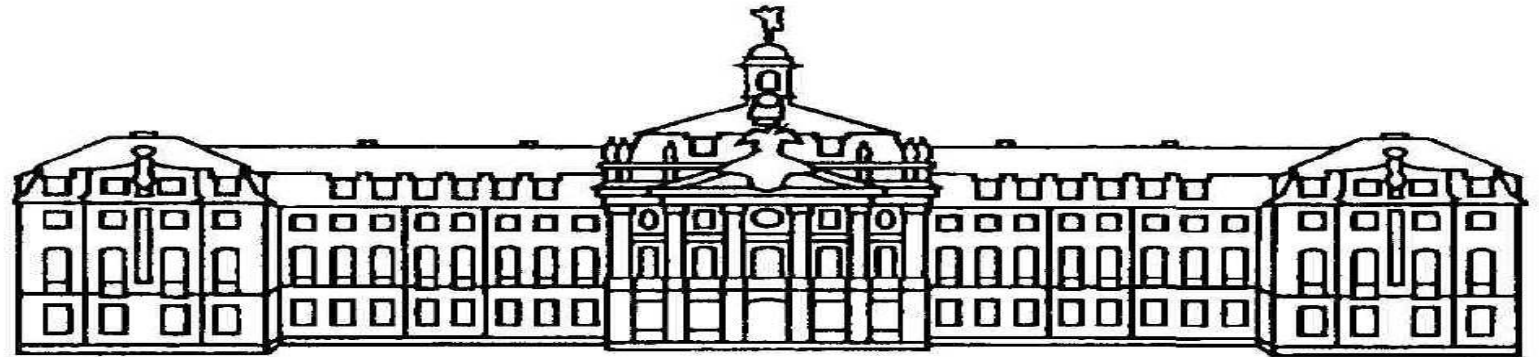




Quantencomputer – Steuerbare Entanglement-Quelle in elastischer Elektron-Austausch-Streuung von chaotischen Spin-Systemen

Kolloquium der Gesellschaft für Informatik Dortmund, *Römischer Kaiser*

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Introduction

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Introduction

Most intriguing phenomenon in nature.
Continuously at the center of intense research activities,
Brunner *et al* (2014); Chandra and Ghosh (2013);
Gühne and Tóth (2009); Horodecki *et al* (2009); Reid *et al* (2009).

Entanglement



Fundamental to quantum mechanics

non-locality, superposition principle, *Verschränkung* by Schrödinger (1935).



Local realism vs. Quantum mechanics

Bell's theorem (Bell, 1964)

Hensen *et al* (2015); Giustina *et al* (2015); Shalm *et al* (2015).



AND



Moreover

Entanglement

QI & QC – Viable resource for:

- Quantum cryptography
Herbert (1975); Ekert (1991),
- Quantum teleportation
Bennett *et al* (1993),
- Quantum computation
Gottesmann and Chuang (1999);
Raussendorf and Briegel (2001).

New field in scattering physics:

- Scattering process yields tunable entanglement resource.
- Proof of intrinsic non-locality in exchange processes.
- Relating scattering physics and Bell's theorem.
- Maximal violation of Bell's inequalities.

👉 **This talk and our results shall interrelate all these areas.** 👈

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Scattering Theory

- Consider the **incoming state** of the particles as the state vector $|\psi_{in}\rangle$ at an **infinitely remote past** when the **interaction** between the particles **can be neglected**.

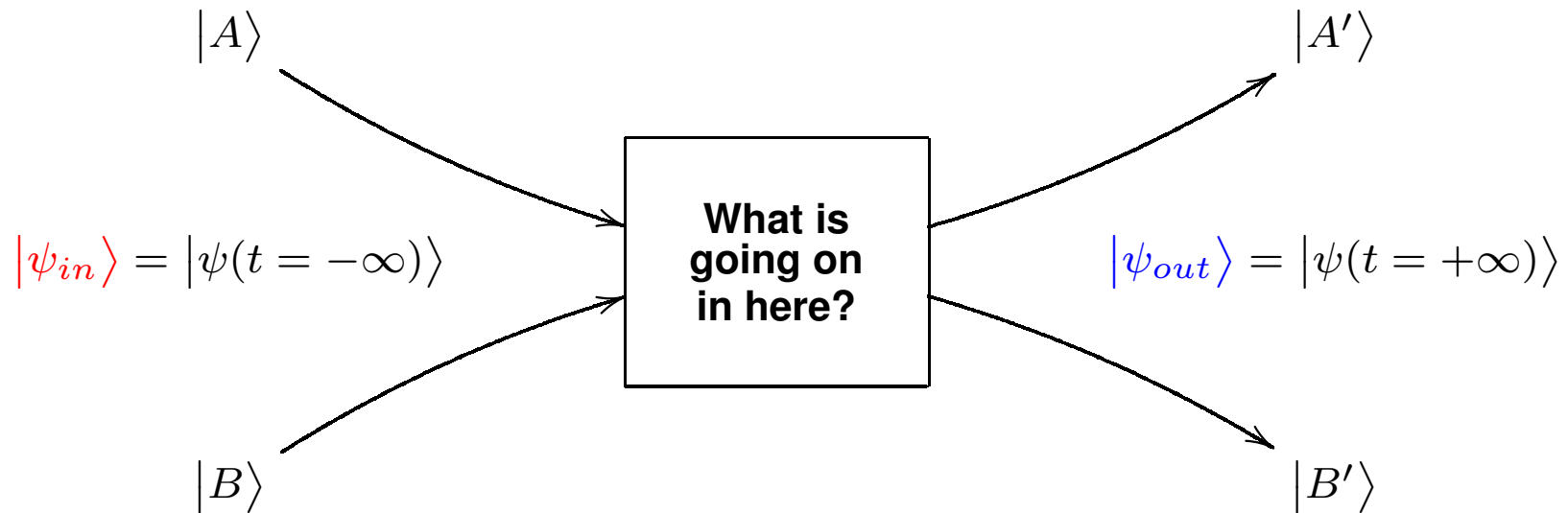


FIG. 1 A typical *black box* scattering scenario.

- The **outgoing state** $|\psi_{out}\rangle$ describes the state in a **large distance** from the collision at an **infinitely late future** instant.
- The distance between the particles is assumed as large enough for the **interaction to be neglected again**.

- The collision is thought of as a **black box**, mathematically represented by the **unitary operator** S , which transforms the **in** states into the **out** states.



The S **matrix** can then be defined by the relation

$$|\psi_{out}\rangle = S |\psi_{in}\rangle . \quad (1)$$

- When the **initial state** is represented by the **density matrix**

$$\rho_{in} = \sum_i p_i |\psi_{in}^{(i)}\rangle \langle \psi_{in}^{(i)}| , \quad (2)$$

with probabilities $p_i \geq 0$.

