SCHRÖDINGER'S THOUGHTS ON PERFECT KNOWLEDGE

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> What is one is one
> What is not one is also one
>
> Chuang Tsu

ABSTRACT. Perfect knowledge of the many-body system is contained in the wavefunction but, as Schrödinger has already emphasized, best possible knowledge of a whole does not include the best possible knowledge of its parts. Separability from the point of view of quantum mechanics is discussed. General "entangled" systems are analysed in terms of knowledge. If the state vector is defined for a whole system its parts are described only by mixed density operators. Correlations violating Bell's inequality are necessary to avoid superluminal signaling and result from the lack of independent reality of subsystems. Model calculations on two separated atoms and on non-interacting gas show that the perfect knowledge of the whole system or the total wavefunction is not sufficient to calculate local properties without actually solving the local problem.

1. INTRODUCTION

The history of modern civilization spans roughly about 5000 years. Civilization is clearly in its infancy because a single lifetime may still span as much as 2% of its history. Only a few men have been privileged to contribute so much to the development of human thought as Erwin Schrödinger, whose centenary of birth we are now celebrating. He has introduced the concept of wavefunction to physics and never stopped bothering himself with its meaning. Quantum Mechanics (QM) is a strange theory already at the level of single-particle phenomena but, accepting the wave-particle dualism in one form or another [1], one can still form a reasonable picture of reality. It is the holistic nature of QM at the multi-particle level or, technically speaking, the existence of multi-particle nonfactorizable states, that is more bothering. A few months after the famous Einstein, Podolsky and Rosen (EPR) paper [2] appeared Schrödinger made a profound analysis of the problem [3]. He summarized the conclusion

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in one sentence: "Best possible knowledge of a whole does <u>not</u> include best possible knowledge of its parts - and that is what keeps coming back to haunt us".

It is my feeling that we have just started to explore the consequences of this statement. The present paper is an attempt to look at it from modern perspective. In the second section separability in QM is discussed. Next, two sections deal with the spatially extended quantum states, EPR paradox and Bell inequality. In section 5 general "entangled systems" are considered. Finally Schrödinger's statement about the knowledge of a whole is exemplified in section 6 on a model of non-interacting gas.

2. SEPARABILITY IN QUANTUM MECHANICS

The question "When can one consider two physical systems to be separate?" is rather subtle. Naively, if I could isolate one system and perform experiments on this system without influence from the second system I would call it "a separate system". From the QM point of view such a definition would be naive indeed: how can one be sure that the results of experiments are really not determined by what happens to the other system? Maybe the wavefunction of my system was changed by someone experimenting with the second system? The only way to know is by computing correlations between the results of measurements on the two systems and checking if these correlations are trivial, i.e. if they can be explained assuming that the systems are independent. I will come to this point in the next section.

Leaving aside the subtleties concerned with isolation of physical systems let us consider the question of separation. The common knowledge is that "when two systems interact, their ψ - functions... consist, to mention this briefly, at first simply of the product of the two individual functions...", as Schrödinger [3] has put it. Quite recently Rosen [4], discussing separability, made a similar statement. Is it really true?

There is no smooth connection between distinguishability and indistinguishability, and thus between the simple product of two functions and a total function with a definite permutational symmetry. If there was, is, or will be a possibility of an interaction the product function is a false start. No matter how small, the interaction makes the total Hamiltonian symmetric and forces a definite permutational symmetry on the total wave function. By setting the interaction to zero one switches off the possibility of any interaction in the future. But, to rephrase the famous remark of Pauli [5], "Was Gott vereint hat, soll der Mensch nicht trennen" (what God has united men should not separate). We cannot start with the product function without "playing God's role".

