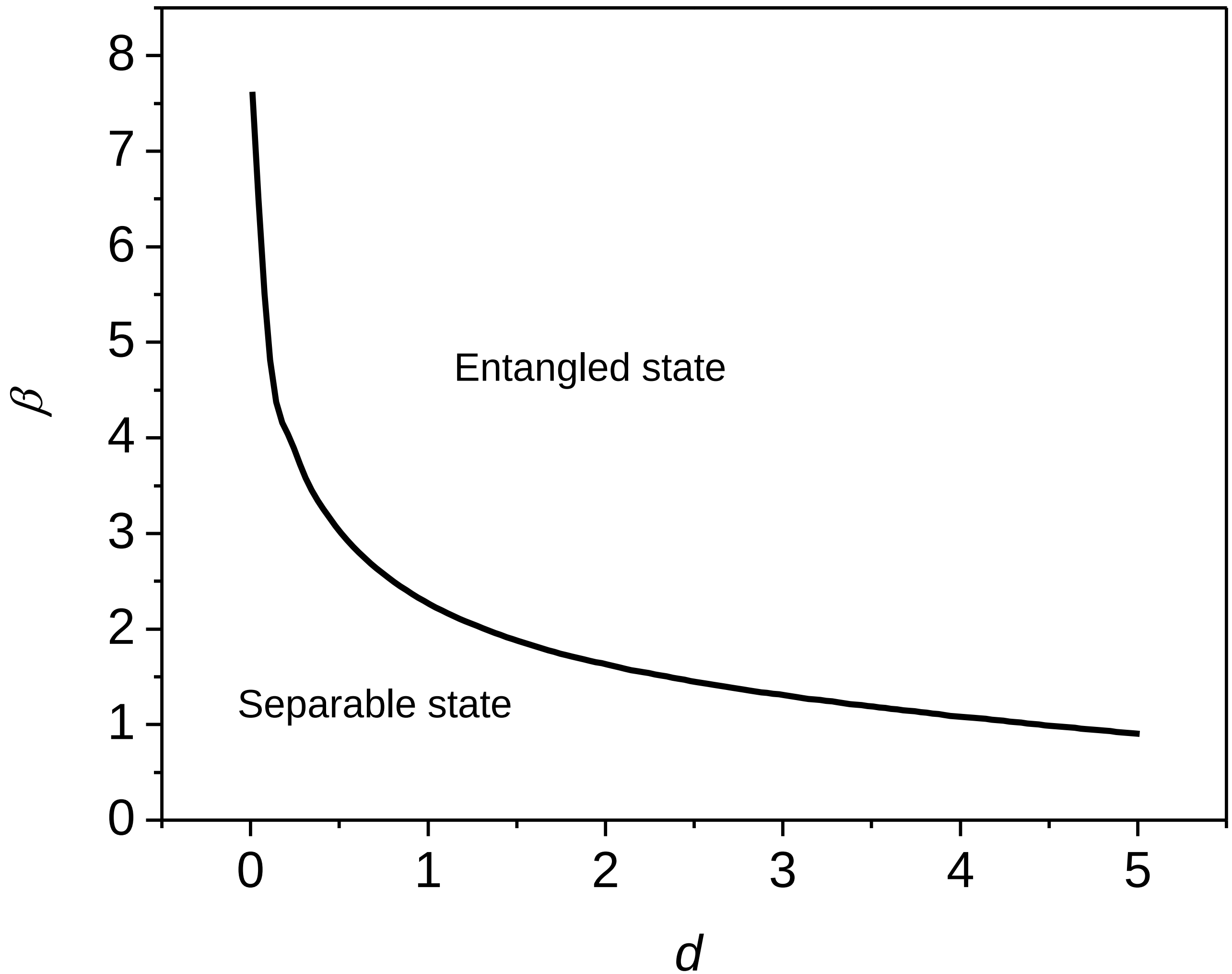
Entanglement in system of two dipolar coupling spins (concurrence between nuclear spins ½)

We examine dependence of the concurrence, ***C***, between states of the two spins ***1/2*** on the magnetic field strength and its direction, dipolar coupling constant, and temperature. The results of the numerical calculation show that concurrence reaches its maximum at the case of $\theta=\pi/2$ and $\phi=0$ and we will consider this case below.

G. B. Furman, V. M. Meerovich, and V. L. Sokolovsky,
Quantum Inf. Process. 9, 283 (2010).

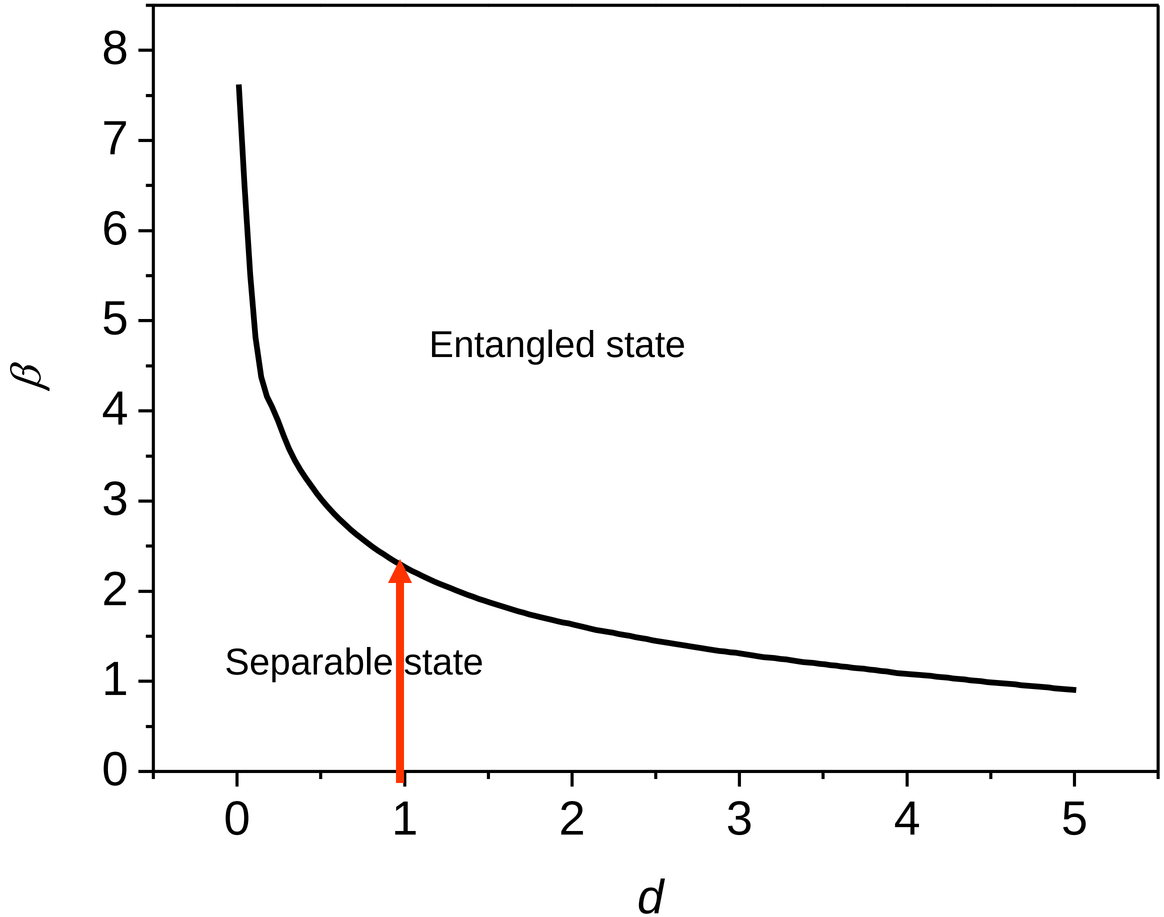


Concurrence as a function of the parameter $\beta=\omega_0/k_B T$ and magnetic field direction at $\phi=0$



The phase diagram. Line presents boundary between the entangled and separated states in the plane ***β-d***.

at *d=1* entanglement can be achieved at *β>2.26*.

