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Entanglement, coherent states; a quantum rotor passing through an aperture

Synopsis of Ph.D. Thesis

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Introduction

In the quantum-mechanical description of a physical system the superposition principle plays a fundamental role, and this is the reason why the quantum and the classical descriptions show significant differences. In the mathematical framework the possibility of the superpositions is ensured by the complex Hilbert-space structure we use to define the states of a system [1]. The actual vectors of the Hilbert space are the so called *pure* states. They contain all the information known about a state what quantum mechanics allows at all. If the physical system is built up of several subsystems, then its Hilbert-space is a tensor product of the spaces belonging to the individual subsystems. This tensor product structure allowing the superpositions by definition provides the possibility of entanglement, which is one of the most pronounced difference between classical and quantum systems.

As an example let us consider a two qubit (or two-state) system, with qubits A and B , where each of which can be described by a two-dimensional Hilbert-space \mathcal{H}_2 . We assume that each of these Hilbert-spaces are spanned by the orthogonal and normalized basis states $|0\rangle$ and $|1\rangle$. The Hilbert space of the composite system is then the tensor product $\mathcal{H}_2^{(A)} \otimes \mathcal{H}_2^{(B)}$, which is naturally spanned by the following states:

$$\begin{aligned} |00\rangle &:= |0\rangle_A \otimes |0\rangle_B, & |01\rangle &:= |0\rangle_A \otimes |1\rangle_B, \\ |10\rangle &:= |1\rangle_A \otimes |0\rangle_B, & |11\rangle &:= |1\rangle_A \otimes |1\rangle_B. \end{aligned} \quad (1)$$

The superposition principle, however, allows the linear combinations of these basis states, as well. For example combinations like

$$|\Psi_{\pm}\rangle := \frac{1}{\sqrt{2}} (|0\rangle_A \otimes |1\rangle_B \pm |1\rangle_A \otimes |0\rangle_B). \quad (2)$$

do also belong to the state space of the composite system. These latter linear combinations (2) cannot be factorised into a single tensor product of a vector in $\mathcal{H}_2^{(A)}$ and a vector in $\mathcal{H}_2^{(B)}$. Vectors with this property are called *entangled* states, which grasps this non-separability property in a single word.

These type of states, introduced by D. Bohm [2] for spins, raise fundamental questions, which appeared in the literature soon after the emergence of quantum theory. The recognition of the problems having their roots in entanglement appeared in a paper by Schrödinger in 1935 [3]. In that work he considered a gedanken experiment about the entanglement of a macroscopic body (a cat) with different states of a radioactive atom, and emphasised the paradoxical nature of the situation. He also formulated his doubts on quantum theory itself, if it was a complete theory or not. Einstein, Podolsky and

Rosen (EPR) in their famous paradox [4] formulated the same question, and discussed it on a much deeper physical and philosophical level. The authors of the EPR paper considered the so called realistic viewpoint, and argued that if the value of a physical quantity can be predicted without making any measurement on it, then a complete theory must provide a well defined value for that quantity. A detailed analysis of a gedanken experiment showed that quantum mechanics violated either this seemingly natural preconception of realism or the locality principle. In 1964 J. S. Bell formulated his famous inequalities [5], which together with its later variants [6] opened the possibility to perform experiments and provide an evidence based decision of the question. The first experiments were carried out by J. Clauser and A. Aspect and by their co-workers [7, 8] with polarization states of entangled photon pairs. Later on the group of A. Zeilinger [9] and several other experimental teams worked on the problem of Bell-type tests. The actual experimental results showed that quantum mechanics violates the local realistic viewpoint and this was due to the presence of entanglement in the state of the two particles.

While the significance of entanglement is invaluable from the point of view of understanding the fundamental principles in nature, it promises useful practical applications, as well. The stronger than classical quantum correlations appearing in the entangled states can serve as a resource for quantum computation and for quantum communication protocols [10, 11].

There is another important concept in quantum mechanics, the notion of coherent states, showing quasi-classical behaviour. These are most well known as special quantum states of the harmonic oscillator, or in the context of quantum optics, as special states of a single or many field modes [12]. The construction of coherent states can also be interpreted as a problem in group theory, and thus similar coherent states can be associated to groups different from the Heisenberg-Weyl group pertinent to the oscillator problem [13].