<u>Formal proof</u>: consider two systems, S_A and S_B, with N_A and N_B particles, respectively. Each system is described by its own function, χ_A antisymmetric in N_A particles and χ_B in N_B . It is easy to show that the product function $\chi=\chi_A\chi_B$ is always "far" from the antisymmetric function $\psi=\hat{A}\chi$ looking at the norm $||\chi-\psi||$. If χ and ψ are normalized then the antisymmetrizer $\hat{A}$ is

$$(1) \qquad \hat{A} = (N_A!N_B!/N!)^{1/2} \sum_P \epsilon(P)P$$

where $N = N_A + N_B$ and P is either identity or permutes particles of S_A with those of S_B. Therefore

$$(2) \qquad \|\chi-\psi\|^2 = \langle\chi-\hat{A}\chi|\chi-\hat{A}\chi\rangle = 2-2\mathrm{Re}\langle\chi|\hat{A}\chi\rangle \geq 2-2^{1/2}$$

because the integral $\langle\chi|\hat{A}\chi\rangle = (N_A!N_B!/N!)^{1/2}$ is not smaller than $2^{-1/2}$.

Quantum mechanics is thus unable to describe two separated systems. The minority attitude towards this fact is to beat the drum: "quantum mechanics is dead", as Piron does [6]. His criticism is based primarily on his own quantum logic approach and on the axiomatic approach of Aerts [7], who emphasized many times that "it is impossible in quantum mechanics to describe two separated physical systems". Aerts presented a theory of the quantum-logic type that allows for such a description. The majority adopts a "so what?" attitude. As long as QM calculations agree with experimental results everything is O.K. Axiomatic approaches are not important because they do not give numbers. I would like to adopt here the Middle Way: with the "so what" attitude we may easily overlook things that are important but we never dreamed of. On the other hand it is too soon to mourn over the death of quantum mechanics before we will find predictions in direct conflict with experimental results. After all, separation may be just one of these illusions acquired in the childhood. It is simply impossible to measure correlations among more than a few bodies but concentrating on just two particles correlations proving their nonseparability should be seen. Let us look closer at the consequences of quantum mechanics.

3. SPATIALLY EXTENDED QUANTUM STATES

Suppose that two spatially separated particles are in a pure quantum state. There are basically two ways in which such a state could be prepared. First, by breaking one system into fragments, for example in the two-photon cascade emission or photodissociation of H_2 into H + H in a triplet state, spatially extended systems in pure states are obtained. A second possibility, peculiar to QM, is to prepare the two systems in such a way that in future they will fit together into a single system in a definite way. As an example one may think of a particle or an odd-electron atom with total spin $S = ½$ crossing a magnetic field that separates $M_S = +½$ states. If one has two atoms in $|S=½, M_S=+½\rangle$ states coming from the opposite directions even before they start to interact they must be in $|S=1, M_S=1\rangle$ combined state. It is not a question of interaction at an earlier time but of the wave functions that we are allowed to write. The first possibility of forming a spatially separated quantum state is due to the common past and the second due to the common future [8].

Are there observable consequences of the existence of such quantum states? Obvious consequences were noted by Einstein, Podolsky and Rosen [2] and by Schrödinger [3] already in 1935. There are also less obvious consequences noted by Bell [9] in 1965. To see the obvious consequences let us write the state of the two systems as

$$(3) \quad |\psi\rangle = 2^{-1/2}(|a_1\rangle|b_1\rangle + |a_2\rangle|b_2\rangle)$$

where $|a_k\rangle$ ($|b_k\rangle$) are states of the system S_A (S_B). If a measurement on S_A finds the system in the state $|a_k\rangle$ then S_B should be in $|b_k\rangle$, so a measurement on one system selects the state of the other system! This is the essence of the EPR paradox, a feature of quantum mechanics entirely unacceptable to Einstein [10]. This is also the reason why the definition of separated systems given previously is naive. It is tempting to assume that the state $|\psi\rangle$ describes an ensemble of systems, half of them in the $|a_1\rangle|b_1\rangle$ and half in $|a_2\rangle|b_2\rangle$ state. Einstein himself has advocated such interpretation. Unfortunately this would remove all interference and exchange effects. Superposition of states is not just the question of our knowledge but of potential reality.