- The density matrix ρ'_{out} describing the **final particles** is obtained by sandwiching ρ_{in} between S and S^+ ,

$$\rho'_{out} \equiv S \rho_{in} S^+ = \sum_i p_i S |\psi_{in}^{(i)}\rangle \langle \psi_{in}^{(i)}| S^+ = \sum_i p_i |\psi_{out}^{(i)}\rangle \langle \psi_{out}^{(i)}| . \quad (3)$$



Since we are only interested in **transitions between different states** it is convenient to extract from S the identity operator $\mathbb{1}$ and define the **transition operator T** as

$$T = S - \mathbb{1} . \quad (4)$$

- It follows

$$T|\psi_{in}\rangle = |\psi_{out}\rangle - |\psi_{in}\rangle . \quad (5)$$

- All possible transitions (scattering, reactions) in the collision system will be connected with the **dissimilarity between initial and final state**.



The T operator transforms the **in** state into the scattered **out** state.

- Thus, the **interesting part** of the density matrix ρ'_{out} is that one which contains the information on the **scattered states alone**, which is given by

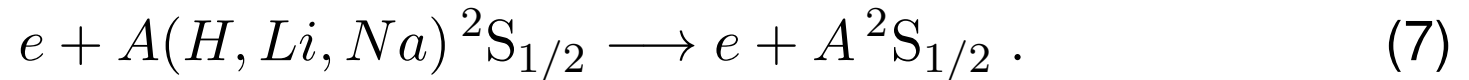
$$\rho_{out} = T \rho_{in} T^+ . \quad (6)$$



The **central problem of scattering theory** is the determination of T , that is to **determine all elements of the T matrix**.

Density Matrix of the Scattering System

- Initially unpolarized electrons and unpolarized atoms:



- Quasi **hydrogen-like** (one electron) atoms; H, Li, Na .
 - ◆ **Light atoms** $\longrightarrow$ spin-orbit interaction can be neglected.
 - ◆ **Coulomb- and exchange forces**, only.

 **Initial unpolarized state density matrix:**

$$\rho_{in} = \frac{1}{4} \sum_{m_1 m_2} |m_1 m_2\rangle \langle m_1 m_2| . \quad (8)$$

- Calculate **final state density matrix** after scattering:

$$\rho = T \rho_{in} T^+ , \quad (9)$$

where T is the transition operator.

☞ Clebsch-Gordan Algebra yields:

$$\rho = \frac{1}{8\sigma} \begin{pmatrix} 2|f^{(1)}|^2 & 0 & 0 & 0 \\ 0 & |f^{(1)}|^2 + |f^{(0)}|^2 & |f^{(1)}|^2 - |f^{(0)}|^2 & 0 \\ 0 & |f^{(1)}|^2 - |f^{(0)}|^2 & |f^{(1)}|^2 + |f^{(0)}|^2 & 0 \\ 0 & 0 & 0 & 2|f^{(1)}|^2 \end{pmatrix} , \quad (10)$$

$f^{(S)} = \langle SM_s | T | SM_s \rangle$, denotes the **triplet** ($S = 1$) and **singlet** ($S = 0$) **scattering amplitudes** (T matrix is independent of M_s).

- Here, ρ is **normalized** by the **differential cross section**:

$$\sigma = \frac{1}{4} \left(3|f^{(1)}|^2 + |f^{(0)}|^2 \right) , \quad \text{and} \quad \text{tr } \rho = 1 . \quad (11)$$

- **Characterization** of the 4×4 spin density matrix (10):

$$\rho = \frac{1}{4} \left[\mathbb{1} \times \mathbb{1} + \sum_i P_i^{(1)} (\sigma_i \times \mathbb{1}) + \sum_j P_j^{(2)} (\mathbb{1} \times \sigma_j) + \sum_{ij} \left(P_i^{(1)} \times P_j^{(2)} \right) (\sigma_i \times \sigma_j) \right]. \quad (12)$$

- ◆ **Two** individually measured **spin polarization** vectors $\mathbf{P}^{(1)}$ and $\mathbf{P}^{(2)}$, referring to particles 1 and 2:

$$P_i^{(1)} = \text{tr } \rho (\sigma_i \times \mathbb{1}) , \quad \text{and} \quad P_i^{(2)} = \text{tr } \rho (\mathbb{1} \times \sigma_i) , \quad (13)$$

($i = x, y, z$), 2-dim. unit matrix $\mathbb{1}$, and $\times$ denotes the direct product.

- ◆ **Nine** direct product components $P_i^{(1)} \times P_j^{(2)}$ of the **spin–spin correlation tensor** ($i, j = x, y, z$):

$$P_i^{(1)} \times P_j^{(2)} = \text{tr } \rho (\sigma_i \times \sigma_j) . \quad (14)$$

- σ_i ($i = x, y, z$) abbreviates the Pauli matrices.

- The **simple structure** of the density matrix (10) allows for quickly calculating the **relevant parameters**.
- The individual polarization vectors of the two sub-systems cancel,

$$\mathbf{P}^{(1)} = 0 \quad \text{and} \quad \mathbf{P}^{(2)} = 0 . \quad (15)$$

- All spin-spin correlation tensors with $i \neq j$ vanish.

 **The only non-vanishing** spin correlation parameters are

$$P = P_i^{(1)} \times P_i^{(2)} = \frac{|f^{(1)}|^2 - |f^{(0)}|^2}{3|f^{(1)}|^2 + |f^{(0)}|^2} , \quad i = x, y, z , \quad (16)$$

- Introducing the **parameter** $\mathbf{P} = \mathbf{P}(\boldsymbol{\theta}, \mathbf{E})$ which is a function of scattering angle and energy.
- ✓ In general, **P is restricted** to the interval $[-1, 1]$. From(16) we get the further restriction

$$-1 \leq P \leq \frac{1}{3} . \quad (17)$$

$$\rho = \rho(P)$$

- The **spin density matrix** (10) can be expressed in terms of the spin correlation parameter. We obtain

$$\rho = \frac{1}{4} \begin{pmatrix} 1+P & 0 & 0 & 0 \\ 0 & 1-P & 2P & 0 \\ 0 & 2P & 1-P & 0 \\ 0 & 0 & 0 & 1+P \end{pmatrix}. \quad (18)$$

👉 The **key equation** (18) shows that the spin system is completely characterized by the **single parameter** P .

- For **negative values** of $P = -|P|$, that is **anticorrelated spins**, we can write the scattering matrix ρ in form of a **Werner state** (Werner, 1989)

$$\rho = \frac{1-|P|}{4} \mathbb{1} + |P| |00\rangle\langle 00|, \quad (19)$$

with the **singlet state** $|00\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle).$ (20)

Coincidence Measurements of Spin-Spin Correlation Parameter

- The **correlation parameters** refer to experiments where both scattered particles are measured in **coincidence by two observers**.
- E.g., $P_z^{(1)} \times P_z^{(2)}$ gives the outcome of an experiment where **both** analyzer-detector sets are oriented **along the z-direction**, which yields (Blum, 2012)

$$P_z^{(1)} \times P_z^{(2)} = \frac{1}{N} (N(z)_{\uparrow\uparrow} + N(z)_{\downarrow\downarrow} - N(z)_{\uparrow\downarrow} - N(z)_{\downarrow\uparrow}) , \quad (21)$$

where, e.g. $N(z)_{\uparrow\uparrow}$ denotes the number of measurements finding both particles with spin up with respect to the z -axis.