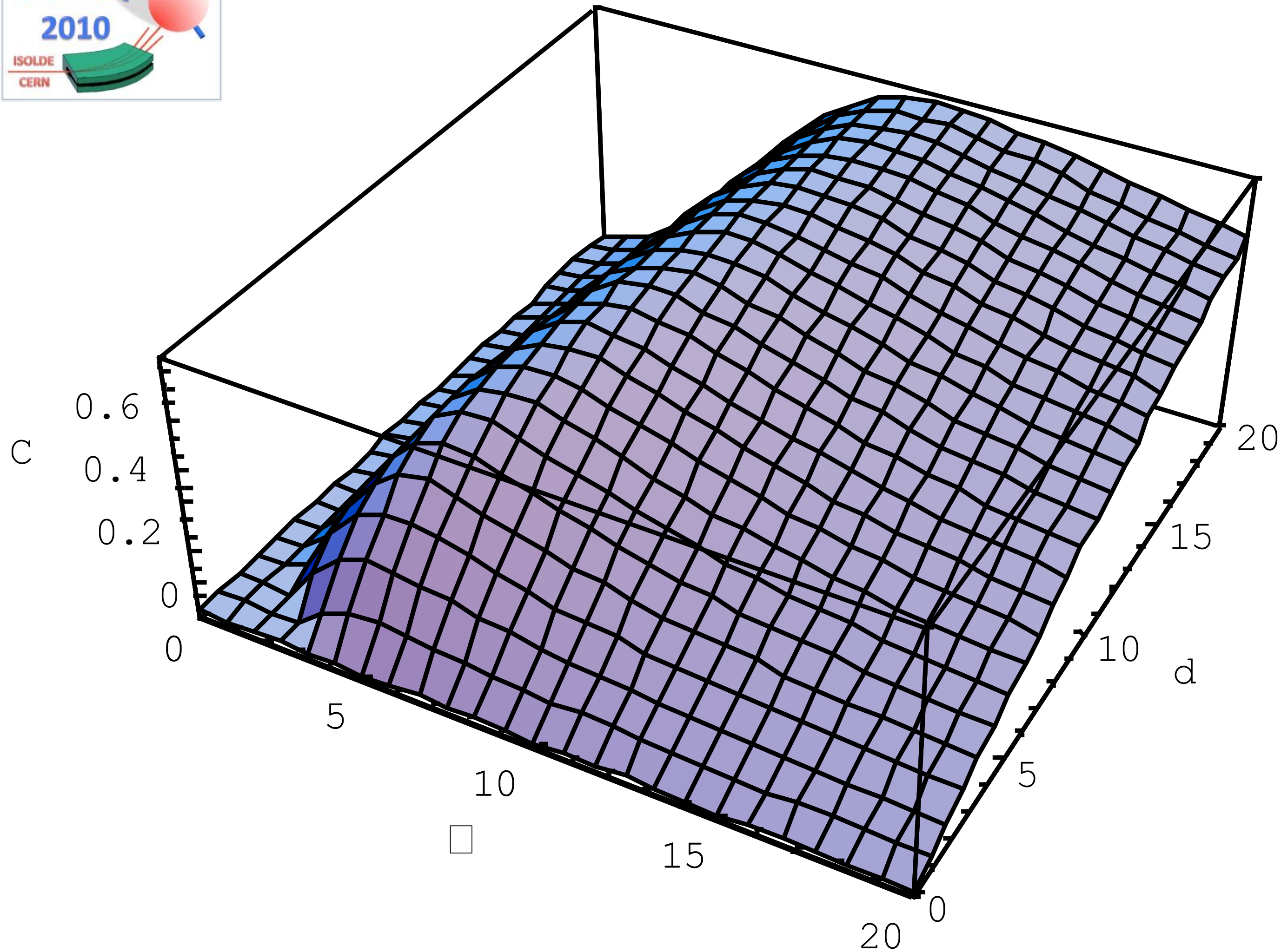


The phase diagram. Line presents boundary between the entangled and separated states in the plane ***β-d***.

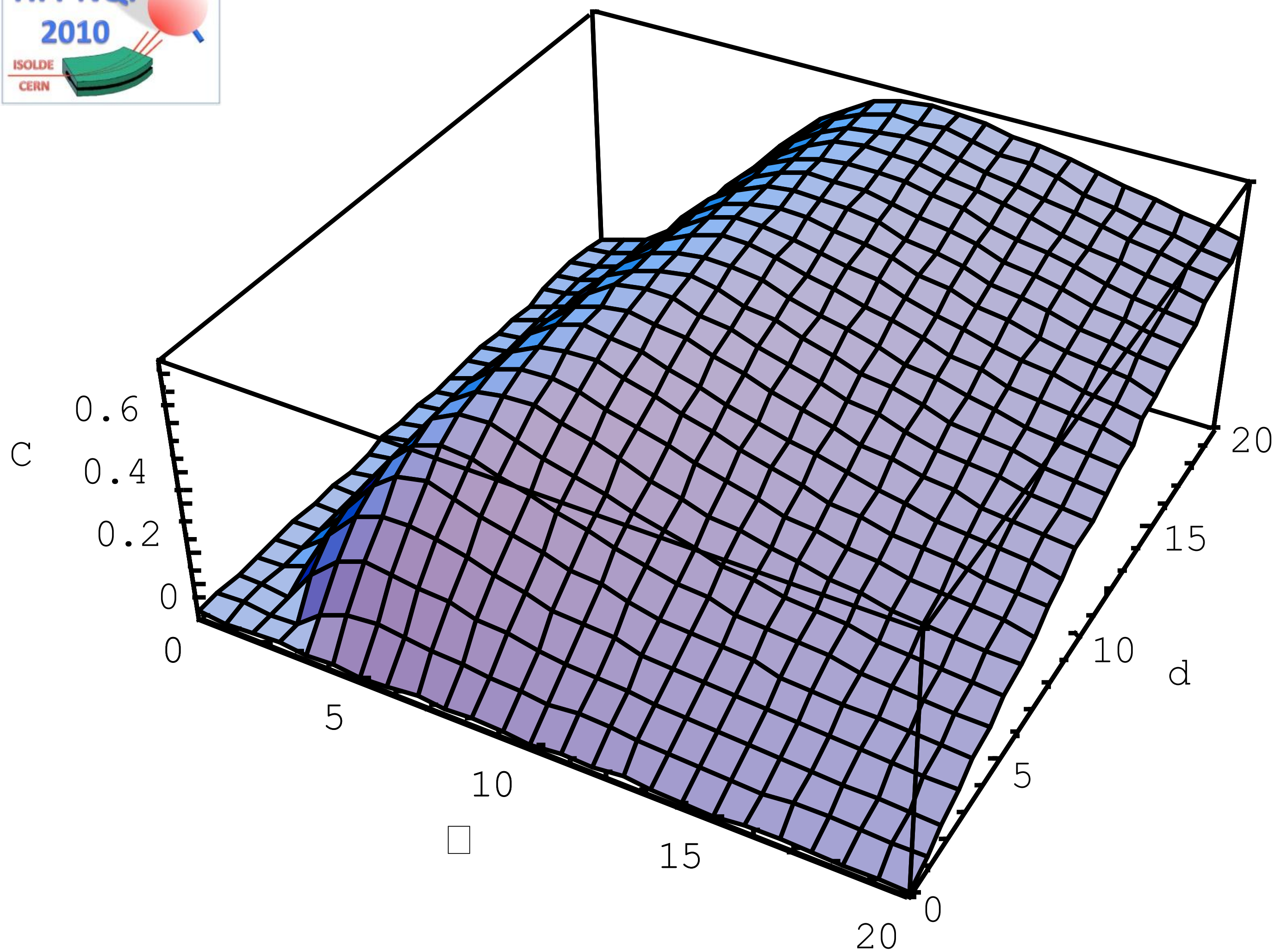
Let us consider fluorine with ***γ= 4. 0025kHz/G*** and the dipolar interaction energy typically of order of a few kHz. Taking ***H_0= 3 G*** we have ***ω_0=12 kHz***, which leads to ***Tc=0.33 μK***

It is interesting that the ordered states, such as antiferromagnetic, of nuclear spins were observed in a calcium-fluoride ***CaF_2*** single crystal at ***T= 0.34 μK***