<u>Formal argument</u> against ensemble interpretation of $|\psi\rangle$ is the following: density operator ρ_m corresponding to the two ensembles $|a_1\rangle|b_1\rangle$ and $|a_2\rangle|b_2\rangle$ is:

$$(4) \quad \rho_m = \tfrac{1}{2}(|a_1\rangle|b_1\rangle\langle a_1|\langle b_1| + |a_2\rangle|b_2\rangle\langle a_2|\langle b_2|)$$

This operator does not correspond to the pure state (3) nor any other pure state because it is not idempotent ($\rho_m^2 \neq \rho_m$). It means that ρ_m does not represent the maximal knowledge about the total system. It misses precisely the correlation between the two systems, included in the true density operator $|\psi\rangle\langle\psi|$

$$(5) \quad \rho = \rho_m + \tfrac{1}{2}(|a_1\rangle|b_1\rangle\langle a_2|\langle b_2| + |a_2\rangle|b_2\rangle\langle a_1|\langle b_1|)$$

One may still think that there is some physical mechanism that reduces the pure state ρ to the mixture ρ_m as the distance between the two systems S_A and S_B increases, thus localizing the states around S_A and S_B. A proposition in this spirit has been most recently advocated by Piccioni [11], but it has a longer history. Einstein himself suggested that "the current formulation of the many-body problem in quantum mechanics may break down when particles are far enough apart" (in a private communication to Bohm [12]). The possibility of such a localization process has been also considered by other authors [1]. In particular some physicist believe that when the wave packets of the two systems are localized and do not overlap there should be no correlations between measurements on the two systems, i.e. the reduced density operator ρ_m should be used. In this context Bohm and Hiley [13] analyzed the anisotropy measurements of the gamma rays, showing that pure states extend over macroscopic distances, more than an order of magnitude exceeding the width of the wave packet associated with each photon. The situation is qualitatively different from that which one finds in the self-interference experiments of Jánossy-Náray type or in the neutron interferometry (see the review on "empty waves" by Selleri [14]) because the experiments involving single-particle states are easily explained using the wave picture. The wavefunction in the two-particle case exists in 6-dimensional space and cannot be pictured as a real wave.

Less obvious consequences of the existence of the extended pure states were found by J.S. Bell. I will discuss them briefly now.

4. EPR AND BELL INEQUALITY REVISITED

Let E_{ab} be the usual correlation coefficient between simultaneous measurements [cf. 15]. Under a very general assumptions of locality and realism one may then prove the Bell inequality: combination of four correlation coefficients with the parameters (in particular angles) (ab), (ab'), (a'b) and (a'b') must not exceed 2:

$$(6) \qquad \begin{array}{l} C(a,b,a',b') = E_{ab} - E_{ab'} + E_{a'b} + E_{a'b'} \\ |C(a,b,a',b')| \le 2, \quad |E_{ab}| \le 1 \end{array}$$

Correlations computed with the extended quantum states (3) violate this inequality. In singlet and triplet spin states correlation coefficients are

$$(7) \qquad \begin{array}{ll} |0,0\rangle \text{ state:} & E_{ab} = -\cos(a-b) \\ |1,0\rangle \text{ state:} & E_{ab} = -\cos(a+b) \\ |1,\pm1\rangle \text{ state:} & E_{ab} = \cos a \cos b \end{array}$$

In the singlet state inequality (6) is strongly violated because $C(0,45,90,135) = 2\cdot 2^{1/2}$. The same violation is observed in the triplet $|10\rangle$ state. Thus the existence of pure, spatially extended, nonfactorizable states is manifested by non-trivial correlations between the results of measurements on the two systems, correlations greater than allowed by Bell's inequality. Correlations that do not violate the Bell inequality are trivial if the two systems interacted in the past because one can explain them easily by local realistic models.

Is it possible to find non-trivial correlations between the systems that never interacted? In triplet $|1,\pm1\rangle$ states correlations are just as large as allowed by the Bell inequality, with $C(a,b,a',b')$ reaching at most 2. This is not surprising because $|1,+1\rangle = |\alpha\alpha\rangle$ and $|1,-1\rangle = |\beta\beta\rangle$, both are factorizable and therefore there are no interference terms in the density matrix [cf. 16]. But these are the only pure states that we know how to prepare externally! Mixture of all 4 states does not give any correlation, as one may expect. Going to higher spins, like $s = 3/2$, does not help either. Thus unless there is a way to prepare a pure state or a non-trivial mixture there will be no way to observe EPR correlations without previous interaction.