- $\longrightarrow$ **This is a difficult experiment.**

- **Measuring** the spin-spin correlations along **directions** a and b is given by

$$\text{👉} \quad P_a^{(1)} \times P_b^{(2)} = P(\theta, E) \cos \beta . \quad \text{👈} \quad (22)$$

- This and (16) exhibit the **rotational symmetry** of the spin–spin system.

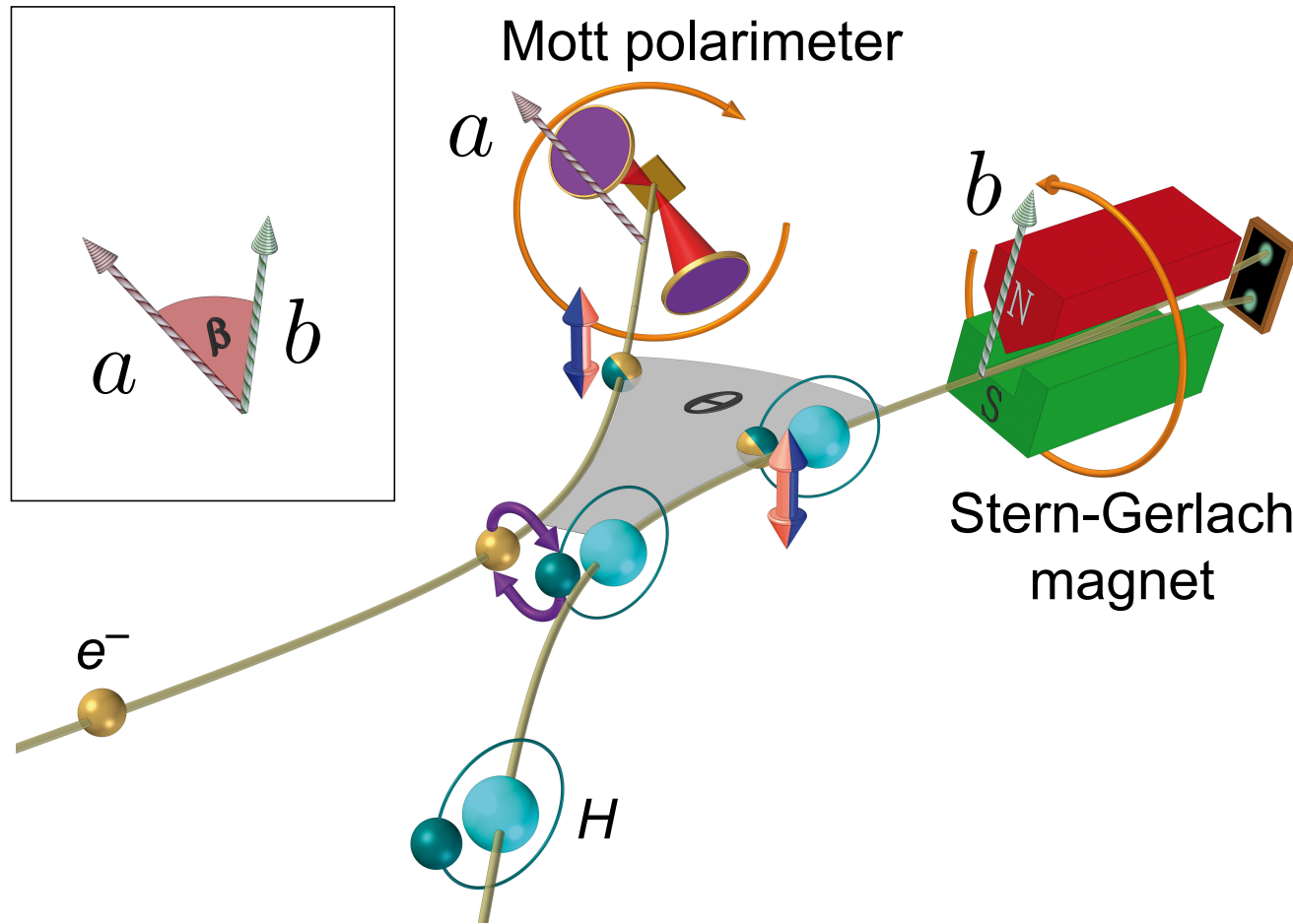


FIG. 2 Scheme of an e – H spin correlation coincidence experiment.

- A spin selective coincidence experiment as described above is not easy to perform.



Important: the correlation parameter (16) can also be obtained from the results of a **different type of experiment**.



Many experimental and numerical results are already available.

- Consider the case where electrons and atoms, **both**, are **initially polarized**.

$$e\uparrow + A\uparrow \longrightarrow e + A \quad \Longrightarrow \quad \sigma_{\uparrow\uparrow}, \quad (23)$$

$$e\uparrow + A\downarrow \longrightarrow e + A \quad \Longrightarrow \quad \sigma_{\uparrow\downarrow}, \quad (24)$$

where $\sigma_{\uparrow\downarrow}$ and $\sigma_{\uparrow\uparrow}$ denote differential cross sections for incident parallel and antiparallel spins, respectively.



In this case, the **spin asymmetry** A_{ex} can be measured

$$A_{ex} = \frac{\sigma_{\uparrow\downarrow} - \sigma_{\uparrow\uparrow}}{\sigma_{\uparrow\downarrow} + \sigma_{\uparrow\uparrow}}, \quad (25)$$

- Expressing A_{ex} in terms of the **scattering amplitudes** $f^{(0)}$ and $f^{(1)}$, we obtain (Lorentz *et al*, 1991)

$$A_{ex} = \frac{|f^{(0)}|^2 - |f^{(1)}|^2}{3|f^{(1)}|^2 + |f^{(0)}|^2} . \quad (26)$$

- 👍 A comparison with (16) yields the **simple relation**

$$\text{👉} \quad P(\theta, E) = -A_{ex}(\theta, E) . \quad \text{👈} \quad (27)$$

- Using published data for the spin asymmetry A_{ex} , then (27) allows to immediately obtain the spin correlation parameter P for our considered **experimental setup with initially unpolarized particles**.

- 👉 See the discussion of data later on.

Entanglement versus Separability

- Under **which conditions** is the density matrix ρ , i.e. the mixed spin state (18), separable or entangled, or a combination of both?
- Generally, a density matrix of a bi-partite mixed state is **separable if and only if**

$$\rho = \sum_{i=1}^n p_i |a_i\rangle\langle a_i| \times |b_i\rangle\langle b_i|, \quad p_i \geq 0, \quad (28)$$

where the **pure one-particle states** $|a_i\rangle$ and $|b_i\rangle$ refer to the first (electron) and second (atom) particle, respectively.

- If **no transformation** of a given density matrix ρ to the form (28) can be given, the system is said to be **non-separable or entangled**.
- Generally, this can be a **hard task**.
- **Convenient criterion** by **Peres (1996)** and **Horodecki *et al* (1996)**.
 In our case of a 4×4 density matrix, yields a **necessary and sufficient condition** for separability.