M. Goldman, M. Chapellier, Vu Hoang Chau, and A. Abragam , Phys. Rev. B 10, 226 (1974).

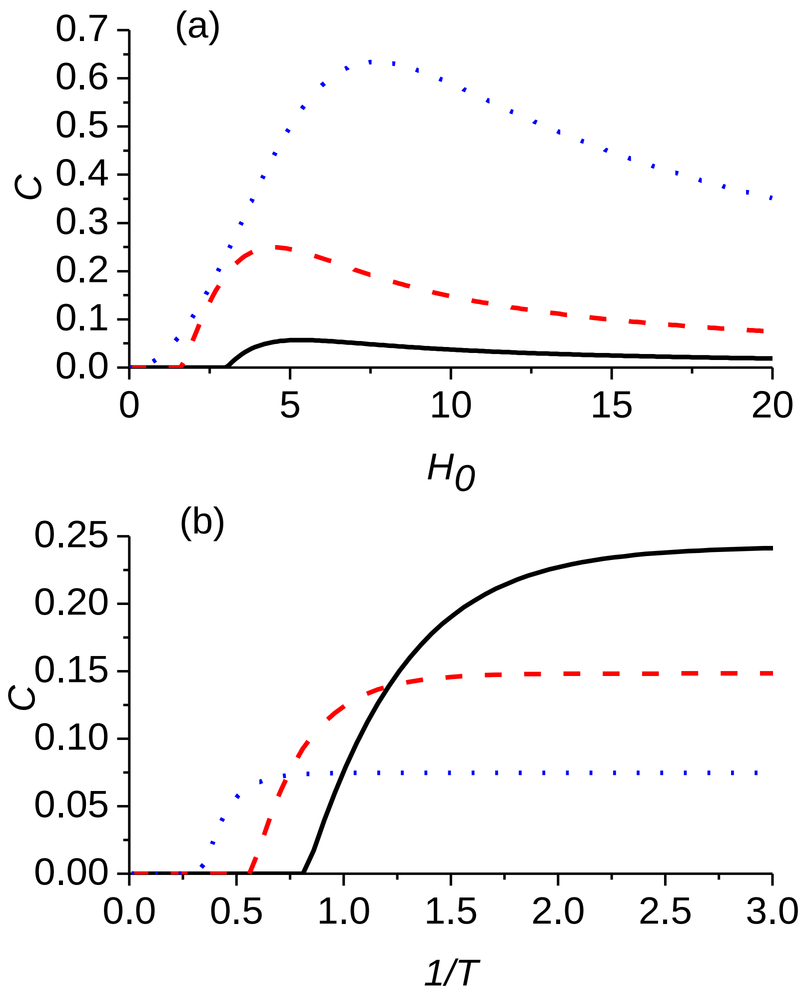


Concurrence as a function of the ratios of the magnetic field strength (ω_0) and dipolar coupling constant γ^2/r^3 to $k_B T$.

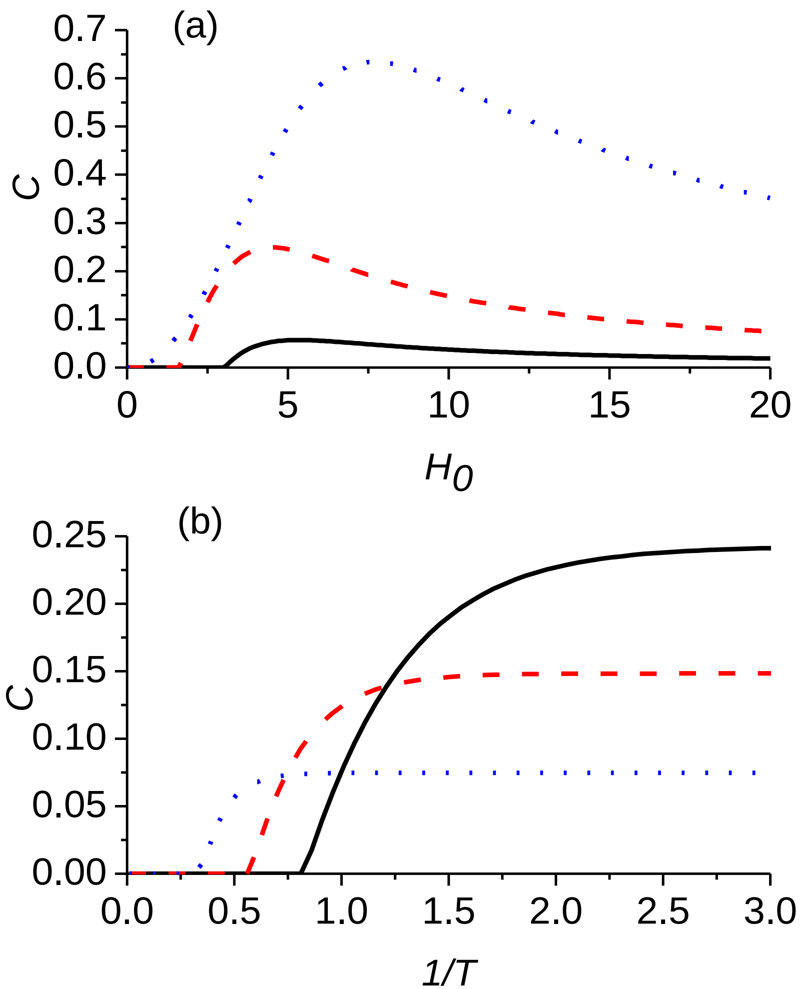


At large temperature and low magnetic field concurrence is zero. The concurrence increases with the magnetic field and inverse temperature and reaches its maximum. Then the concurrence decreases.

Concurrence as a function of the ratios of the magnetic field strength (ω_0) and dipolar coupling constant γ^2/r^3 to k_BT.

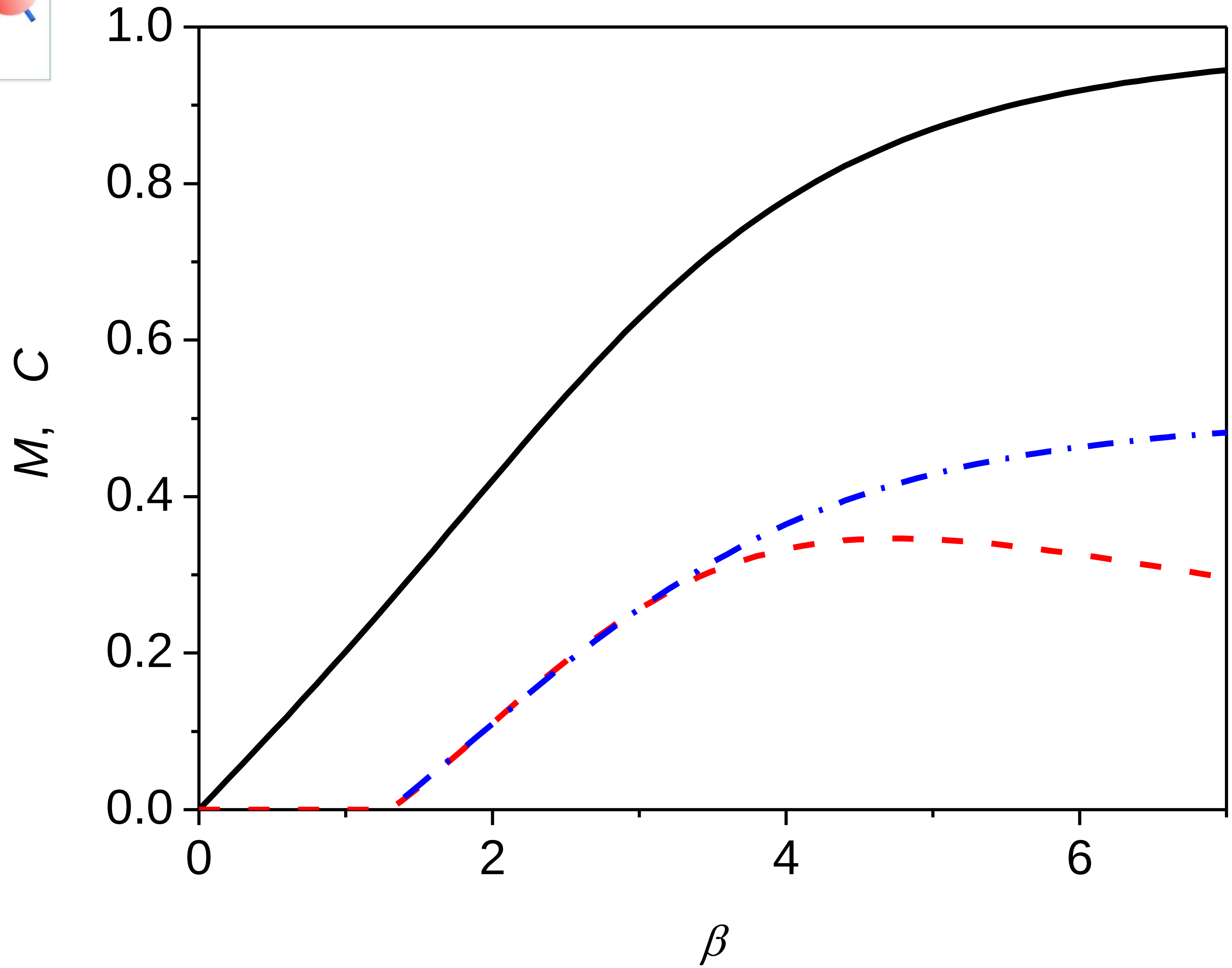


Concurrence vs. magnetic field at ***T***=const (a) and vs. temperature at $\boldsymbol{H_0}$=const (b) for various dipole interaction constants.