In the case of a qubit system, modelling spin one-half particles, or two-level atoms, the mathematical conditions for a useful coherent state definition are readily given [14]. The Hilbert-space of one qubit carries the defining representation of the $SU(2, \mathbb{C})$ Lie-group, where the usual spin operators are the elements of the corresponding Lie-algebra. In case of a multi qubit system the tensor product representation enters, and the $\{J_z, J_+, J_-\}$ global spin operators, well known from the algebraic theory of angular momentum, play the crucial role. Coherent states are then defined by continuously parametrized exponential transformations of a reference state. Since these states emerged in the literature first in the context of two-level atomic systems [15], we often refer to them as *atomic coherent* states. The composite tensor product

structure suggests, that it is reasonable to investigate these states from the point of view of entanglement or separability.

In the example of a two qubit entangled state as given by (2) we can think about system A and system B as different particles. But entanglement is possible not just in this sense, namely as a property of a state of a set of different particles. Entanglement can also be created in the case of one single particle with different degrees of freedom. Here we can think of the Stern-Gerlach experiment, where the interaction of a silver atom with the inhomogeneous magnetic field induces entanglement between the spin and momentum degrees of freedom. Entanglement is thus a general property of quantum systems described by a tensor product space, and it can appear either in the context of independently measurable particles, or in the context of a single particle with different degrees of freedom.

This latter kind of entanglement is the subject of the second part of our dissertation. We consider the quantum mechanical scattering of a particle, with rigid but orientable internal structure, from a single slit in a thin screen. Progress in the experimental techniques has made it possible to study the transmission of particles through apertures, or aperture arrays, where the characteristic size of the projectile is comparable to the aperture. The observed phenomena include the scattering and interference from mechanical gratings of atoms, molecules, and clusters [16, 17, 18].

In connection with these experiments one may address the simple question: what is the effect of the aperture on the transmission of the particle with an internal structure, is the passage enhanced or hindered? In our simple model we assume a rigid rotation as internal structure and constrain the centre-of-mass motion to be along the symmetry axis of the aperture, so the motion has only two degrees of freedom. Far away from the aperture the translational and rotational degrees of freedom are uncoupled, so the energy eigenfunctions of the Hamiltonian separate into a product of a plane wave, corresponding to the centre-of-mass motion, and a transversal mode function of the free rotation. We take into account the interaction with the aperture through boundary conditions, prescribed for the energy eigenfunctions, which results in the entanglement of translational and rotational degrees of freedom. In this way we are left with a stationary scattering problem on a complicated two-dimensional boundary. In the region of free motion the rotational part of the energy eigenfunctions experience a periodic boundary condition, giving rise to a discrete spectrum with respect to the rotation. In this sense our scattering problem is *quasi one-dimensional*, where the interaction-free regions are represented by *leads*, leading to and leading away the incoming and outgoing probability currents. Throughout the interaction the different

plane wave modes of these leads are scattered into each other.

In this construction the translational and rotational motions can be entangled even when we consider only the incident particle, thus a specific incident energy supports multiple separable eigenfunctions. But even if the incident rotor had a separable wavefunction (as in the cases we investigated), the state at the output would necessarily become an entangled combination of the mode functions determined by the S-matrix of the problem. Different incident energies refer to different linear combinations i.e. different entangled states. The amplitudes of these combinations contain the useful physical information, the transmission or the reflection coefficients with depending on the energy of the incident wave.

Research aims, methods and outline of the thesis

Part I.: Coherent states and entanglement

Both the concept of entanglement and the concept of coherent states play an important role in several quantum mechanical problems, but their strong connection is hardly ever mentioned in the literature. We are aware of only one earlier paper, where Brif et al. [19] pointed out a relation between coherent states and entanglement. They have shown what happens if a system is split into two parts, while we investigate the question of total separability in a multi-partite system.

The aim of the first part of our work is to investigate the atomic coherent states of an N qubit system from the point of view of entanglement or separability. Throughout of our proofs and calculations we rely on the Hilbert space structure of the problem, and use arguments familiar from the theory of angular momentum algebra.