☞ For this, we construct the **partial transpose** density matrix ρ^{PT}

$$\langle M'm' | \rho^{PT} | Mm \rangle = \langle Mm' | \rho | M'm \rangle . \quad (29)$$

✓ Applying this to the density matrix (18) we obtain

$$\rho^{PT} = \frac{1}{4} \begin{pmatrix} 1+P & 0 & 0 & 2P \\ 0 & 1-P & 0 & 0 \\ 0 & 0 & 1-P & 0 \\ 2P & 0 & 0 & 1+P \end{pmatrix} . \quad (30)$$

■ A given density matrix ρ describes a separable state if **all** eigenvalues of ρ^{PT} are **positive**.

☞ In contrast, ρ describes an entangled system if **at least one** eigenvalue is **negative** (Horodecki *et al*, 1996; Peres, 1996).

■ Calculating the **eigenvalues** λ_i of ρ^{PT} yields

$$\lambda_{1,2,3} = \frac{1}{4}(1-P) , \quad \text{and} \quad \lambda_4 = \frac{1}{4}(1+3P) . \quad (31)$$

- Eq. (31) indicate that all eigenvalues are positive for P -values in the range

$$-\frac{1}{3} \leq P \leq \frac{1}{3}, \quad (32a)$$

- ρ is **separable** in this region.

- 👍 ρ describes an **entangled** system in the range

$$-1 \leq P < -\frac{1}{3}, \quad (32b)$$

where λ_4 becomes negative.

- The system is **maximally entangled** for $P = -1$; see Fig. 3.

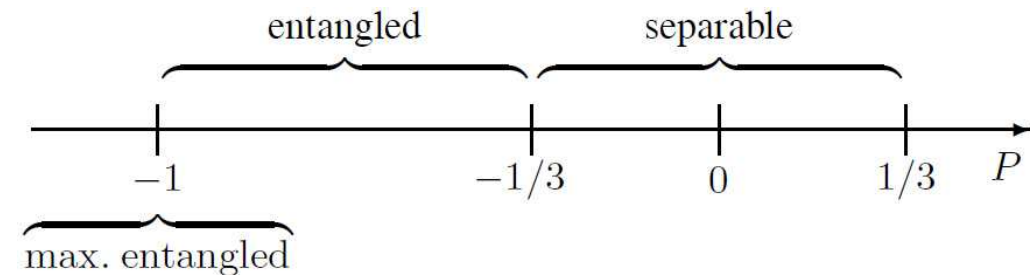


FIG. 3 Separable and entangled areas.

- Whether a given collision system is separable or non-separable depends on the **strength of the spin correlation** and can be decided experimentally by **measuring P**.



Interrelation between spin-spin correlation and Bell's theorem (Bell, 1964).

Bell correlations

- ✓ Entanglement is inherently a **non-local phenomenon**.
 - In order to **avoid this *strange* feature** of quantum mechanics hypothetical **hidden variables** have been introduced ([Einstein *et al*, 1935](#); [Bell, 1964](#)).
 - Hoping to **reinststate** the results of **conventional quantum mechanics** in a local realistic way.
 - Although designed to preserve locality it has turned out that attempts to do so failed in all circumstances.
 - As a consequence of **Bell's theorem** ([Bell, 1964](#)) a set of inequalities have been derived, collectively known as **Bell inequalities**, which must be satisfied by any local theory, and which can be used as a **test of its validity**.
- 👉 A quantum mechanical state is said to display non-local correlations, or being **Bell (or EPR) correlated**, if it **violates** any of the **Bell inequalities**.

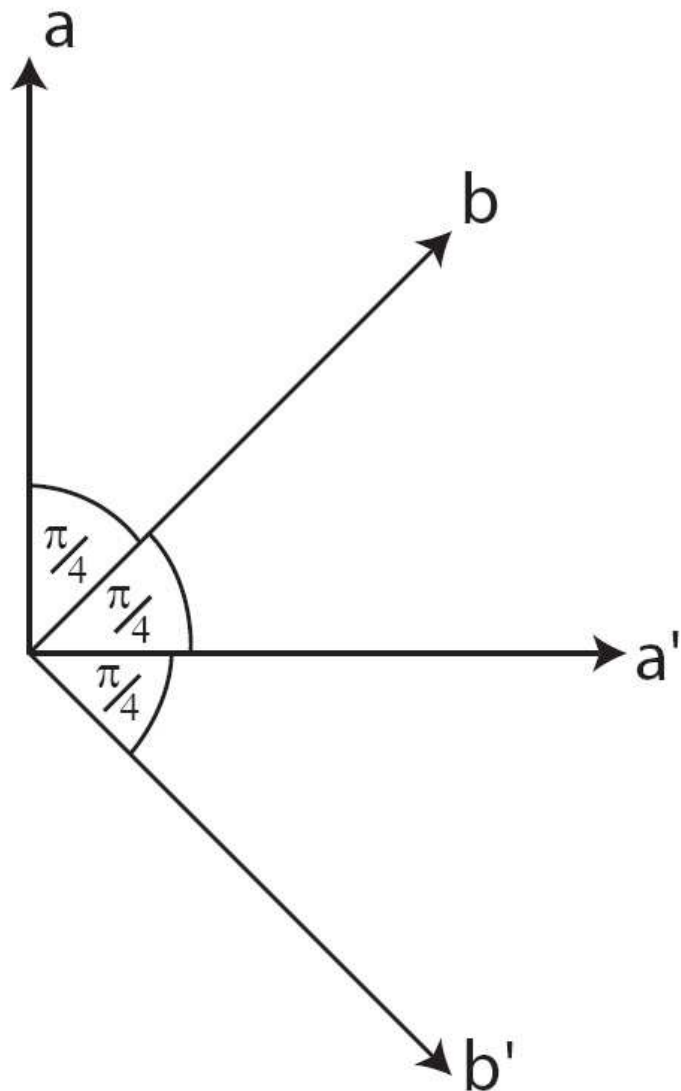


FIG. 4 Coplanar directions of the detector-spin-analyzer sets.

- Following *Aspect et al* (1982), we will adapt this to our case of interest.



Consider the following **combination of correlation parameters**

$$\Delta(a, a', b, b') \quad (33)$$

$$= |P_a^{(1)} \times P_b^{(2)} - P_a^{(1)} \times P_{b'}^{(2)}| \\ + |P_{a'}^{(1)} \times P_b^{(2)} + P_{a'}^{(1)} \times P_{b'}^{(2)}| ,$$

- where $a, a', b,$ and b' denote the **four directions** of the detector-spin-analyzer sets in the corresponding coincidence measurement of the first (directions a and a') and second beam (directions b and b'), respectively.

- ✓ It has been shown by Clauser *et al* (1969) that **local realism** implies the familiar **CHSH-inequality**

$$\Delta(a, a', b, b') \leq 2, \quad (34)$$

- ✓ Quantum mechanics allows for a **larger bound** (Cirel'son, 1980)

$$\Delta(a, a', b, b') \leq 2\sqrt{2}. \quad (35)$$

- In order to demonstrate that *local hidden variable theories* are **inconsistent with quantum mechanics** it is only necessary to show that condition (34) is **violated** for a particular setting.



Consider **coplanar vectors**; Fig. 4.

- Calculating the correlation parameters using (22) one obtains from (33)

$$\Delta = 2\sqrt{2} |P|. \quad (36)$$



Inequality (34) is **violated** for all correlation parameters with $P < -1/\sqrt{2}$.



