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# Bell's theorem and chemical potential

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## Abstract

Chemical potential is a property which involves the effect of interaction between the components of a system, and it results from the whole system. In this paper, we argue that for two particles which have interacted via their spins and are now spatially separated, the so-called Bell's locality condition implies that the chemical potential of each particle is an individual property. Here is a point where quantum statistical mechanics and the local hidden variable theories are in conflict. Based on two distinct concepts of chemical potential, the two theories predict two different patterns for the energy levels of a system of two entangled particles. In this manner, we show how one can distinguish the non-separable features of a two-particle system.

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## 1. Introduction

Bell's theorem [1, 2] has a distinguished place in the contemporary research on the foundations of physics. In general terms, this theorem concerns two spin  $\frac{1}{2}$  particles which were together once and now have a space-like separation. According to this theorem, one cannot, *using a certain definition of locality*, construct a hidden variable theory that can reproduce all the predictions of quantum mechanics (QM). By a *certain definition of locality*, we mean 'Bell's locality condition' which in a local stochastic hidden variable (LSHV) theory is equivalent to the statistical independence of the values of the spin components of the two particles. While people agree that according to QM Bell's locality condition cannot hold at a sub-quantum level, there is no unanimous agreement on the scope of such non-locality [3]. Does it mean the existence of superluminal communication between the two particles or does it imply that two particles that have once interacted can never be considered to be independent of each other (or being separable), even though there is no exchange of information between them? Here

we are confronted with two quite distinct interpretations of Bell's locality condition which are usually referred to as 'locality' and 'separability' in the literature [4]. In a multi-component system, the locality assumption means that for a given component, the value of an observable does not depend on the measurements which are performed simultaneously on any other spatially separated component. This is Einstein's view of locality. In his view, however, the separability criterion implies that each component in a spacetime region has its own intrinsic physical state and that the entire physical state of a multi-component system is specified once one has determined the intrinsic state of each component [5]. In Bell's theorem, the two notions seem to be indistinguishable [6]: the spin correlations are the properties of the whole system, i.e. the correlations result from the entire singlet state, while the empirical verification of them would be possible once the spin measurements are performed simultaneously on two particles which have space-like separation.

There have been many attempts to give an interpretation of the context of Bell's theorem [7–9]. Here, we try to present a new perspective of this matter by explaining how it is possible to identify the non-separable trait of Bell's locality condition in a proposed experiment. Our argument shows that the distinction between the notions of non-locality and non-separability is actually realizable. Furthermore, our work gives a new insight into Bell's theorem in a broader sense in which the effective spin–spin interaction between any two particles with the same spin can be considered as a special factor for describing the non-separable nature of composite systems. The role of such interactions in understanding and formulation of the chemistry of solutions and mixtures is an open problem.

In our paper, we consider a system of two spin  $\frac{1}{2}$  particles which have been interacted via their spins in the past and then are spatially separated from each other. For such a system, we *do not* consider the spin correlations, i.e. we suppose *no* spin measurements are made on each individual particle. We introduce the idea of using the chemical potential as a classical property, instead of using spin correlations which have a quantum mechanical origin. Then, we carry out some simple quantum statistical mechanics (QSM) calculations for a singlet state to show that Bell's locality condition is equivalent to the assumption that those properties of each particle which result from the whole system can effectively be taken as individual properties. A physical consequence of this is that the energy pattern of the system can be obtained from the energy states of the individual particles. This is an implication of the separability criterion which is in conflict with what we get from QSM.

In section 2, we consider a method for producing pairs of entangled spin  $\frac{1}{2}$  particles in a singlet state and we review the QSM calculations for an effective spin–spin Hamiltonian. In section 3, we calculate the chemical potential of each particle in the quantum limit. We shall argue that Bell's locality condition is equivalent to the separability criterion when the whole system is taken into account. The non-separable character of the system is recognizable through a unique energy pattern which, in turn, can be identified by an appropriate spectroscopic measurement. Finally, in the last section, we review the significance of our analysis.