5. ENTANGLED SYSTEMS

Let us look from a more general point of view at the problem of "entanglement", as Schrödinger [3] calls it, manifested in EPR correlations violating local realism. If such correlations exist, as all experiments performed so far seem to indicate, then the ensemble interpretation of quantum mechanics cannot be maintained and local modifications of quantum mechanics are not admissible.

Two particles with spin ½ are in one of four spin states $|S,M\rangle$ but in experimental situations we usually have an ensemble described by a mixed state ($|\alpha\rangle$ and $|\beta\rangle$ are the single-particle spin functions):

$$(8) \qquad \rho(1,2) = \tfrac{1}{4}\Big(|0,0\rangle\langle 0,0| + \sum_M |1,M\rangle\langle 1,M|\Big) =$$
$$\tfrac{1}{2}(|\alpha\rangle\langle\alpha| + |\beta\rangle\langle\beta|)\,\tfrac{1}{2}(|\alpha\rangle\langle\alpha| + |\beta\rangle\langle\beta|) = \rho_1(1)\rho_1(2)$$

In general for N particles with spin ½ the number of states degenerate at large distance is 2^N and the mixed state is factorized

$$(9) \qquad \rho(1,2..N) = 2^{-N}\sum_S\sum_M |S,M\rangle\langle S,M| = \prod_i \rho_1(i)$$

It is very hard to avoid mixed states in real experimental situations and mixed spin-density operators are nicely separated into products of single-particle operators which represent mixtures, i.e. half of the particles with spin α and half with spin β in an ensemble of particles. This is an answer to the question why EPR correlations are not seen more often.

Factorizability of the density matrix is a stronger requirement than separability which should require no more than the lack of correlations between measurements on the two spatially separated systems. Indeed if one takes two spatial states, $|a\rangle$ localized around the system S_A and $|b\rangle$ around S_B, antisymmetric two-particle singlet and triplet functions give

$$(10) \qquad \begin{aligned} |\psi_{00}\rangle &= 2^{-1/2}(|ab\rangle+|ba\rangle)2^{-1/2}(|\alpha\beta\rangle-|\beta\alpha\rangle) \\ |\psi_{1M}\rangle &= 2^{-1/2}(|ab\rangle-|ba\rangle)|1,M\rangle \\ \rho &= \tfrac{1}{4}\sum_{SM}|\psi_{SM}\rangle\langle\psi_{SM}| = \tfrac{1}{2}(|ab\rangle-|ba\rangle)(\langle ab|-\langle ba|)\rho_1(1)\rho_1(2) \end{aligned}$$

The spin part is factorized but the spatial part is not. Off-diagonal matrix elements $|ab\rangle\langle ba|$ correspond to the exchange of particles between systems S_A and S_B and may be neglected at large separations of the two systems. Of course the (negligibly small) possibility of such an exchange always exists and the cross terms in the density operator simply remind us of this, but all operators $\hat{F}$ corresponding to physical observables have vanishing matrix elements $\langle a|\hat{F}|b\rangle = 0$. One may call it practical separability. Claims that quantum mechanics is not able to describe separated systems [6,7] are true but irrelevant. It is rather axiomatic approach to quantum mechanics ("new quantum theory" as Piron calls it [6]) that is unable to describe the process of separation because it washes out all physics inherent in this process. It is completely artificial to base separation on pure states requiring factorizability at large separations. Real processes must involve other bodies exerting forces breaking the system or processes like photodissociation, with all its subtleties, that no axiomatic approach can describe.