In the both cases concurrence remains zero up to a certain value of the magnetic field (a) or of the inverse temperature (b), which depends on the coupling constant.

Concurrence vs. magnetic field at T=const (a) and vs. temperature at H_0=const (b) for various dipole interaction constants.



Absolute value of magnetization (black solid line) and concurrence (red dash line) as a function of $\beta = \omega_0 / k_B T$. Fitting of the concurrence (blue dash-dot line) by C=-0.71(M+0.26) at d=3

Entanglement between states of single quadrupole nuclear spin

a) A single spin 3/2 is isomorphic to a system consists of two dipolar coupling spins ½.

b) The quantum states of single spin 3/2 can be considered as two qubits.

c) Our purpose is to investigate entanglement between these qubits.

The Hamiltonian H consists of the Zeeman H_M and the quadrupole H_Q parts:

$$H=H_M+H_Q$$

A suitable system for studying by NQR technique:
a high temperature superconductor $YBa_2Cu_3O_{7-\delta}$

^{63}Cu : $S = 3/2$, $Q = -0.211 \; 10^{-24} cm^2$, $eQq_{ZZ} = 38.2$ MHz (in the four-coordinated copper ion site) and $eQq_{ZZ} = 62.8$ MHz (in the five-coordinated copper ion site) [1]

^{65}Cu : $S = 3/2$, $Q = -0.195 \; 10^{-24} cm^2$

There are two different locations of copper ions in this structure:

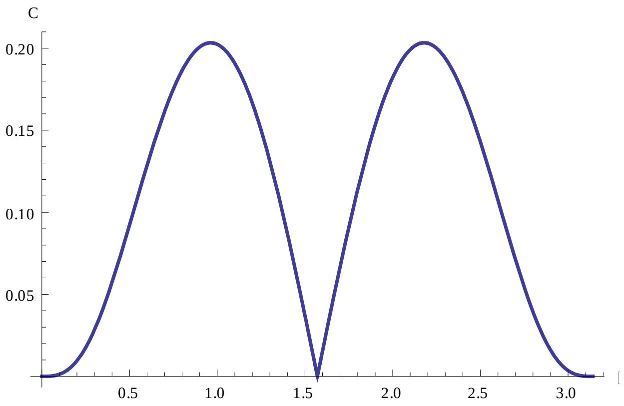
the first is the copper ion sites at the center of an oxygen rhombus-like plane while the second one is five-coordinated by an apically elongated rhombic pyramid. The four-coordinated copper ion site, EFG is highly asymmetric ($\eta \geq 0.92$) while the five-coordinated copper ion site, EFG is nearly axially symmetric ($\eta = 0.14$) [1].

1. M. Mali, D. Brinkmann, L. Pauli, J. Roos, H. Zimmermenn, Phys. Lett. A, 124, 112 (1987).

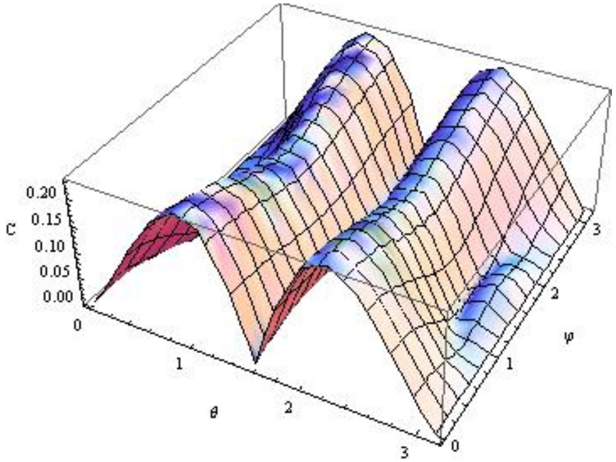
Concurrence as a function of the angles ϕ and θ at