Thus, as depicted in Fig. 5, the spin-spin correlation system is entangled in the range $-\frac{1}{3} > P \geq -\frac{1}{\sqrt{2}}$ but **does not violate** any Bell inequalities.

The spin correlation in this region is not sufficiently strong.

- Thus, it is in principle possible to **simulate the quantum correlations** within local theories (**hidden variables**).



This possibility is **ruled out** for values $-1 \leq P < -\frac{1}{\sqrt{2}}$ by Bell's theorem.

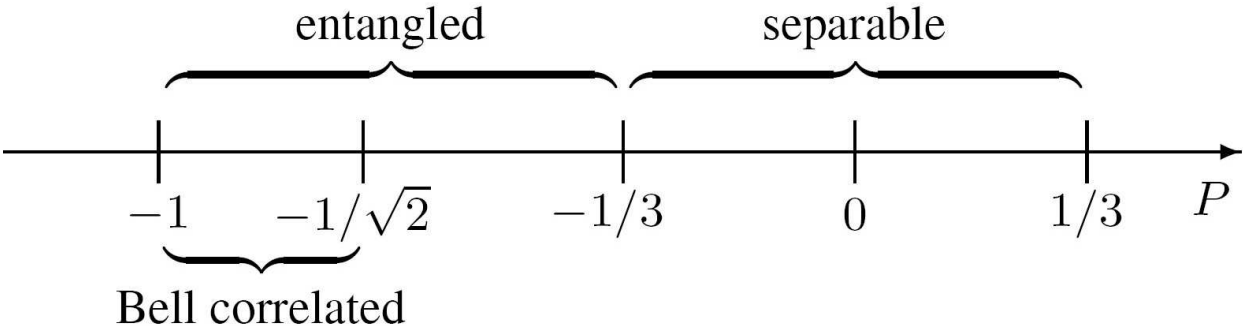


FIG. 5 Separable, entangled, and Bell correlated areas.

- In this case, the **correlations, generated by the spin-exchange collision, are stronger** than could ever be created by classical means and **cannot be described by local realistic theories**.



For $P = -1$, (36) yields a **maximal violation of the CHSH inequality (34)**, or any other of the Bell inequalities.

Experimental and Numerical Results

 $P(\theta, E) = -A_{\text{ex}}(\theta, E)$ 

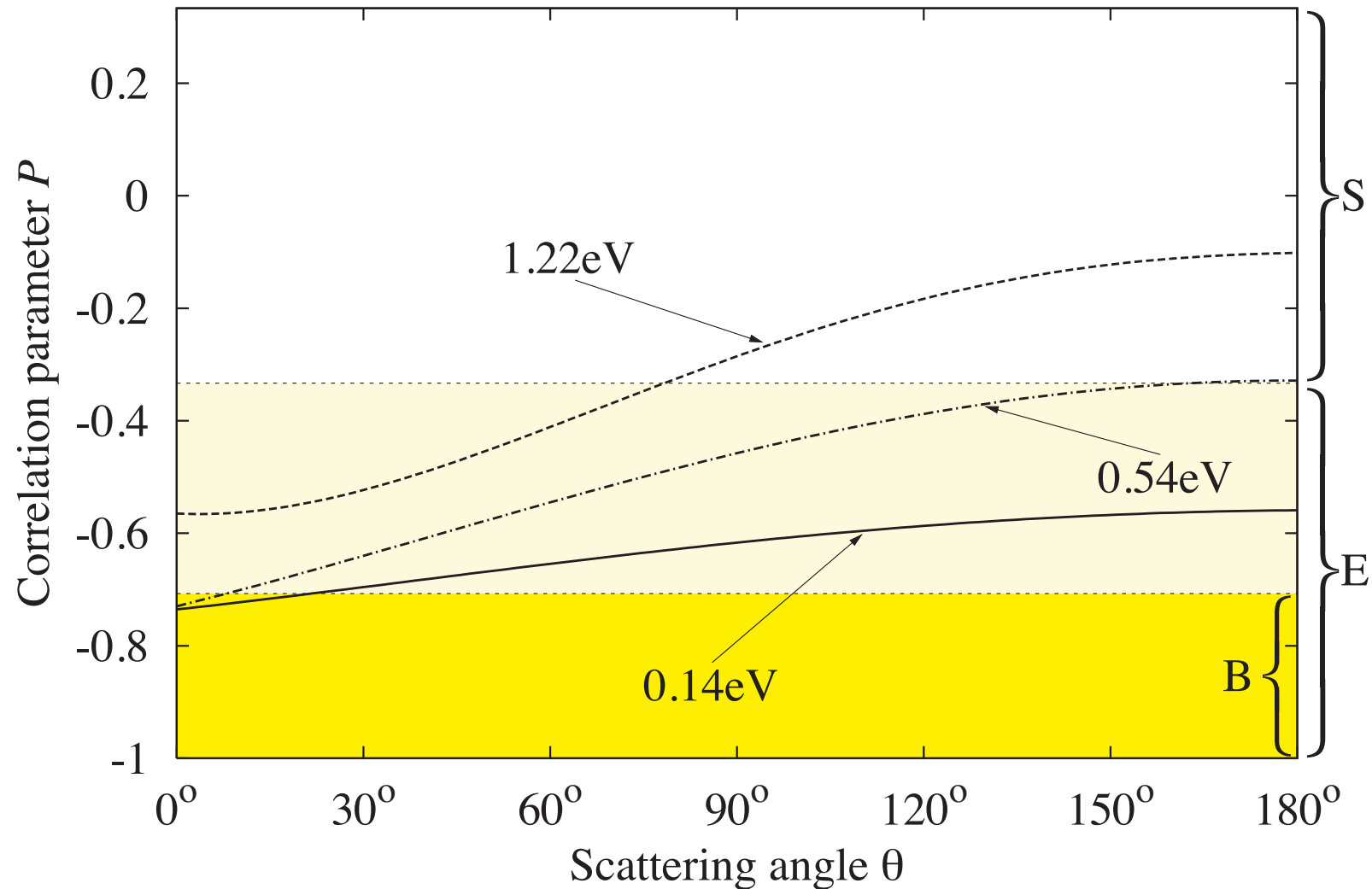


FIG. 6 Correlation parameter P of hydrogen versus scattering angle θ for different scattering energies. Num. data: 0.14 eV, 0.54 eV, and 1.22 eV, (MPCC) [van Wyngaarden and Walters \(1986\)](#). Horizontal lines divide separable (S), entangled (E), and Bell correlated (B) regions. The Bell correlated region can almost not be reached.