## 2. QSM calculations for an effective spin–spin interaction

Suppose we produce an ensemble of systems, each system containing a pair of spin  $\frac{1}{2}$  particles (e.g. two electrons). We send each pair of spin  $\frac{1}{2}$  particles towards an entangler which is assumed to be a device in which the two particles interact via their spins and thereby the entangled states are generated. After the interaction, we let the particles recede from each other. We assume that the temperature of the ensemble is very low and the other experimental conditions (if relevant) are so adjusted that the two emerging particles are in a singlet state.

We represent the spin–spin interaction of a pair of particles of our ensemble by the Hamiltonian

$$H_{\text{int}} = \alpha \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \quad (1)$$

where  $\vec{\sigma}^{(i)}$  represent Pauli spin matrices of the  $i$ th particle ( $i = 1, 2$ ) and  $\alpha$  is the exchange coupling coefficient between the two spins  $\vec{\sigma}^{(1)}$  and  $\vec{\sigma}^{(2)}$  and here we assume it to be a positive constant for a specific pair of spin  $\frac{1}{2}$  particles. Here, by  $\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}$  we mean  $\sigma_x^{(1)}\sigma_x^{(2)} + \sigma_y^{(1)}\sigma_y^{(2)} + \sigma_z^{(1)}\sigma_z^{(2)}$ .

A particular realization of producing the singlet states which is relevant to our discussion has been recently provided by using coupled quantum dot systems [10, 11]. Quantum dots are small semiconductor structures which can host a single electron in a three-dimensional confined region [12]. If two nearby single electrons in each quantum dot are being weakly coupled (e.g. by tunnelling between the dots), a double-dot system will be produced which is the result of a combined action of the Coulomb interaction and the Pauli exclusion principle. It has been shown that at low temperatures (typically about 0.2 K) and in the absence of magnetic fields, the ground state of a double-dot system is a spin singlet while the excited state is a spin triplet. Each pair of the entangled electrons can be injected into two distinct leads (one electron in each lead) and, then, the outgoing electrons are separated [13].

Considering the dynamics of the spins of two electrons which are confined in a double-dot system, the real Hamiltonian of the system can be replaced by the effective Heisenberg Hamiltonian (1), where  $\alpha$  is equal to  $\frac{1}{4}$  of the difference between the triplet and the singlet states. The order of magnitude of  $\alpha$  is about 0.05 meV, which is a typical value for the exchange energy between two electrons in a double-dot system [11].

In QSM, the density matrix of a coupled system, which is described by the Hamiltonian (1), can be written as

$$\rho = \frac{e^{-\alpha\beta \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}}}{z} \quad (2)$$

where  $\beta = \frac{1}{kT}$ ,  $T$  is the temperature,  $k$  is the Boltzmann constant and  $z = \text{Tr}(e^{-\beta H_{\text{int}}})$  denotes the partition function of the two-particle system.

Using the properties of Pauli matrices, one can show that

$$e^{-\alpha\beta \sigma_j^{(1)} \sigma_j^{(2)}} = \cosh(\alpha\beta) - \sigma_j^{(1)} \sigma_j^{(2)} \sinh(\alpha\beta) \quad (3)$$

where  $j = x, y, z$ ;  $\cosh(\alpha\beta) = \frac{e^{\alpha\beta} + e^{-\alpha\beta}}{2}$  and  $\sinh(\alpha\beta) = \frac{e^{\alpha\beta} - e^{-\alpha\beta}}{2}$ .