$\alpha = \gamma H_0/k_B T = 5$

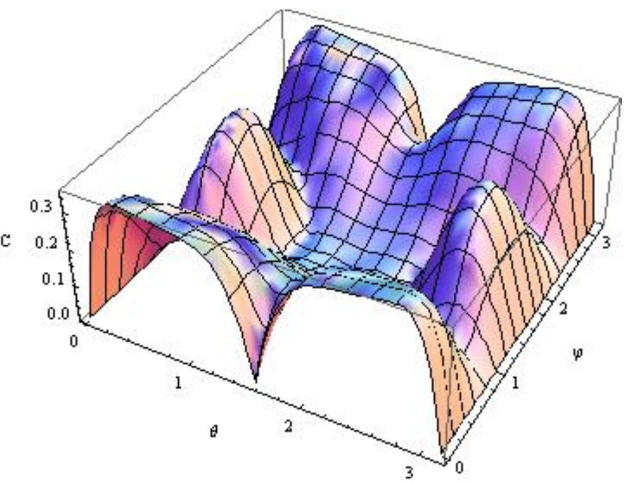
$\beta = eQq_{ZZ}/(4I(2I-1)k_B T)) = 5$



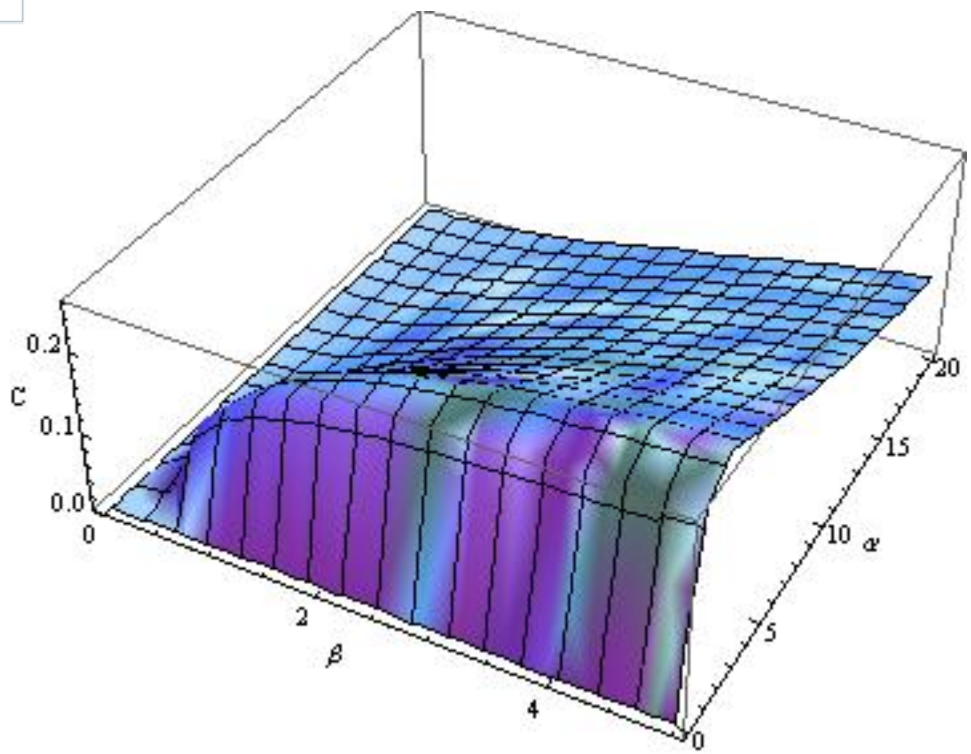
a) η=0



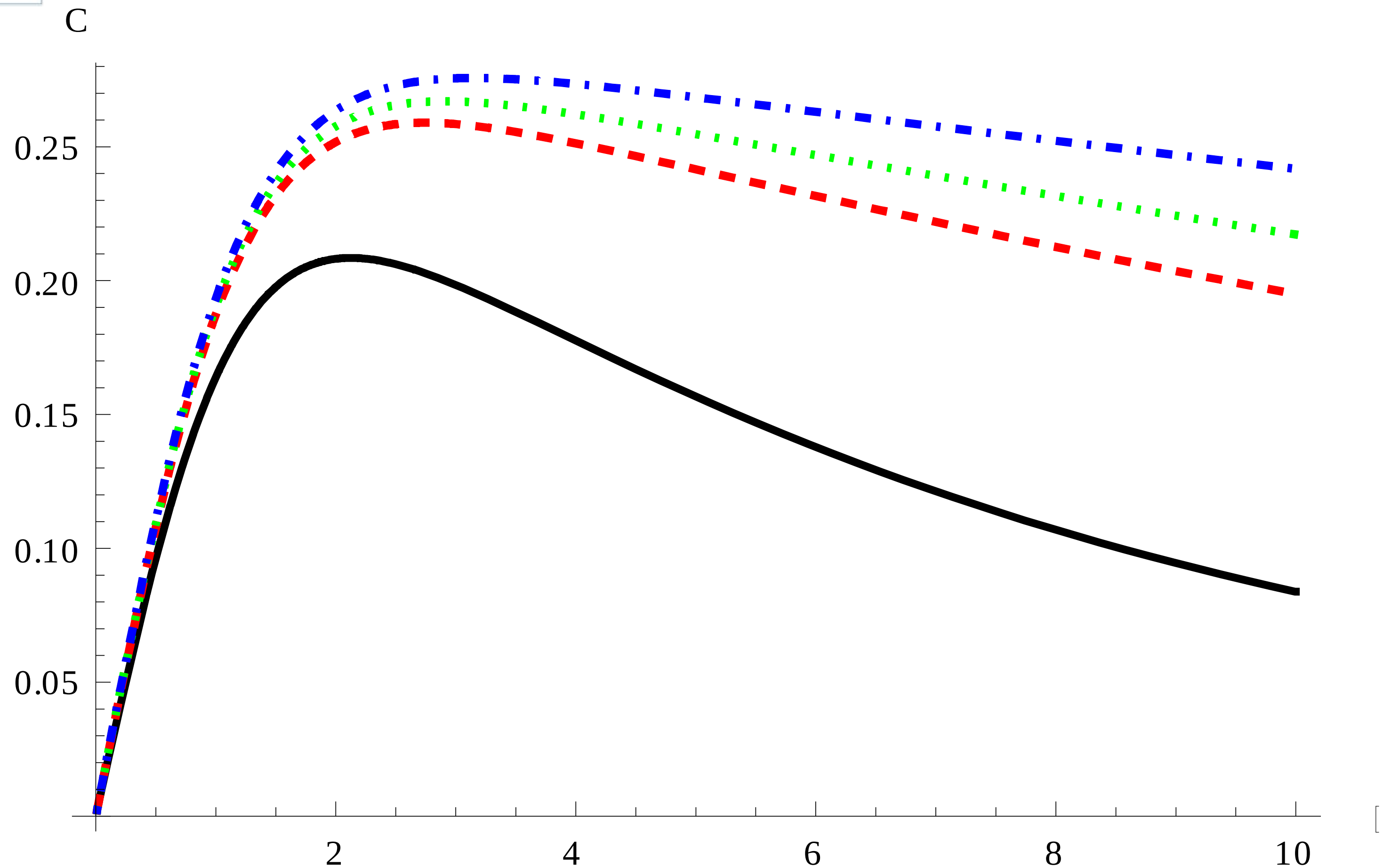
b) η=0.14



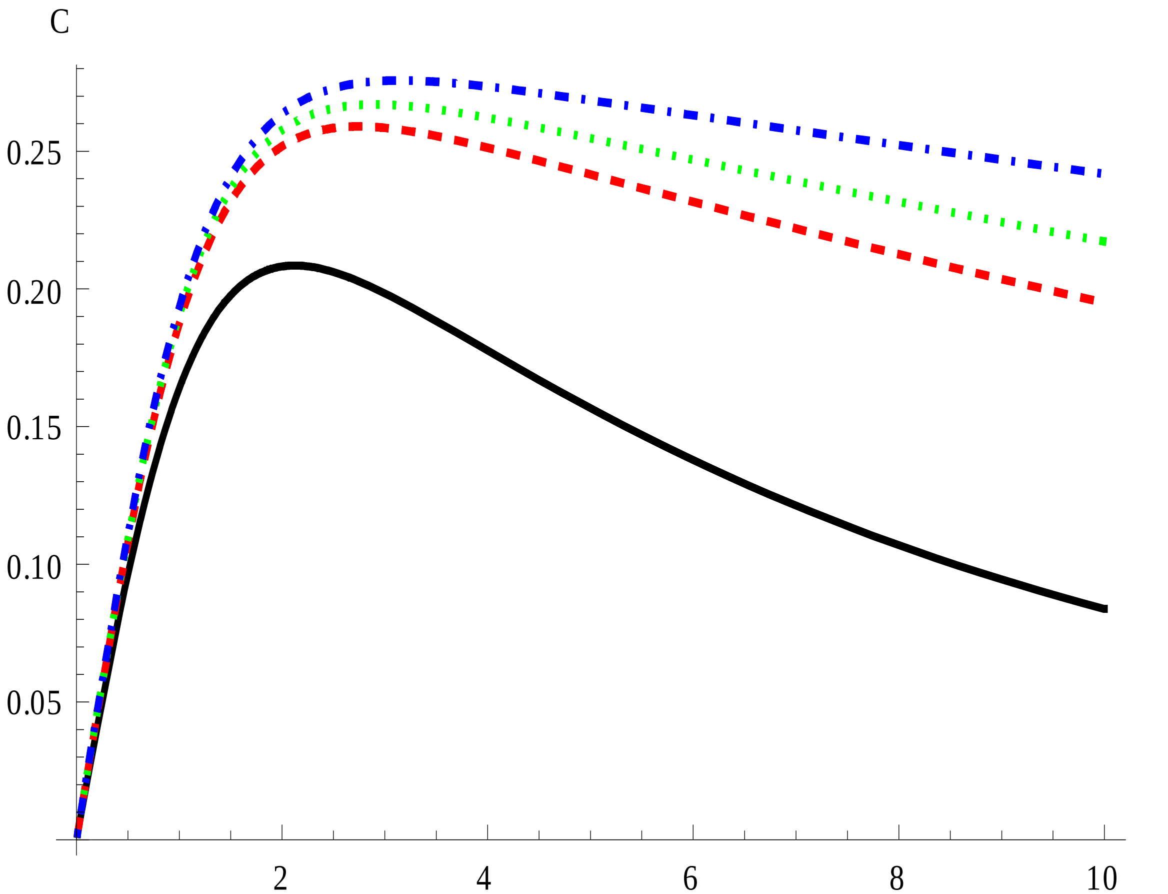
c) η=0.92



The maximum concurrence as a function of
the parameters α and β at η=0.14, θ=0.94, ϕ=0