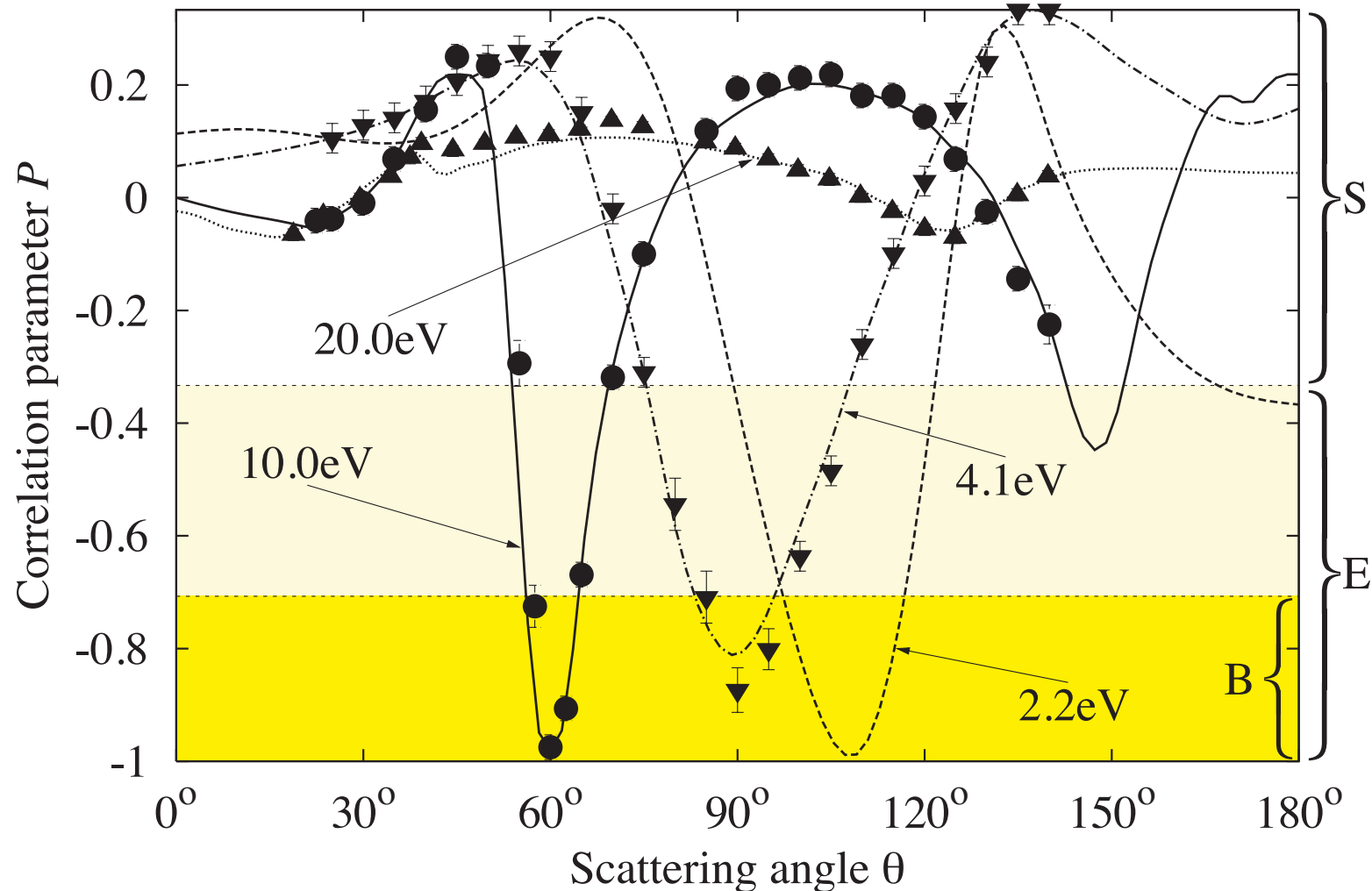


FIG. 7 Correlation parameter P of sodium versus scattering angle θ for different scattering energies. Exp. data by NIST group: 4.1 eV (∇), McClelland *et al* (1989, 1992); 10 eV ($\bullet$), and 20 eV ($\blacktriangle$), Kelley *et al* (1992). Num. data: 2.2 eV, (CC) Moores and Norcross (1972); 4.1 eV, 10 eV, and 20 eV (CCC) Bray (1994a,b). Horizontal lines divide separable (S), entangled (E), and Bell correlated (B) regions.