Inserting (3) in (2), we obtain

$$e^{-\alpha\beta \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}} = \prod_{j=x,y,z} \left[ \cosh(\alpha\beta) - \sigma_j^{(1)} \sigma_j^{(2)} \sinh(\alpha\beta) \right]. \quad (4)$$

Using the properties of Pauli matrices again, (4) reduces to

$$e^{-\alpha\beta \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}} = \frac{1}{4} (e^{3\alpha\beta} + 3e^{-\alpha\beta}) (1 - \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} S_{\alpha\beta}) \quad (5)$$

where  $S_{\alpha\beta} = \frac{e^{2\alpha\beta} - e^{-2\alpha\beta}}{e^{2\alpha\beta} + 3e^{-2\alpha\beta}}$ . The eigenstates of  $\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}$  consist of  $|\Phi_1\rangle = |++\rangle$ ,  $|\Phi_2\rangle = |--\rangle$  and  $|\Phi_3\rangle = \frac{1}{\sqrt{2}} [|+-\rangle + |-+\rangle]$  with the eigenvalue +1 and  $|\Phi_4\rangle = \frac{1}{\sqrt{2}} [|+-\rangle - |-+\rangle]$  with the eigenvalue -3. Here,  $|+-\rangle$  indicates that the values of the  $z$ -components of both  $\sigma_z^{(1)}$  and  $\sigma_z^{(2)}$  are +1, and a similar definition holds for the other cases.

Using a complete set of these eigenstates, we can calculate the partition function  $z$ :

$$z = \text{Tr} \left( e^{-\alpha\beta \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}} \right) = e^{3\alpha\beta} + 3e^{-\alpha\beta}. \quad (6)$$

Thus, (2) is reduced to

$$\rho = \frac{1}{4}(1 - \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} S_{\alpha\beta}). \quad (7)$$

At very low temperatures ( $T \rightarrow 0$  or  $\beta \rightarrow \infty$ ), we have  $\lim_{\beta \rightarrow \infty} S_{\alpha\beta} = 1$ . This limit is known as the quantum limit. According to QSM and in the quantum limit, we have

$$\rho_{\text{QM}} = \frac{1}{4}(1 - \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}). \quad (8)$$

The states  $|\Phi_1\rangle$ ,  $|\Phi_2\rangle$  and  $|\Phi_3\rangle$  are three eigenstates of  $\rho_{\text{QM}}$  with the eigenvalue zero and  $|\Phi_4\rangle$  is the singlet state with the eigenvalue +1. Thus  $\rho_{\text{QM}}$  can be written as  $\rho_{\text{QM}} = |\Psi_0\rangle\langle\Psi_0|$ , where  $|\Psi_0\rangle = |\Phi_4\rangle$ , i.e. the singlet state. This can also be shown by writing  $|+\rangle\langle+| = \frac{1}{2}(1 + \sigma_z)$ ,  $|-\rangle\langle-| = \frac{1}{2}(1 - \sigma_z)$ ,  $|+\rangle\langle-| = \frac{1}{2}(\sigma_x + i\sigma_y)$  and  $|-\rangle\langle+| = \frac{1}{2}(\sigma_x - i\sigma_y)$  and substituting these in the  $|\Psi_0\rangle\langle\Psi_0|$  expression.

Relation (8) shows that for a pair of spin  $\frac{1}{2}$  particles which have interacted through the Hamiltonian (1), the spin state of the system in the quantum limit is described by a singlet state. When these two spin  $\frac{1}{2}$  particles interact, we get two energy levels: one having a lower energy  $-3\alpha$  belonging to the singlet state; the other having a higher energy  $+\alpha$ , belonging to the triplet state. At very low temperatures, the lowest occupied energy state is the one having the energy  $-3\alpha$  and so the quantum state of the system is a pure singlet state. When no perturbation is introduced, the system will remain in the singlet state. But, if the temperature is raised the pure singlet state is lost. Similarly, once we measure a spin component of a particle, there is going to be an interaction with an external field (e.g. a magnetic field in the case of Stern–Gerlach apparatus). Then, the energy pattern of the system is changed and a new pattern will be formed which is composed of the single-particle energy states.