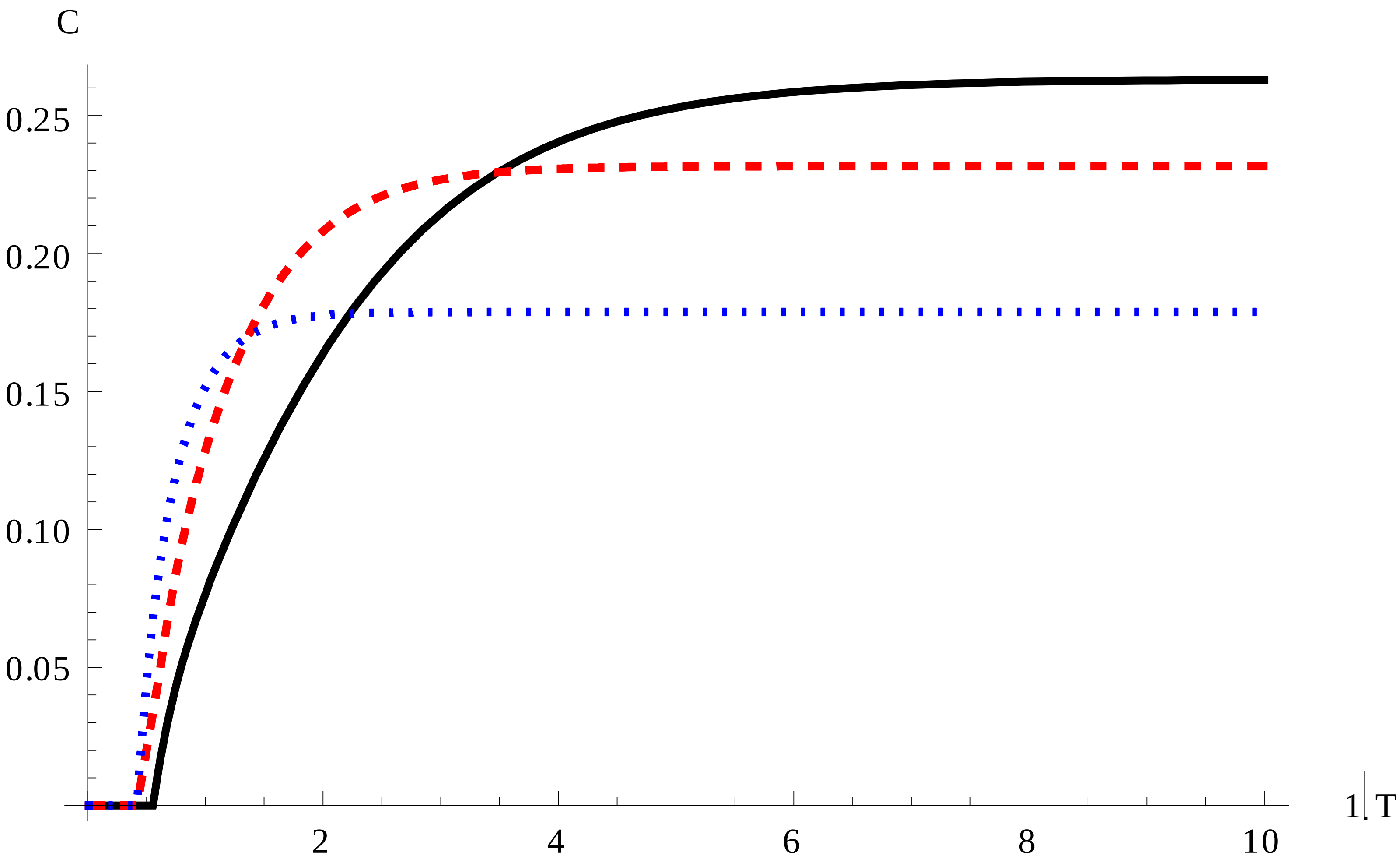


Concurrence vs. magnetic field at ***T*** = const for various quadrupole interaction constants: black solid line -- ***β=2***; red dashed line --***β=6*** ; green dotted line -- ***β=8***; blue dash-doted line -- ***β=12***.

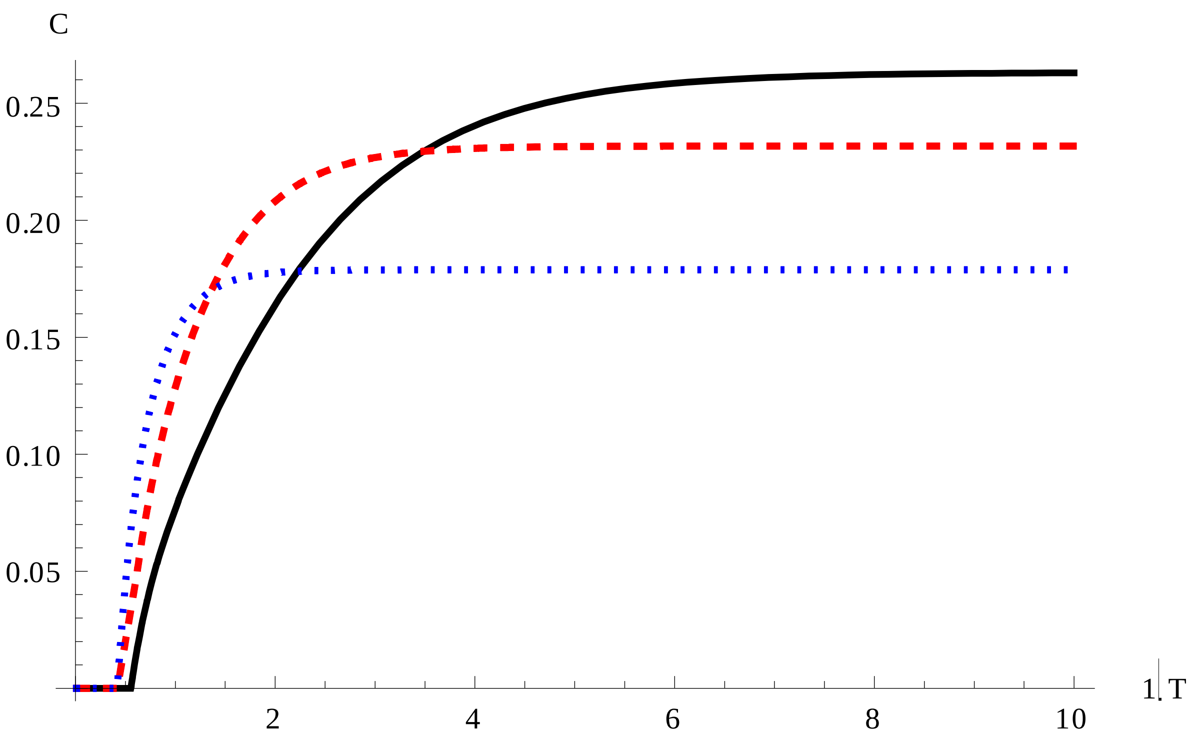


The concurrence increases with the magnetic field strength and reaches its maximum value. Then the concurrence decreases with increasing the magnetic field strength

Concurrence vs. magnetic field at T = const for various quadrupole interaction constants:: black solid line -- $\beta=2$; red dashed line --$\beta=6$; green dotted line -- $\beta=8$; blue dash-doted line -- $\beta=12$.

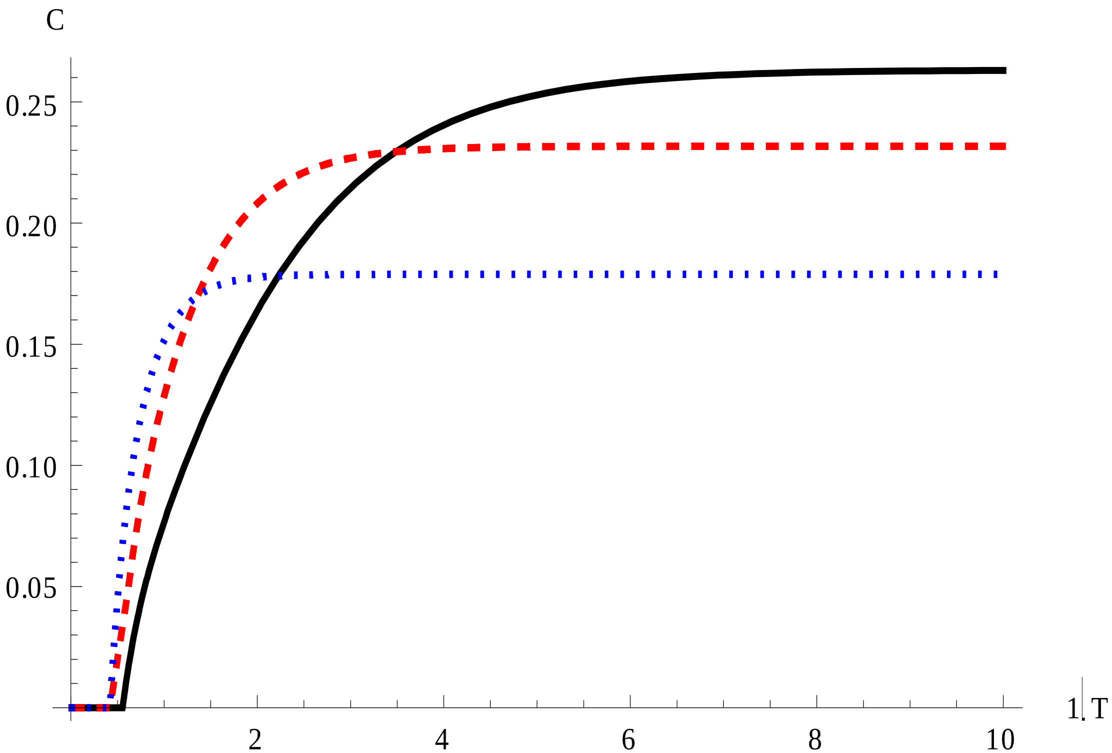


Concurrence as a function of temperature at ***α/β=0.5*** (black solid line), ***α/β=1*** (red dashed line), and ***α/β=2*** (blue dotted line) at ***η=0.14***, ***θ=0.94***, ***ϕ=0*** Temperature is given in units of $eQqZZ/(4I(2I-1)k_B)$



At a high temperature concurrence is zero. With a decrease of temperature below a critical value the concurrence monotonically increases till a limiting value. The critical temperature and limiting value are determined by a ratio of the Zeeman and quadrupole coupling energies, ***α/β***.