Let us come back to Schrödinger's analysis of entanglement. For the two systems in a pure state $|\psi_{AB}\rangle$ with the density operator ρ_{AB} one has

$$(11) \qquad |\psi_{AB}\rangle = \sum_n \lambda_n|A_n\rangle|B_n\rangle; \quad \rho_{AB} = \sum_{nm}\lambda_n\lambda_m^*|A_n\rangle|B_n\rangle\langle A_m|\langle B_m|$$

where ρ_{AB} is idempotent. If more than one λ_n value is non-zero there are non-trivial correlations between the two systems - they are entangled. A pure state represents the best possible or perfect knowledge about the whole system and that of course includes the correlations between the two subsystems. Maximal knowledge of S_A must include also the knowledge of its correlation with S_B, therefore it should not be possible to describe the S_A system separately by a wavefunction. Indeed, reducing ρ_{AB} to the subsystem,

$$(12) \qquad \rho_A = Tr_B(\rho_{AB}) = \sum |\lambda_n|^2 |A_n\rangle\langle A_n|$$

and similarly for ρ_B. These density operators correspond to mixed states because they are not idempotent. Taking

$$(13) \qquad 0 \leq \mu(\rho) = Tr(\rho-\rho^2) \leq 1$$

as the measure of loss of information one has $\mu(\rho) = 0$ for a pure state and $\mu(\rho) = 1$ or complete loss of knowledge for the worst mixed state possible. If the number of particles in both subsystems is large $\mu(\rho_A) \approx 1$. Almost all information about the whole system concerns the correlations between the two subsystems. Of course density operators do not tell us which part of the knowledge is interesting - it may be just the tiny local one, contained in the reduced density matrix.

Perfect knowledge of the whole is not the best possible knowledge of all parts even when the parts are not interacting. What does it imply in practice? It implies that non-trivial EPR correlations are necessary to avoid non-locality! This seems to be rather paradoxical because one is tempted to think about EPR correlations as proving non-locality. In fact it is the existence of extended quantum states that saves Einstein's locality introducing instead non-local correlations that cannot be used to send information [17].

7. REDUCING THE PERFECT KNOWLEDGE.

As another illustration of Schrödinger's statement that the best possible knowledge of the whole does not give the best possible knowledge of the parts consider two hydrogen-like atoms separated by a large distance R. It is the starting point of the Heitler-London theory of hydrogen molecule [cf. 18]. In this case the wavefunction is

$$(14) \qquad |\psi\rangle = 2^{-1/2}(|a\rangle|b\rangle \pm |b\rangle|a\rangle)|SM\rangle$$

where $|a\rangle$ is the 1s orbital centered on the atom A and $|SM\rangle$ is the corresponding spin function. The spinless Hamiltonian

$$(15) \qquad \begin{aligned} &H(1,2) = H_A(1) + H_B(2) + V(1,2); \quad T_i = -\tfrac{1}{2}\Delta_i \\ &H_A(1) = T_1 - Z_A/r_{A1}; \; H_B(2) = T_2 - Z_B/r_{B2}; \\ &V(1,2) = -Z_A/r_{A2} - Z_B/r_{B1} + Z_AZ_B/R + 1/r_{12} \end{aligned}$$

where the meaning of various terms is obvious [18]. For a large separation R the overlap integral $\langle a|b\rangle$ is zero and the energy is

(16) $\langle\psi|H|\psi\rangle = E_A + E_B$

We know that $|\psi\rangle$ is never reduced to a simple product of $|a\rangle$ and $|b\rangle$. Still we do hope that a local energy operator exists. Such is not the case! Take for example H_A and calculate

(17) $$\langle H_A\rangle = \langle\psi|H_A|\psi\rangle = \tfrac{1}{2}(\langle ab|H_A|ab\rangle + \langle ba|H_A|ab\rangle) = \tfrac{1}{2}(E_A + \langle b|H_A|b\rangle)$$

Calculating the last element directly or via the virial theorem one obtains

(18) $$\langle b|H_A|b\rangle = \langle b|T+V_A|b\rangle = \langle b|T|b\rangle = -\langle b|H_B|b\rangle = -E_B$$

This result may seem surprising but the state $|b\rangle$ belongs to the continuum of the H_A Hamiltonian. As a result the average value is