In the first chapter of the dissertation we shortly recall the concept of qubits, the operators acting on them, and the algebraic structure coded in their commutation relations, which determines the possible dynamics in the two-state system. Then in a short survey we review the construction of atomic coherent states [15] as special states of the symmetric subspace in the multi-partite qubit system. The N -partite symmetric subspace \mathbb{S} is spanned by those Dicke-states [20] which can be indexed with quantum numbers $j = N/2$ and $m \in \{-N/2, \dots, N/2\}$ known from the theory of angular momentum.

We present our results and the proofs in the second and third chapter. Here we first formulate a formal criterion of N qubit pure state separability

inspired by an idea behind the entanglement measure introduced by Meyer and Wallach [21].

We present first the results for the qubit system, which can be grasped more easily, in chapter 2. Then in the third chapter we generalize our results derived earlier for the qubit system, for the case of *qudits*, where the subsystems are d -dimensional Hilbert spaces. Compared to the qubit case the number of rising and lowering operators increase together with the number of zero trace diagonal operators. We define the coherent states generalized for the case of $SU(d, \mathbb{C})$ symmetry with help of these step operators. Then we prove the generalised statements following the logical steps of the qubit case.

Part II. The transmission of a rotating diatomic molecules through an aperture

In the second part of the dissertation starting with the fourth chapter, we consider the energy eigenvalue problem modelling a rigidly rotating diatomic molecule that passes through a thin aperture. The problem is simplified and reformulated to a quasi one-dimensional scattering problem with unconventional boundary conditions prescribed for the wavefunction through the classical constraints. Our goal is to solve the scattering problem and investigate the effect of the inner structure on the transmission probability of the particles.

In the fifth chapter we obtained results for incident particles of low energy by means of analytic approximations. Starting from a suitable ansatz, we decoupled the translational and rotational motions by preserving only the diagonal coupling terms, allowing analytical solution of the effective eigenvalue equation. The transmission as function of incident energy is calculated by fitting the solutions for the full two-dimensional problem at the boundaries of the interaction region and the free regions (so called leads) far from the aperture. The approximations we use can only be valid for low energy (non rotating) particles, but even in that case they may seem to be oversimplified. The verification of our analytical approximative results necessitates to use a numerical method that enables us to check the validity of the approximations, as well as to obtain the solution for the whole scattering problem, valid for an arbitrary incoming state.

We introduce a discrete lattice representation in the sixth chapter, where the complicated boundary conditions can be taken into account naturally, using only the lattice points where the wavefunction is declared to be nonzero. Complications in this case still appear, as the matrices of the relevant opera-

tors become infinite due to the free regions. A similar problem occurs in the modelling of quantum transport properties of nano-scale solid state systems, where the scattering problem is solved by calculating the Green's function for a relevant finite size region [22, 23, 24]. The Green's function is connected to the S-matrix through the Fisher-Lee relation [25]. Using the above analogy we derive in detail this connection for our case, where the periodic boundary condition prescribed for the rotation introduces complex transversal mode functions.

By a proper partitioning of the problem, it is possible to show that only a restricted part of the Green's function is necessary to describe the interaction. This restricted part can be calculated by "dressing up" the original Hamilton operator with the so called self-energy corrections. These corrections – though only on a discrete lattice – take into account the effect of the connection with the infinite parts exactly [22].

The characteristic features of the continuous energy spectra, containing for example long-living resonant states, are embodied in the spectral function, that provides us the density-of-states (DOS), as well as the local density-of-states (LDOS). All of these characteristic quantities can be calculated with help of the Green's function.