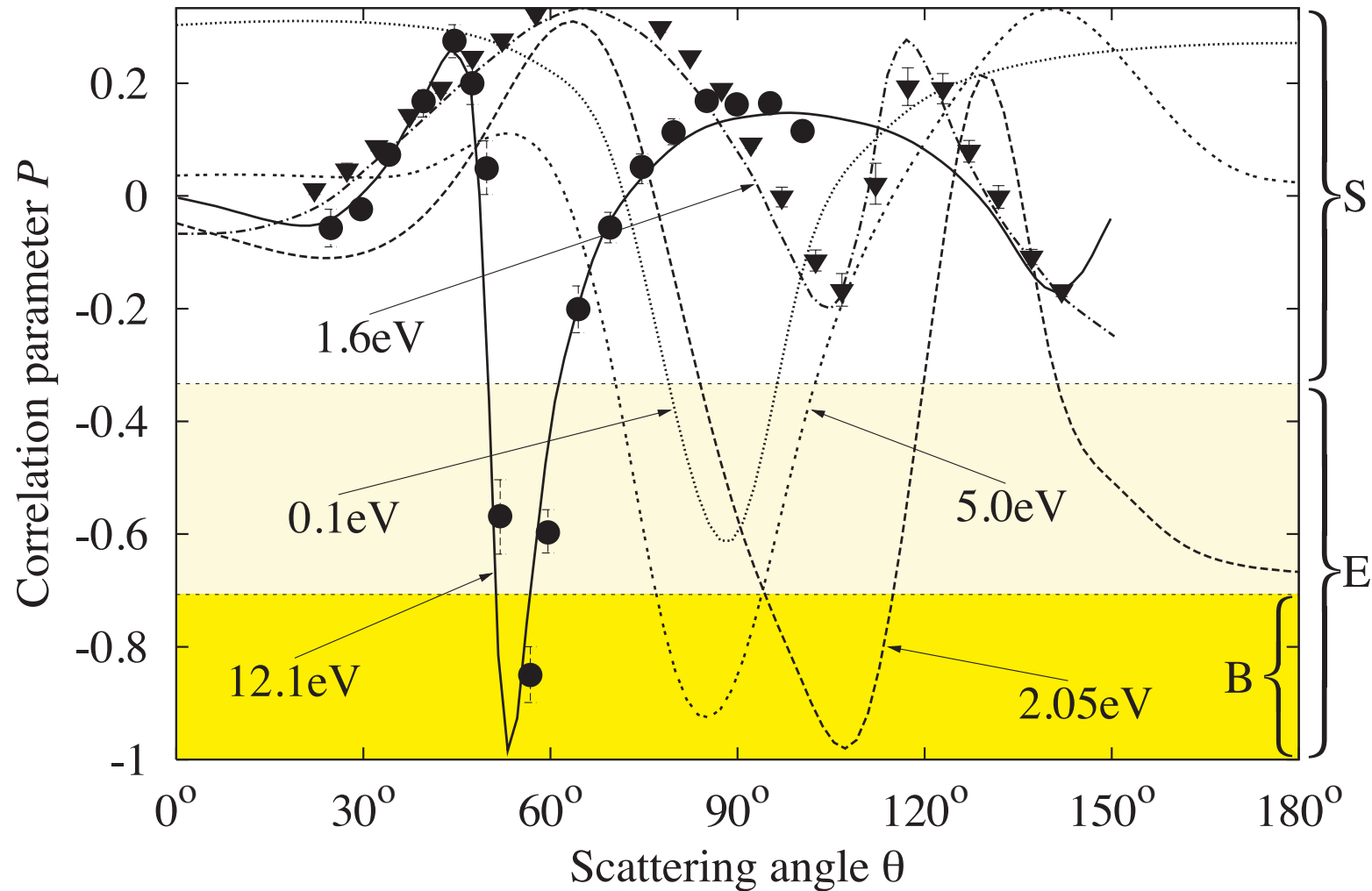


FIG. 8 Correlation parameter P of sodium versus scattering angle θ for different scattering energies. Exp. data by NIST group: 1.6 eV ($\blacktriangledown$), Lorentz *et al* (1991); 12.1 eV ($\bullet$), McClelland *et al* (1992). Num. data: 0.1 eV, 2.05 eV, and 5.0 eV (CC) Moores and Norcross (1972); 1.6 eV, (CCC) Bray (1994b); 12.1 eV, (CCO) Bray and McCarthy (1993). Horizontal lines divide separable (S), entangled (E), and Bell correlated (B) regions.

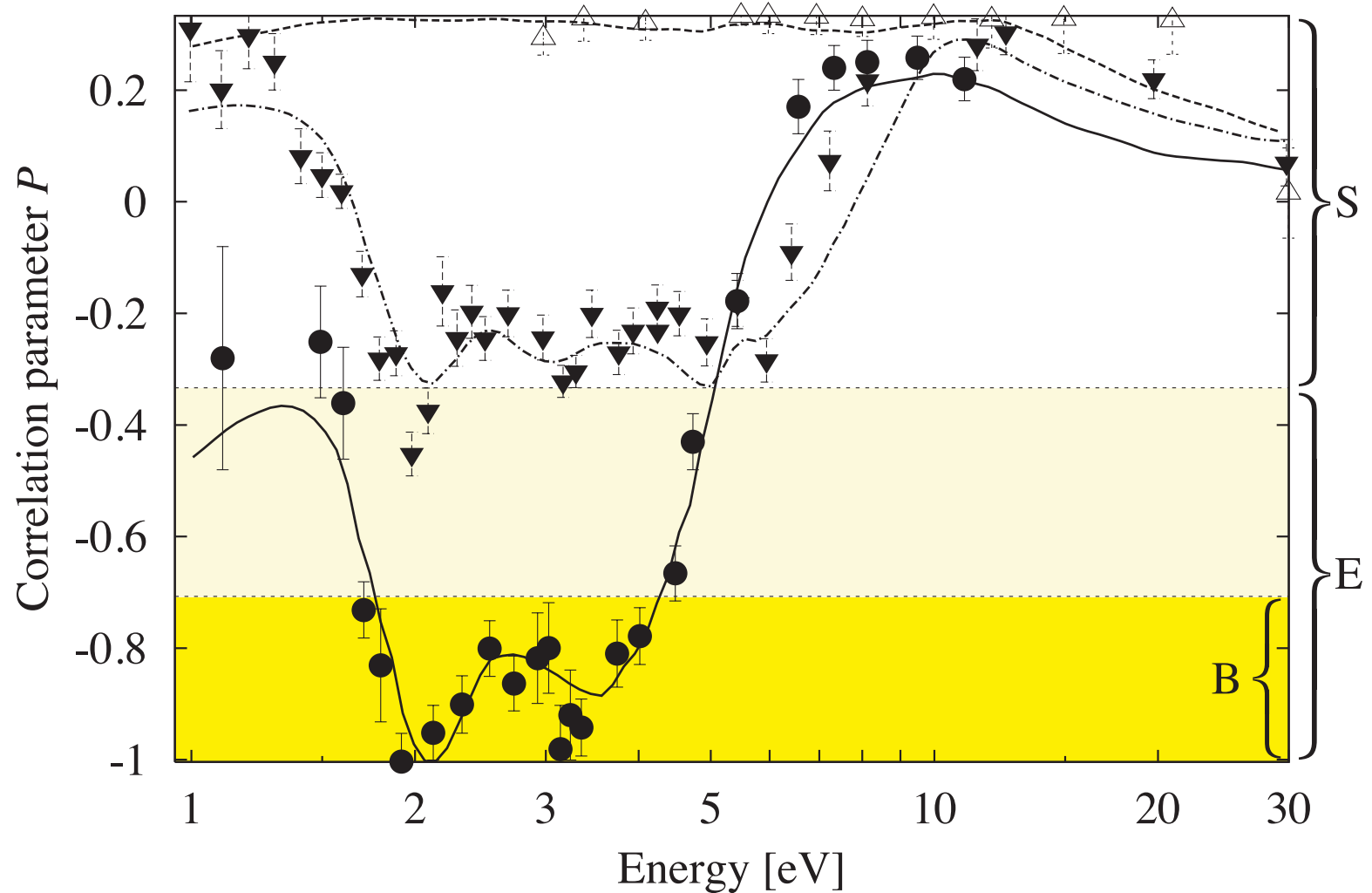


FIG. 9 Correlation parameter P of Li versus electron projectile energy in the range $E = 1 - 30$ eV for fixed scattering angles $\theta = 65^\circ$ ($\triangle$), 90° ($\blacktriangledown$), 107.5° ($\bullet$). Exp. data: [Baum *et al.* \(1986\)](#). Num. data: 13CCO8 calculation, [Bray *et al.* \(1993\)](#). Horizontal lines divide separable (S), entangled (E), and Bell correlated (B) regions.