### 3. QSM versus LSHV theories

Consider a canonical ensemble consisting of  $N$  identical distinguishable coupled systems, e.g.  $N$  double quantum dot systems in a semiconductor heterostructure [12] which are distinguishable because of their locations. The partition function of the canonical ensemble is  $Z = z^N$ , where  $z$  is the partition function of the two-particle system and is obtained from (6). If we denote the number of particles 1 and 2 in the ensemble by  $N_1$  and  $N_2$ , respectively, then  $N = \frac{N_1 + N_2}{2}$ . For this ensemble, the chemical potential of each particle resulting from the spin interaction of each pair (which is a coupling process), under the condition of a definite temperature, is equal to

$$\mu_i = -\frac{1}{\beta} \left( \frac{\partial \ln Z}{\partial N_i} \right) = -\frac{1}{2\beta} \ln z \quad (9)$$

where  $i = 1, 2$ . Using (6) and (9), we get

$$\mu_1 = \mu_2 = -\frac{3}{2}\alpha - \frac{1}{2\beta} \ln(1 + 3e^{-4\alpha\beta}). \quad (10)$$

In the limit  $\beta \rightarrow \infty$ , the chemical potential reduces to  $-\frac{3}{2}\alpha$ . Chemical potential can be defined for any species of particles in the pair, but *it is not an individual property*. From (9), it is clear that the chemical potential of each particle can be calculated from the partition function of the two-particle system, and here one cannot reduce  $z$  to the single-particle case. In other words, the chemical potential for each particle is a property which involves the effect of interaction and results from the whole system. From (10), it is clear that the effect of interaction on the chemical potential enters through the parameter  $\alpha$  and in the quantum limit, it approaches the value  $-\frac{3}{2}\alpha$ . On the other hand, in the quantum limit, the canonical ensemble reduces to a pure ensemble in which only the ground state is occupied. In this case, we

have the maximum amount of order in the system and the entropy of each system, which is  $S = -k\text{Tr}(\rho_{\text{QM}} \ln \rho_{\text{QM}})$ , is equal to zero. Thus, due to the existence of thermodynamic equilibrium in the system, the chemical potential of the whole system, which is in the ground state, is equal to the sum of single-particle chemical potentials in a coupling process, and we have  $\mu_1 + \mu_2 = -3\alpha$ .

Now, suppose that we have a sub-quantum level describable by some hidden variables, in which the principle of separability is honoured. After the spin–spin interaction of the two-particle system and when the two particles are spatially separated, we assume that the joint probability for the spin of particle 1 along  $\hat{a}$  ( $\sigma_a^{(1)}$ ) being  $r$  ( $r = \pm 1$ ) and the spin of particle 2 along  $\hat{b}$  ( $\sigma_b^{(2)}$ ) being  $q$  ( $q = \pm 1$ ), is equal to

$$p_{r,q}^{(1,2)}(\hat{a}, \hat{b}, \lambda_r^{(1)}, \lambda_q^{(2)}) = p_r^{(1)}(\hat{a}, \lambda_r^{(1)}) p_q^{(2)}(\hat{b}, \lambda_q^{(2)}) \quad (11)$$

where  $p_r^{(1)}(\hat{a}, \lambda_r^{(1)})$  and  $p_q^{(2)}(\hat{b}, \lambda_q^{(2)})$  are individual probabilities for particles 1 and 2, respectively. Here, we are assuming that the spin state corresponding to  $\sigma_a^{(1)} = +1$  or  $-1$  ( $\sigma_b^{(2)} = +1$  or  $-1$ ) for particle 1 (2) could be made to correspond to *different* collections of hidden variables  $\lambda_+^{(1)}$  or  $\lambda_-^{(1)}$  ( $\lambda_+^{(2)}$  or  $\lambda_-^{(2)}$ ) respectively, although in Bell's theorem, they are usually characterized by a unique set of hidden variables  $\lambda$ . Thus, with a broader attitude, we consider relation (11) as a criterion for the so-called Bell's locality condition in an LSHV theory. In a canonical ensemble, the individual probabilities are equal to

$$p_r^{(1)}(\hat{a}, \lambda_r^{(1)}) = \frac{e^{-\beta\epsilon_r^{(1)}(\hat{a}, \lambda_r^{(1)})}}{z^{(1)}} \quad (12)$$

and

$$p_q^{(2)}(\hat{b}, \lambda_q^{(2)}) = \frac{e^{-\beta\epsilon_q^{(2)}(\hat{b}, \lambda_q^{(2)})}}{z^{(2)}}. \quad (13)$$