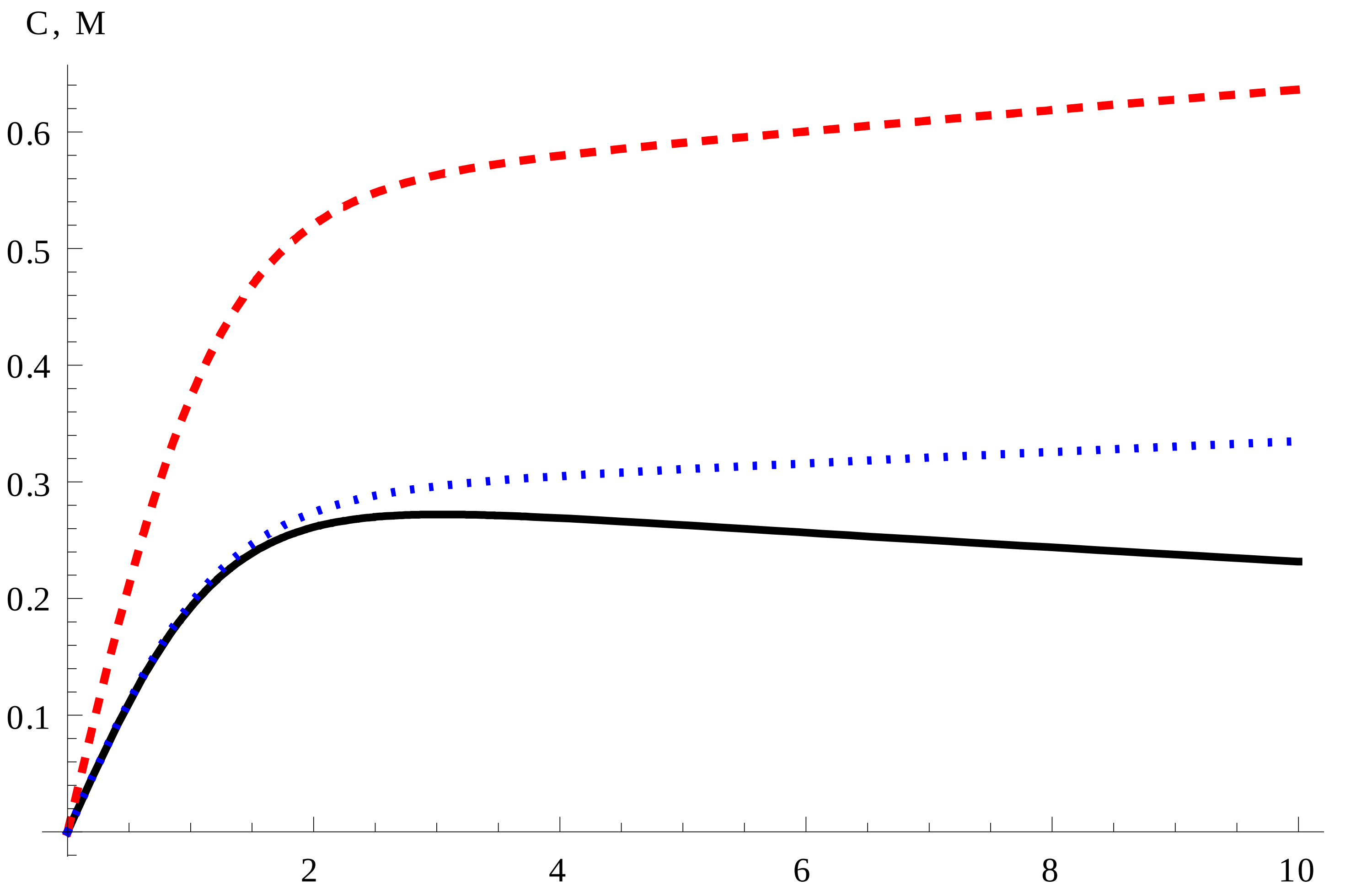
Concurrence as a function of temperature at ***α/β=0.5*** (black solid line), ***α/β=1*** (red dashed line), and ***α/β=2*** (blue dotted line) at ***η=0.14***, ***θ=0.94***, ***ϕ=0*** Temperature is given in units of $eQqZZ/(4I(2I-1)k_B))$



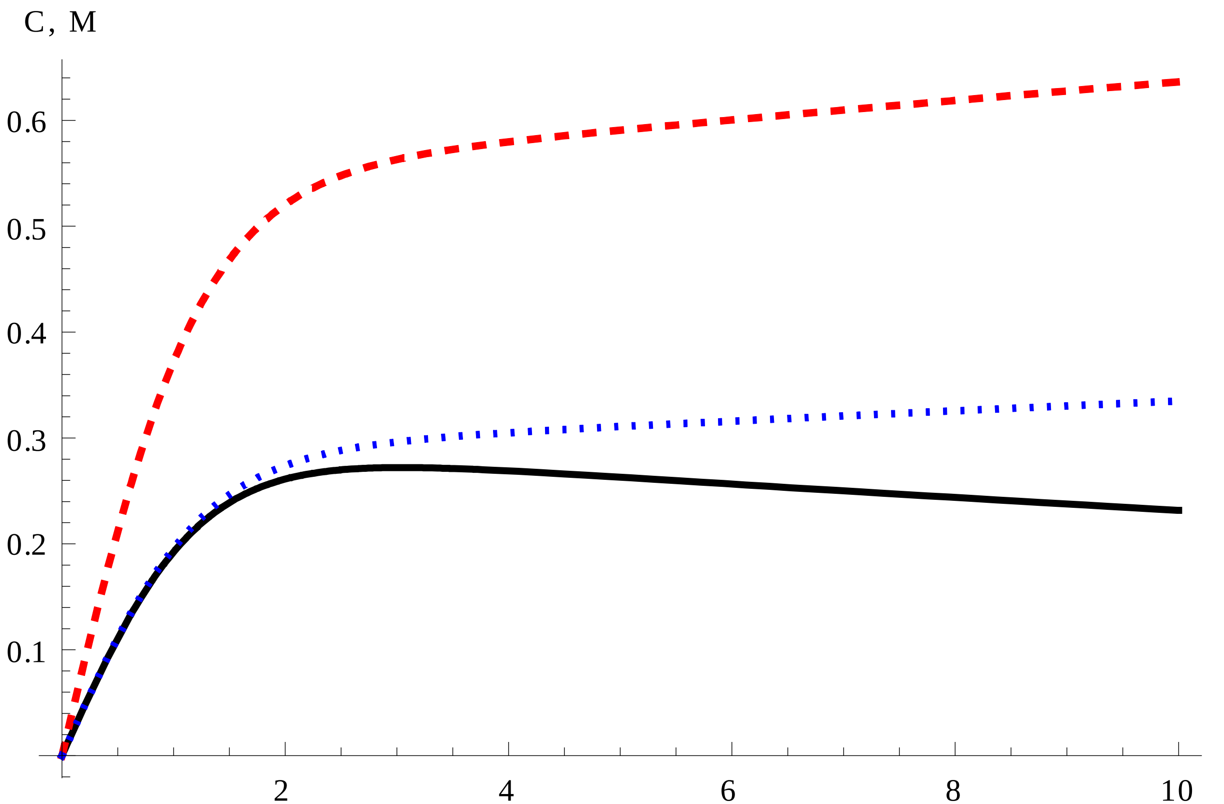
Concurrence as a function of temperature at *$\alpha/\beta=0.5$* (black solid line), *$\alpha/\beta=1$* (red dashed line), and *$\alpha/\beta=2$* (blue dotted line) at *$\eta=0.14$*, *$\theta=0.94$*, *$\phi=0$* Temperature is given in units of *$eQqZZ/(4I(2I-1)k_B))$*

The calculation for ^{63}Cu in the five-coordinated copper ion site of $YBa_2Cu_3O_{7-\delta}$ at $\alpha/\beta=1$, $\eta=0.14$ and *eQqzz= 62.8 MHz*, gives that the concurrence appears at *$\beta=0.6$* . This *β* value corresponds to temperature *$T\approx5$ mK*.

This estimated value of critical temperature is by three orders greater than the critical temperature estimated for the two dipolar coupling spins under the thermodynamic equilibrium



Concurrence (black solid line) and magnetization (red dashed line) as functions of the magnetic field at ***β=10***, ***θ=0.94***. Blue dotted line is (***-M/1.9***)



Concurrence (black solid line) and magnetization (red dashed line) as functions of the magnetic field at ***β=10***, ***θ=0.94***. Blue dotted line is (***-M/1.9***)

To distinguish an entangled state from a separable one, it is important to determine an entanglement witness applicable to the given quantum system

The concurrence is well fitted by a linear dependence on the magnetization in the temperature and magnetic field range up to a deviation of the magnetization from Curie's law and, following, the magnetization can be used as an entanglement witness for such systems

An important measure is the entanglement entropy

Definition of entanglement entropy

Divide a given quantum system into two parts A and B.

Then the total Hilbert space becomes factorized

$$H_{tot} = H_A \otimes H_B \quad .$$

We define the reduced density matrix ρ_A for A by

$$\rho_A = \mathrm{Tr}_B \rho_{tot} \quad ,$$

taking trace over the Hilbert space of B .

