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Research Article

# Hydrogen-like quantum Hamiltonians & Einstein separability in the case of charged radical molecules

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Abstract. In the history of the debate about the completeness of quantum theory, Schrödinger and Einstein exchanged letters concerning the fact hat, according to Schrödinger, quantized classical mechanics in the form of the Schrödinger equation cannot be Einstein separable. In the present paper the question is raised if, next to wave-particle duality and quantum tunneling, a Schrödinger wave function can transform itself such that it no longer "feels" the (non-relativistic instantaneous and omnipresent) Coulomb attraction of opposite charges. Looking at the separability debate between Einstein and Schrödinger this appears to be a, strange but, meaningful question. Should such transformation be possible then we can conclude that the particles described by a Schrödinger equation would be Coulomb separable. This is contrary to what Schrödinger said. Translating the mathematics to chemistry, we will look at a mesoscopic inter-molecular description of the behavior of charged radical molecules. Firstly, given a restricted experimental geometry set-up such as described in the paper. Secondly, given that the intra-molecular wave function of a charged radical molecule does not prevent the mescoscopic inter-molecular wave function to be described in the present paper. Then it is found that a transformation of mesoscopic inter-molecular wave functions is possible that entails a kind of "immunization" for Coulomb interaction. The author acknowledges that immunization is a medical term. He has not a better term at this moment. In the appendix of the present paper, an experiment is proposed where micelle based molecules are turned into opposite charged radical molecules and are separated in the special geometry of the experiment. The generation of the opposite charged radicals can be performed with light. The method is borrowed from spin-chemistry. The separation is with "dipole radiation". The method is borrowed from Positronium separation. After the mathematical proof, we ask the question what kind of chemical transformation is possible to mimic the mathematical transformation of the wave function provided here in the paper. The theory given here is that the Coulomb immunity can be approximated through the geometry of the oligomerization of charged radical molecules.

Keywords. Coulomb interaction, Einstein-Schrödinger discussion, unexpected separability, charged radicals, spin-chemistry.

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#### 1. INTRODUCTION

In the philosophy of physics there is every now and then some debate about the exact meaning of Einstein's seminal criticism [1] on the completeness of the quantum theory.

#### 1.1 Philosophy of physics and chemistry

Einstein's idea of entanglement was to let two particles A and B have a brief interaction and then to separate them [2] and [3]. The wave function is writtenas  $\psi_{a,B}$ . Einstein reformulated his criticism, which still contained the Heisenberg uncertainty in [1], into the following. If the wave fuction of A, denoted by  $\psi_A$ , can be manipulated by observer  $O_A$ , then, the wave function to be observed by the distant  $O_B$  and denoted with  $\psi_B$  is not uniquely attached to B. This is Einstein's *inseparability* criticism. Don Howard [2] argues that, because of e.g. Bose statistics, already far before the publication of the EPR paper, Einstein had his doubts about the separability of quantum particles.

In later developments Bohm [4] replaced the brief interaction between A and B with the singlet spin state to entangle spins of particles A and B. Bohm's paradigmatic particle was para Positronium. Bohm's work gave rise to Bell his formula and the inequality derived there of [5].

The present author has shown a critical flaw in Bell's work [6]. This flaw is in fact a reference to concrete mathematical incompleteness: the Gödel incompleteness phenonmenon, as quoted by [8], in concrete mathematics. Non inequality research supported the idea that Bell inequalities are perhaps not the only way to establish that, in nature, the quantum mechanical non-relativistic analogue of classical mechanics is effectively at work. A non-quantum mechanics falls short to explain the outcome of the experiment. Historically, one of the earliest proofs thereof is by Kocher and Commins [12].

The study of Kocher and Commins is an example of a photon correlation experiment without the need for a Bell correlation formula based inequality. Recently, Nordén [14] discussed the question how wrong Einstein was after all. The mathematical incompleteness of Bell's inequalities in [6] and [7] questions  $\approx 40$  years of experimental research into non-locality. It will not receive a warm welcome in certain quarters of research. It does, however,not invalidate quantum mechanics as a statistical theory. The latter view on quantum mechanics was Einstein's conception [2]. In a sense, Nordén [15] supports this idea with an explanation that comes close to a Hanbury-Brown Twiss view of spin-spin correlation. It must, in addition, be noted also that Wenneström [16] advances criticism on the conclusions of Bell inequality experiments. He based his criticism on the physics of measurement instruments. A famous experiment that deserves mentioning here is Aspect's [18].

To continue, it must be noted that in his letter to Schrödinger, Einstein was interested in the physics of a brief interaction followed by a spatial separation. This means a transformation of the joint wave function  $\psi(\mathbf{x}_A, \mathbf{x}_B)$  into a product of two separate wave functions  $\psi_A(\mathbf{x}_A)$   $\psi_B(\mathbf{x}_B)$  for distant particles *A* and *B*. a.