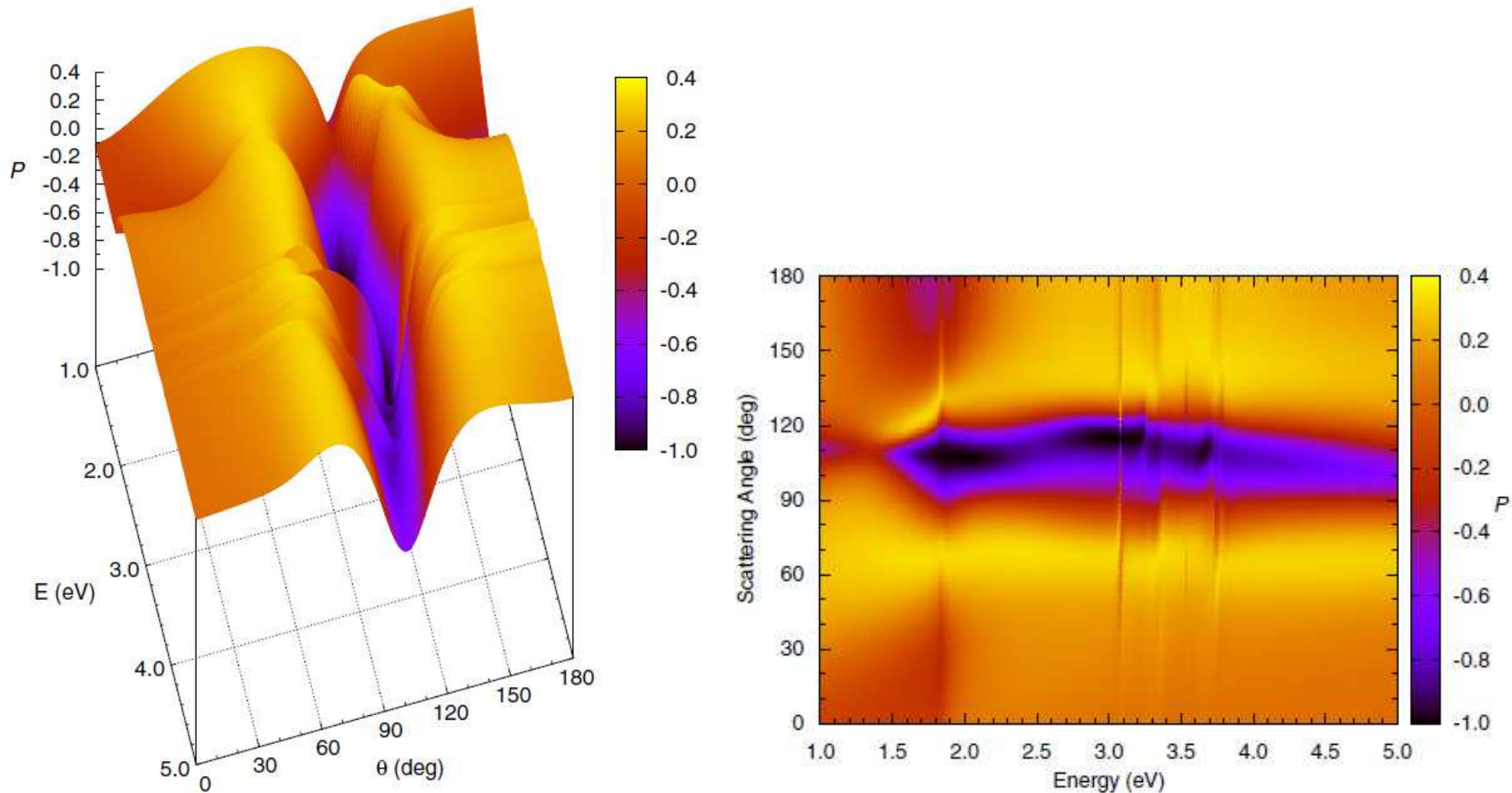


FIG. 10 Spin-correlation parameter P of Li versus electron projectile energy E and scattering angle θ as (left) 3D- and (right) contour plots, respectively. Num. data: 5-state close coupling R-matrix calculation, (Bartschat and Fonseca dos Santos, 2017).

Conclusions

- **Analysis** of numerical and experimental **spin asymmetry** A_{ex} yields results for the **spin correlation parameter** P .
- **Li and Na data** reveal surprisingly **strong spin correlations**, created out of an initially **totally chaotic spin system**. – Unexpected result. –
- **Experimentally**, the entangled spin pairs can be determined via **one local measurement of P** .
- In particular, **Bell correlated spin pairs** have been obtained.



The **CHSH-equation is maximally violated**, with $P \simeq -1$.

- This is **proof** that the discussed **electron exchange process** is intrinsically **non-local**.
- Considering the remarkable experiments with photons ([Hensen *et al*, 2015](#); [Giustina *et al*, 2015](#); [Shalm *et al*, 2015](#)), $\longrightarrow$ we **emphasize** that



our results originate from a **completely unrelated field** of research and refer to experiments with **massive particles**.



Therefore, our results yield **additional support** to the thesis that **nature behaves quantum mechanically and non-local**.

- By the scattering experiment **Bell pairs** can be produced **quickly and repeatable** in the full range between $-\frac{1}{\sqrt{2}} > P \geq -1$.
- Studying the Li and Na data (Figs. **6–10**) one can **tune to a particular scattering angle and energy**.
- 👉 Creating pairs of collision partners with any **desired degree of spin entanglement** $1/3 \geq P \geq -1$.
 - In particular, the **singlet state** ($P = -1$) can readily be generated in the collision.
 - These **pairs** can then be used for **further experiments** where pairs of particles with a **high degree of correlation** are required.
- 👍 This might be of interest for quantum **communication** or **teleportation** studies and might lead to a certain **entanglement** between **scattering physics** and **quantum information**.
 - New data for potassium are on their way (R-matrix); Bartschat *et al* (2017).



Quantification of Entanglement

Werner States and Negativity

- For negative values of $P = -|P|$, that is anticorrelated spins, we can write the scattering matrix ρ in form of a Werner state (Werner, 1989)

$$\rho = \frac{1 - |P|}{4} \mathbb{1} + |P| |00\rangle\langle 00|, \quad (37)$$

$$\text{with the singlet state } |00\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \quad (38)$$

- The Werner state (37) represents a mixture of the completely uncorrelated state $\sim \mathbb{1}$ (with amount $1 - |P|$) and the maximally entangled singlet state.
- The magnitude $|P|$ of the correlation parameter plays the role of a mixing parameter in the Werner state.
- In the range $-\frac{1}{3} > P \geq -1$ the density matrix ρ (37) represents an entangled spin state (Peres-Horodecki condition).
- Presence of entangled spin pairs $\iff$ verified experimentally by one local coincidence measurement, the determination of P .

- The amount of entanglement can be quantified using the concept of negativity (Zyczkowski *et al*, 1998; Vidal and Werner, 2002). Directly related to the Peres–Horodecki criterion.



Definition:

$$N(\rho) = -2 \sum_i n_i , \quad (39)$$

n_i are the negative eigenvalues of the partial transpose density matrix ρ^{PT} .

- If all eigenvalues > 0 , ρ is separable, $\implies N(\rho) = 0$.
- Thus, $N(\rho)$ *measures* the amount by which ρ^{PT} fails to be positive definite.
- $N(\rho) \sim |P|$ as a measure for the entanglement in the system ρ (Vidal and Werner, 2002).
- Only the eigenvalue λ_4 can become negative. Hence, for $P < -\frac{1}{3}$,

$$N(\rho) = -2\lambda_4 = \frac{1}{2} (3|P| - 1) , \quad (40)$$

$$N(\rho) = 1 \quad \text{for maximal entanglement, } P = -1 , \quad (41)$$

$$N(\rho) = 0 \quad \text{for zero entanglement, } P = -\frac{1}{3} . \quad (42)$$

- Using (40), we are able to rewrite the Werner state (37) in the form $(-\frac{1}{3} > P \geq -1)$

$$\rho = (1 - N)\rho_2 + N|00\rangle\langle 00| . \quad (43)$$

- ρ_2 denotes the clearly separable density matrix with anticorrelated spins

$$\rho_2 = \frac{1}{6} \sum_i |\uparrow_i\rangle\langle\uparrow_i| \times |\downarrow_i\rangle\langle\downarrow_i| + |\downarrow_i\rangle\langle\downarrow_i| \times |\uparrow_i\rangle\langle\uparrow_i| \quad i = x, y, z . \quad (44)$$

👉 Thus, the negativity $N(\rho)$ *measures* the amount of entanglement, contained in the system ρ , after all *classical* correlation $\sim \rho_2$ has been separated off from the original *non-local* singlet contribution.

- Only this fraction is useful for further entanglement studies.

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