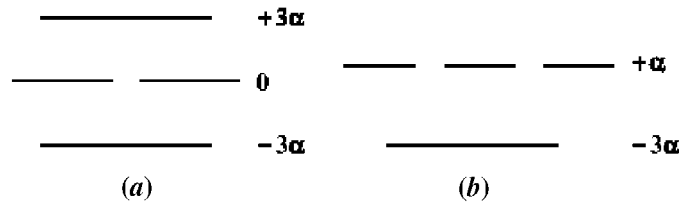
In (12),  $\epsilon_r^{(1)}(\hat{a}, \lambda_r^{(1)})$  refers to two energy levels  $\epsilon_+^{(1)}(\hat{a}, \lambda_+^{(1)})$  (corresponding to  $\sigma_a^{(1)} = +1$ ) and  $\epsilon_-^{(1)}(\hat{a}, \lambda_-^{(1)})$  (corresponding to  $\sigma_a^{(1)} = -1$ ). It is assumed that these levels *split* due to the spin–spin interaction of the pair. Also,  $z^{(1)}$  is the partition function of the particle (1) and is equal to  $z^{(1)} = e^{-\beta\epsilon_+^{(1)}} + e^{-\beta\epsilon_-^{(1)}}$ . The same description holds for (13). In the canonical ensemble, the chemical potential of the first particle is equal to

$$\begin{aligned} \mu_1 &= -\frac{1}{\beta} \ln z^{(1)} \\ &= \epsilon_+^{(1)} - \frac{1}{\beta} \ln \left[ 1 + e^{-\beta(\epsilon_-^{(1)} - \epsilon_+^{(1)})} \right]. \end{aligned} \quad (14)$$

In the quantum limit,  $\beta \rightarrow \infty$ , depending on whether  $\epsilon_+^{(1)}$  is lower or  $\epsilon_-^{(1)}$ ,  $\mu_1$  becomes equal to one of them. In this case,  $\mu_1$  is numerically equal to the energy of the occupied ground state. According to (10), in the limit  $\beta \rightarrow \infty$ , this value must be equal to  $-\frac{3}{2}\alpha$ . Thus, the spin energy level of the first particle, after the interaction with the second particle, splits into two levels:  $-\frac{3}{2}\alpha$  and  $+\frac{3}{2}\alpha$ . But, these are the corresponding hidden variables that determine which of these two levels belongs to  $\epsilon_+^{(1)}$  and which one belongs to  $\epsilon_-^{(1)}$ . The same result holds for the second particle. Thus, we have

$$z^{(1)} = z^{(2)} = e^{-\frac{3}{2}\alpha\beta} + e^{+\frac{3}{2}\alpha\beta}. \quad (15)$$

In relation (15) and consequently relations (12) and (13), the effect of interaction is introduced through the parameter  $\alpha$ . It is also important to note that the equation obtained for



**Figure 1.** The pattern of the energy levels of the two-particle system (a) according to the LSHV theory and (b) according to the QSM calculations.

$z^{(1)}$  and  $z^{(2)}$  in (15) is *independent* of what was assumed about lambda in an LSHV theory, but it is based on the crucial expressions of chemical potential in relations (10) and (14).

Here, we are dealing with *two different concepts* for  $\mu_1$  and  $\mu_2$ . In the sub-quantum level, Bell's locality condition requires that the chemical potential of each particle to be an *individual property* and that in the quantum limit, it represents the lowest occupied energy state for the particle. On the other hand, QSM calculations show that for a system of two entangled particles there are *no* individual energy levels in the limit  $\beta \rightarrow \infty$ , and that  $\mu_1$  and  $\mu_2$  do *not* represent the ground state energy of single particles.