Now the entanglement entropy S_A is defined by the von Neumann entropy

$$S_A = -\mathrm{Tr}_A \rho_A \log \rho_A \quad .$$

Thus the entanglement entropy (E.E.) measures how A and B are entangled quantum mechanically.

(1) E.E. is the entropy for an observer who is only accessible to the subsystem A and not to B.

(2) E.E. is a sort of a `non-local version of correlation functions'.

(3) E.E. is proportional to the degrees of freedom.
It is non-vanishing even at zero temperature.

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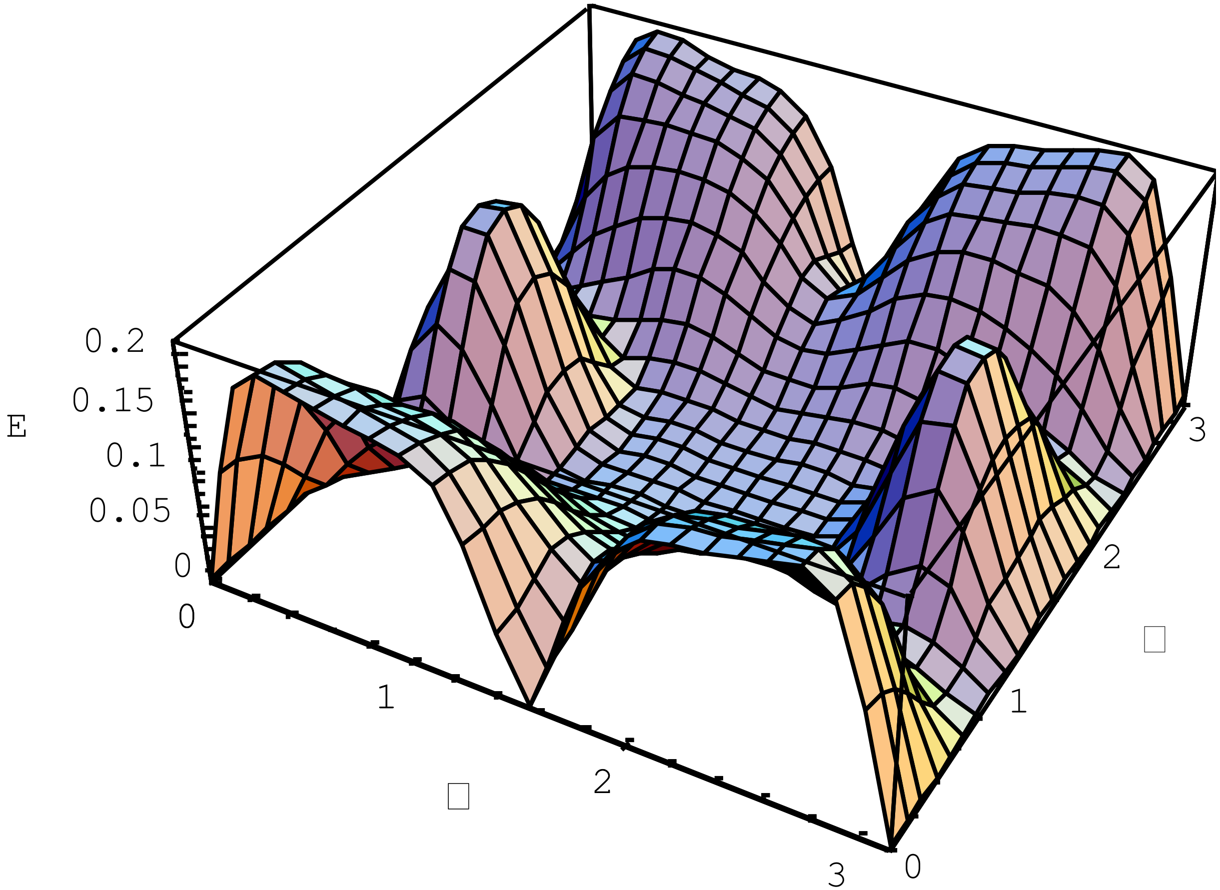

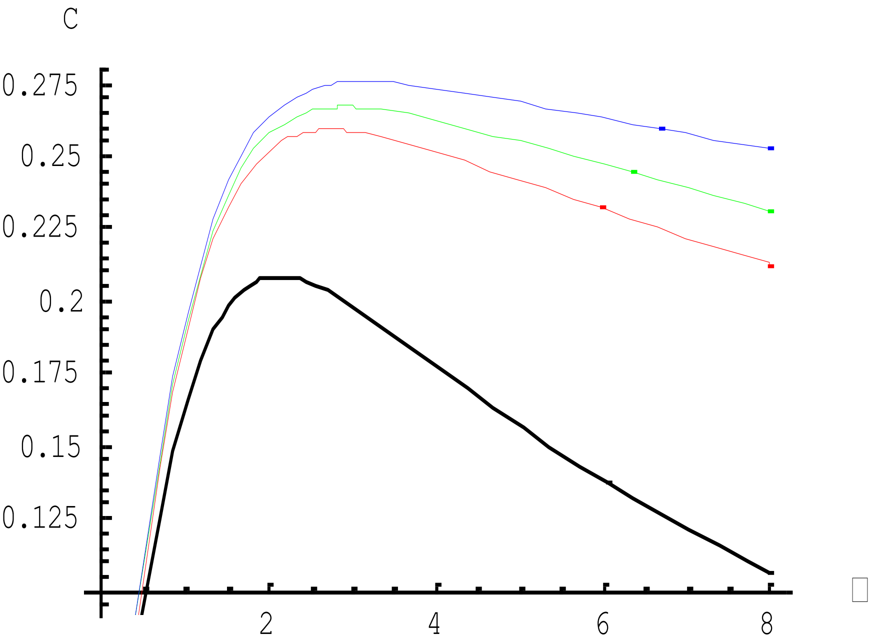

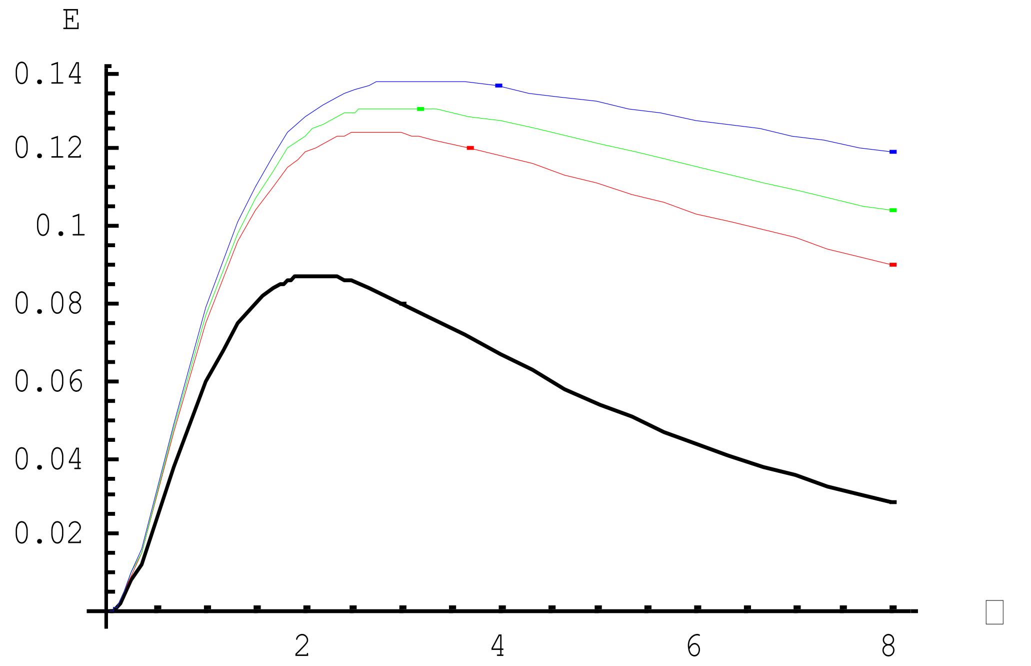

$$E = H((1+\sqrt{1-C^2})/2)$$

$$H(x) = -x\log_2 x - (1-x)\log_2(1-x)$$

Conclusions

1. We study entanglement between quantum states of multi level spin system of a single particle: a special superposition (entanglement) existing in the system of two non-separate subsystems.
2. It was shown that entanglement is achieved by applying a magnetic field to a single particle at low temperature (5 mK).
3. The numerical calculation revealed the coincidence between magnetization and concurrence. As a result, the magnetization can be used as an entanglement witness for such systems.

thanks