New scientific results

Part I.: Coherent states and entanglement

1. We have formulated a new general formal criterion for the separability of a pure state of a multi-partite N qudit system. Accordingly, taking an arbitrary pure N qudit state $|\psi\rangle$, and selecting one of the qudits, say the n -th one, we can decompose $|\psi\rangle$ as

$$|\psi\rangle = |1\rangle_n \otimes |u_n^1\rangle + |2\rangle_n \otimes |u_n^2\rangle + \dots + |d\rangle_n \otimes |u_n^d\rangle, \quad (3)$$

where $|k\rangle_n$ are the standard basis vectors in the n -th d -dimensional Hilbert space, while the $|u_n^k\rangle$ -s are states of a tensor product space of $N - 1$ factors, which are not normalized in general. Based on the decomposition given by (3), we have shown that $|\psi\rangle$ is a product state, if and only if the $|u_n^k\rangle$ vectors are parallel for all k for a given n , and this is valid for all possible n -s [A2, A3].

2. For a multi-partite system consisting of N qubits we have shown that a state in the symmetric subspace \mathbb{S} of the composite system is not entangled, if and only if it is a coherent state [A1]. We have extended

and proved this statement for generalized coherent states of a system consisting of several d -dimensional subsystems (qudits) [A3].

3. We have shown both for qubits and qudits that an arbitrary state which is an element of \mathbb{S}_\perp (which is the orthogonal complement of the symmetric subspace \mathbb{S}) is always an entangled state [A1, A3].

Part II. The transmission of a rotating diatomic molecule through an aperture

4. We have investigated the energy eigenvalue equation of a rotating diatomic molecule. Starting from a suitable ansatz, we decouple the translational and rotational motions thereby obtaining a set of one-dimensional Schrödinger equations for the hindered translation with *effective potentials*. These effective potentials can be further approximated by a fictitious harmonic oscillator, and this allowed us to give an approximate analytic solution for the stationary states in the interaction region. Fitting these solutions to the incoming and outgoing free wavefunctions, we have calculated the transmission coefficient as the function of the energy [A4].
5. For an initially non-rotating rotor we have found resonances in the transmission, which emerge as the consequence of the wave-like nature of quantum-mechanical propagation. The resonances describe a delayed transmission of the rotor, i.e. they correspond to a trapping phenomenon. We have given an approximate expression for the energies of these resonances by expressing them with the ground state energy of the fictitious oscillator potential determined by the geometric parameters [A4].
6. In order to support the analytic results, and to extend the energy range, we have also solved the scattering problem by a numerically exact method. To this end we have reformulated the problem on a discrete grid within an appropriately chosen finite domain inside the interaction region. We have calculated the Green's function restricted to the interaction region by taking into account the self-energy corrections. The S-matrix and the wave function was then determined from the Green's function. The results of the numerical calculations allowed us to characterize the whole continuous spectrum, and we have determined the density of states (DOS), as well as the local density of states (LDOS) as functions of the energy. In the energy dependence of the

density of states we have found peaks again, related to resonances with long lifetimes, i.e. to trapping of the transmitted particles [A5].

7. Among the resonances with long lifetimes, the one with the lowest energy could be identified with the peak in the energy dependence of transmission found previously by our analytic method. Analyzing the energy dependence of the density of states, the resonances could be classified according to the rotational symmetries of the incoming waves. Our numerical calculations approved the analytic results obtained earlier at low energies, and pointed out the limits of the applicability of the analytic method, as well [A5].

Publications

- [A1] P. Dömötör and M. G. Benedict, “Coherent states and global entanglement in an N qubit system,” *Physics Letters A*, vol. 372, no. 21, pp. 3792–3795, 2008.
- [A2] P. Dömötör and M. G. Benedict, “Entanglement and coherent states,” *Physica Scripta*, vol. 2009, no. T135, p. 014030, 2009.
- [A3] P. Dömötör and M. G. Benedict, “Global entanglement and coherent states in an N-partite system,” *European Physical Journal D*, vol. 53, no. 2, pp. 237–242, 2009.
- [A4] B. W. Shore, P. Dömötör, G. Süssmann, E. Sadurní, and W. P. Schleich, “Scattering of a particle with internal structure from a single slit,” *New Journal of Physics*, vol. 17, no. 1, p. 013046, 2015.
- [A5] P. Dömötör, P. Földi, M. G. Benedict, B. W. Shore, and W. P. Schleich, “Scattering of a particle with internal structure from a single slit: Exact numerical solutions,” *New Journal of Physics*, vol. 17, no. 2, p. 023044, 2015.