(19) $$\langle\psi|H_A|\psi\rangle = -\langle\psi|H_B|\psi\rangle = \tfrac{1}{2}(E_A-E_B)$$

Thus the sum of the local energies for the two atoms is zero! Where is all the energy gone? It is easily verified that

(20) $$\langle\psi|V|\psi\rangle = E_A + E_B$$

Calculating local energies using local operators and non-local wave-function gives paradoxical results: all the energy is in the interaction, although the interaction terms are negligibly small. Extension of this simple model to a gas of N noninteracting hydrogen atoms in the 1s states with -1/2 atomic unit of energy gives

(21) $$\langle\psi_{1s}(1..N)|H_A(1)|\psi_{1s}(1..N)\rangle = (N-2)/2N$$
$$\langle\psi_{1s}(1..N)|V_A(1)|\psi_{1s}(1..N)\rangle = 1-N$$

For the excited states $|2s\rangle$ with the energy -1/8 au the local energy comes out as $(N-2)/8N$, i.e. is lower than in the ground state!

These surprising results may be interpreted in different ways. Since the total wave function of the world is not reducible to a product function strictly speaking local energies are not well defined and a kind of "quantum Mach principle" is introduced: it is the interaction, even if negligibly small, that gives meaning to the total properties like energy. If $|\psi\rangle$ is the exact multi-particle state and one-particle approximation is not introduced from the beginning it is not easy to obtain local properties from the knowledge of the whole. Perfect knowledge of the whole should be complemented by the knowledge of local states.

From another point of view the decomposition (15) of the total Hamiltonian, although the most natural one, leaves the interaction $V(1,2)$ in a non-symmetric form. The problem is that there is no better decomposition and thus no way of reducing the description of the whole to the description of one of the non-interacting parts. To obtain a local density operator one has to know local states and project the reduced density operator on these local states. For the two atoms

$$
\begin{aligned}
(22) \qquad \rho_1 &= \mathrm{Tr}_2|\psi\rangle\langle\psi| = ½(|a\rangle\langle a|+|b\rangle\langle b|) \\
\rho_A &= (|a\rangle\langle a|)\ 2\rho_1 = |a\rangle\langle a|
\end{aligned}
$$

In any case although the perfect knowledge is at hand it does not solve the local problem.

8. CONCLUSIONS

Application of quantum mechanics to systems that are not large enough to be treated classically and not small enough to be treated as isolated demands a careful look at separability. Even for small molecules forming weakly interacting van der Waals complexes separability is not a trivial problem. Using perturbation theory for intermolecular interactions one is tempted to think that, if the exchange integrals are small, one may skip antisymmetrization and start from the product function. Computational experience and theoretical analysis [19] have proved that such approach (termed "polarization approximation") is completely inadequate. This fact creates great complications in applications of perturbation theory to many-body systems. Technically these problems are connected with the non-existence of local energy operators when the antisymmetric wavefunctions are used. One could expect problems in the direct determination of the differences between the properties of the whole and the parts (interaction energies) on the basis of the general considerations given in the last section.

So far quantum mechanics has never failed, therefore such strange consequences as non-separability or macroscopic superpositions of pure states [20] should be taken seriously. It is hard to accommodate such notions in the western philosophical tradition; despite experimental verifications still a large number of experts are not ready to accept it [21]. Whole branches of physics, like stochastic electrodynamics, appear motivated by desire to understand physical picture at the quantum level [22]. Such efforts, although so far not successful, should nevertheless be respected: no path should be left unexplored. But, one might ask, is quantum mechanics really "beyond human comprehension"? Non-separability and the complementarity of knowledge about the whole and its constituents would certainly not come as a surprise to the Taoist sages like Czuang-Tsu who wrote:

"The knowledge of the ancients was perfect. How perfect? At first, they did not know that there were things. This is the most perfect knowledge; nothing can be added. Next, they knew that there were things, but did not make distinctions between them. Next, they made distinctions between them but did not pass judgments upon then. When judgments were passed, Tao was destroyed."

One may say: when local predictions are made the Unity (correlations with the other systems) is destroyed.

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