Furthermore, Einstein was displeased with the EPR paper [3, page 175]: "[...] die Hauptsache ist sozusagen durch Gelehrsamkeit verschüttet [...]<sup>2</sup>. In my humble opinion this was not because of a more or less artisitic need for simplicity. The EPR paper formulated something close to, but definitely not identical with, Einstein's inseparability criticism [2].

In an earlier letter to Schrödinger, Einstein writes down after correction [2], a Schrödinger equation for entangled particles in the sense discussed here. The conversation between the two giants of physics continues with Schrödinger noting that with the non-relativistic quantum analogue of classical mechanics, separability cannot be conceived [3, page 177]. One can with a more modern view imagine virtual photons carrying the Coulomb interaction between two opposite charged particles. Because the absence of relativity, the Schrödinger equation with Coulomb potential function is, apparently according to Schrödinger, unfit to describe the separability that Einstein was looking for. End of story according to Schrödinger [3, page 177]. Perhaps that the inseparability notion expressed by Einstein in his exchange of letters with Schrödinger, does not meet the modern standard requirements of entanglement. However the principles, namely brief interaction between A and B leading to a joint wave function  $\psi_{AB}$  and subsequently spatial separation of A and B into separate  $\psi_A$  and  $\psi_B$ , are the same. In this present paper we will look at the "end of story" argument of Schrödinger.

Einstein directed his arrows of criticism to the unexpected inseparability in non-relativistic quantum theory. Let us accept the words of Schrödinger for the quantum analogue of classical mechanics.

But what about unexpected *separability* in non-relativistic quantum theory? What would *that* tell us about the quantum analogue of classical mechanics.

<sup>&</sup>lt;sup>2</sup> The main point is burried under erudition.

#### 1.2 Possible realization in chemistry

Before entering into the mathematics of this question we first may note that this question is most likely not pure philosophy. It is possible to design a real experiment with e.g. charged molecular radicals and perform separation within the boundaries of distances where Coulomb potentials can be felt. This means, we can employ the kind of Schrödinger equation that Einstein considered. However, now we look for unexpected *separability*. We look for disentangling, perhaps better: Coulomb immunity, transformation in the realm where an inevitable "entangling" Coulomb potential function rules. The matter of separeability and therefore disentanglement because of temperature [19] will be discussed later.

In order to find the properly charged radicals we can look at e.g. the interesting field of spin-chemistry and make use of their experimental techniques [10]. Let us look at Figure 1.2. The use of nearly equal mass radicals make sense when we want to approximate a kind of chemical/molecular onium-type of "atom" on the meso scale where quantum theory is still valid. The Schrödinger equation can be similar to the one which approximates the Positronium [9]. In Figure 1.2 the two radicals are presented. The (ideal) molecular mass with  $M_C$ = 12,  $M_N$ = 14,  $M_H$ = 1, is for N-Methyl Car- bazole,  $M_{C13H11N} = M_{NMCZ} = 181$ . For Tetra Cyano Benzene we have  $M_{C10H2N4} = M_{TCNB} = 178$ . The two charged molecular radicals come close to a meso scale type of "onium" atom approach that can also be found with e.g. Positronium but then for electron and positron.

Of course electron and positron are particles with equal mass but also each carrying far less mass. Nevertheless we believe that the radical molecules Hamiltonian show some formal equality with the Positronium one and therefore the following picture isjustified.

Let us suppose a number of plus NMCZ and min TCNB that can, at a certain stage of the separation in the experiment, see Appendix A.1, be described with a Positronium akin Schrödinger equation. We note here that, for clarity, we are dealing with a hydrogenic-like mesoscopic inter-molecular Hamiltonian.

In a paper of Tanimoto and Fujiwara, [10, page 440] we learn about a charged radicals generating reaction for N-Ethyl Carbazole *NECZ* and Tetra Cyano Benzene *TCNB*. This is what we want to accomplish for ( $M_{NMCZ}$  = 181) *NMCZ* and ( $M_{TCNB}$  = 178) *TCNB*. The method is to capture *NECZ* and *TCNB* in a micelle. Upon 308-nm laser excitation, the excited triplet state of NECZ undergoes an electron transfer reaction with TCNB [10]. The generation of the radicals is performed with the use of



**Figure 1.** Left, N-Methyl Carbazole radical R denotes  $N^{\bullet}$ -CH<sub>3</sub> abbreviated as NMCZ<sup>• $\oplus$ </sup> and right Tetra Cyano Benzene radical with R' denoting  $C \equiv N^{\bullet \ominus}$ , abbreviated as TCNB<sup>• $\ominus$ </sup>. In fact, the position of  $\oplus$  in the NMCZ radical and  $\ominus$  in the TCNB radical isunknown.

photons denoted by nv. From [10] we also learn that NMCZ will most likely be less effectively turned into a radical than NECZ. Because we are looking for 1-1 Coulomb interactions this does not seem to be a big problem. In our case we capture *NMCZ* and *TCNB* (Figure 1.2) in micelles and use light to generate theradicals.