According to Bell's locality condition, the partition function of a canonical ensemble is equal to

$$z = z^{(1)}z^{(2)} = e^{-3\alpha\beta} + e^{+3\alpha\beta} + 2. \quad (16)$$

Thus, we are dealing with two different patterns for the energy levels. According to (16), the system has three energy levels with the following characteristics:

- The ground state with an energy of  $-3\alpha$ , where each particle has an energy of  $-\frac{3}{2}\alpha$ .
- The first excited level, involving two states of zero energy, where the first particle has an energy of  $-\frac{3}{2}\alpha$  and the second particle has an energy of  $+\frac{3}{2}\alpha$  and vice versa.
- The second excited state with an energy equal to  $+3\alpha$ , corresponding to the case where each particle has an energy of  $+\frac{3}{2}\alpha$  (figure 1(a)).

The aforementioned description for the energy pattern of the system, which results from different possible combinations of the single-particle energy levels, is an explicit result of the separability condition. On the other hand, according to (6), the system has two energy levels: the ground state with an energy of  $-3\alpha$ , and the first excited level including three states of an energy  $+\alpha$  (figure 1(b)). This pattern cannot be deduced from the sums of individual energy states.

In an LSHV theory, Bell's locality condition implies the first pattern which in turn is a consequence of the separability criterion, but QSM admits the second one. There is an obvious difference in the physics of the problem. Now, suppose, e.g., that the two-particle system is in the ground state (i.e. in the quantum level). Furthermore, suppose that a radiation of energy  $+3\alpha$  is incident on the system. In the first model, there is always a probability for the system to be excited to the zero-energy level (i.e. one of the particles remains in the level  $-\frac{3}{2}\alpha$  and the other one goes to the level  $+\frac{3}{2}\alpha$ ), and then returns to the initial state by the emission of a photon with the energy  $+3\alpha$ . But this process does not take place in the second model, i.e. there would be no change in the system. The spectroscopic study of the coupled quantum dot systems has been cited in [11].

#### 4. Conclusion

We are concerned here with the concept of chemical potential. In a multi-component system, the chemical potential attributed to each component is generally a property which results from the whole system, i.e. it cannot be interpreted to represent an individual property of a specific component of the system. But Bell's locality condition implies that chemical potential can be attributed to each component of the system as an individual property. Here, we use chemical potential as a characteristic feature of the composite systems to demonstrate the (non)separability notion.

Furthermore, after the pioneering work of Guggenheim for electrochemical processes in 1929 [14], it became clear that chemical potential is a quantity in which the interaction with the field can also be included. Then, the formulation of chemical potential was extended to include the potentials due to the interacting fields.

For two spin  $\frac{1}{2}$  particles that interact via their spins at low temperatures and then recede from each other, the calculation of the chemical potential of a particle in a canonical ensemble shows that once the system is described by a singlet state, the effect of the interaction remains in the particles, even if they are spatially separated. Here, there is a common characteristic for the two particles: they are constrained to a unique energy pattern. This is not due to the exchange of information between the particles; rather, it is due to their past interaction which implies the non-separable nature of a two-particle system. In the singlet state, the energy pattern of the system is not reducible. It is a property of the whole system and in the limit of low temperatures, the values of the chemical potential of single particles coincide with none of the individual energy levels. On the other hand, Bell's locality condition requires that at the sub-quantum level, when no spin measurements are performed on each particle, the energy pattern of the whole system can be obtained from the combination of the energy levels of the individual particles. This is a consequence of the separability assumption.

Thus, Bell's theorem is not confined to the evaluation and the comparison of spin correlations in the quantum and sub-quantum levels; rather, it can be used to distinguish the non-separable nature of composite systems which in turn sheds new light on the physics and the chemistry of complex systems, such as solutions and mixtures. Chemical potential is a key property in this context.

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