Other Publications

- [E1] P. Dömötör and M. G. Benedict, “Entanglement and coherent states” [in Hungarian], *P. Ádám, T. Kiss, S. Varró (editors) Kvantumelektronika 2008: VI. szimpózium a hazai kvantumelektronikai kutatások eredményeiről*, 2008.

- [E2] P. Dömötör, P. Földi, M. G. Benedict, B. W. Shore, and W. P. Schleich, “Rotating molecules through an aperture: as simple quantum mechanical model” [in Hungarian], *P. Ádám , G. Almási (editors) Kvantumelektronika 2014: VII. szimpózium a hazai kvantumelektronikai kutatások eredményeiről*, 2014.
- [E3] P. Dömötör, E. Sadurní, and W. P. Schleich, “Trapping cold molecules in an aperture: Effect of internal structure on particle transmission through an opening”, *Book of Abstracts DPG Frühjahrstagung der Sektion AMOP Hannover*, 2010.
- [E4] P. Dömötör, O. Kálmán, K. Papp and M. G. Benedict, “A multimedia course for teachers of physics and science”, *Proc. 12th International Conference on Multimedia in Physics Teaching and Learning*, 2007.

References

- [1] Neumann, J., *Mathematische Grundlagen der Quantenmechanik*, Springer, 1932.
- [2] Bohm, D., *Quantum Theory*, Prentice-Hall, 1951.
- [3] Schrödinger, E., *Naturwissenschaften* **23** (1935) 807.
- [4] Einstein, A., Podolsky, B., and Rosen, N., *Phys. Rev.* **47** (1935) 777.
- [5] Bell, J. S., *Physics* **1** (1964) 195.
- [6] Clauser, J. F., Horne, M. A., Shimony, A., and Holt, R. A., *Phys. Rev. Lett.* **23** (1969) 880.
- [7] Freedman, S. J. and Clauser, J. F., *Phys. Rev. Lett.* **28** (1972) 938.
- [8] Aspect, A., Grangier, P., and Roger, G., *Phys. Rev. Lett.* **49** (1982) 91.
- [9] Weihs, G., Jennewein, T., Simon, C., Weinfurter, H., and Zeilinger, A., *Phys. Rev. Lett.* **81** (1998) 5039.
- [10] Nielsen, M. A. and Chuang, I. L., *Quantum Computation and Quantum Information*, Cambridge University Press, Cambridge, 2000.
- [11] Feynman, R. P., *International Journal of Theoretical Physics* **21** (1982) 467.

- [12] Glauber, R. J., Phys. Rev. **131** (1963) 2766.
- [13] Zhang, W.-M., Feng, D. H., and Gilmore, R., Rev. Mod. Phys. **62** (1990) 867.
- [14] Gilmore, R., Annals of Physics **74** (1972) 391 .
- [15] Arecchi, F. T., Courtens, E., Gilmore, R., and Thomas, H., Phys. Rev. A **6** (1972) 2211.
- [16] Fabre, C., Gross, M., Raimond, J.-M., and Haroche, S., J Phys B **16** (1983) L671.
- [17] Kalinin, A., Kornilov, O., Rusin, L., Toennies, J. P., and Vladimirov, G., Phys Rev Lett **93** (2004) 163402.
- [18] Hackermüller, L. et al., Phys Rev Lett **91** (2003) 090408.
- [19] Brif, C., Mann, A., and Revzen, M., Phys. Rev. A **57** (1998) 742.
- [20] Dicke, R. H., Phys. Rev. **93** (1954) 99.
- [21] Meyer, D. A. and Wallach, N. R., Journal of Mathematical Physics **43** (2002) 4273.
- [22] Datta, S., *Electronic Transport in Mesoscopic Systems*, Cambridge University Press, Cambridge, 1995.
- [23] Di Ventra, M., *Electrical Transport in Nanoscale Systems*, Cambridge University Press, Cambridge, 2008.
- [24] Ferry, D., Goodnick, S., and Bird, J., *Transport in Nanostructures*, Cambridge University Press, Cambridge, 2nd edition, 2009.
- [25] Fisher, D. and Lee, P., Phys. Rev. B **23** (1981) 6851.