The generation of charged molecular radicals in micelles, is presented below

$$\overbrace{NMCZ + TNCB}^{\text{micelle}} + \hbar\nu \longrightarrow \overbrace{NMCZ \bullet \oplus}^{\text{micelle}} + TCNB \bullet \ominus$$

The right hand side of this equation serves as the entangled pair (better: pairs) in a micelle. The spinchemistry literature shows that this step is possible.

A subsequent step is the separation of NMCZ<sup>•</sup> and TCNB<sup>•</sup>. This can be done by e.g. "destroying" the micelle confinement and simultaneously separate NMCZ<sup>•</sup> and TCNB<sup>•</sup> with e.g. dipole radiation. The latter separation method can be compared to the way e.g. Wigner described the separation of entangled electron and positron from Positronium [11]. Hence,

$$\overbrace{NMCZ \bullet \oplus + TCNB \bullet \ominus}^{\text{micelle}} \longrightarrow NMCZ \bullet \oplus \dots TCNB \bullet \ominus$$

The dots denote the spatial separation. We claim that Einstein's treatment of the Schrödinger equation can be applied to NMCZ<sup>•</sup> and TCNB<sup>•</sup> generated in the micelle. What is needed is that, perhaps for a short moment in time upon generation of the radicals, NMCZ<sup>•</sup> and TCNB<sup>•</sup> are in a state where a joint wave function exists. Let us call this the "onium" state. Most likely, similar to spin-chemistry, there will be a loss of free NMCZ<sup>•</sup> and TCNB<sup>•</sup> through chemical reaction. Moreover, the number of "onium" typed but afterwards free NMCZ<sup>•</sup> and TCNB<sup>•</sup> must not be too small compared to the NMCZ<sup>•</sup> and TCNB<sup>•</sup> that never were in the "onium" state.

To be clear, upon the start of the separation of NMCZ<sup>• $\oplus$ </sup> and TCNB<sup>• $\oplus$ </sup> the joint "onium" wave function exists. Then we have a Einstein-Schrödiger Hamiltonian.

Shortly afterwards, the separation of the two wave functions is accomplished according to Appendix A.1.

In relation to that we may note that spin-chemistry experiments [10] do show that separate molecular radicals can be in the spin singlet state. So in case of spinspin entanglement, if this state occurs sufficiently long enough between two charged radical molecules in a micelle, a comparable "onium" is possible. We claim that therefore our "onium" without explicit consideration of the spin, living in the micelle state and described by the compound Schrödinger equation [2, page 26], is not just sheer fantasy. In fact our description here is independent of spin entanglement. We are dealing here with an inspection of Einstein separability on a molecular scale in a Coulomb field without by necessity spin entanglement. This will be made clear in the next section.

Initially there is a jumble of a number of NMCZ and TCNB radical molecules. For a clear picture on intra molecular and inter molecular wave functions we introduce the following. When the separation sets in via dipole radiation, there is a more ordered situation that can be described by the equation. We assume here a number, K, of TCNB particles that form a kind of minus K charged virtual particle. The corresponding K plus charged NMCZ molecules give a virtual positive charged particle. Virtual parti- cles occur in quantum statistical mechanics and can be described by a Schrödinger equation. Quantum quasi-particles see: [17, e.g. page 32 & appendix *A*].

## 2. HAMILTONIAN IN A NON-RELATIVISTIC QUANTUM ANALOGUE OF CLASSICAL MECHANICS

Let us start with the, normalized in form, stationary Schrödinger equation for the Coulomb bound state of two particles. The structure in a sense resembles a Positronium [9] and coincide with [3, page 26]. In the lowest non-relativistic approximation the binding energy is determined by the instantaneous electrostatic interaction, similar to the hydrogen atom but then for, for instance,  $1 \equiv \text{NMCZ}^{\bullet}$  and  $2 \equiv \text{TCNB}^{\bullet}$ . The reduced molecular mass  $M = M_1 M_2 / (M_1 + M_2)$  is close to 179.49/2, e.g.  $m \approx m_{NMCZ}/2$  in e.g. kg, the reduced mass is  $m \approx 1.4987 \times 10^{-25}$  kg. In SI units,  $n \approx 1.055 \times 10^{-34}$  J.s and  $e \approx 1.602 \times 10^{-19}$  coulomb.

$$\left[\nabla_{1}^{2} + \nabla_{2}^{2} + \frac{\alpha'}{r_{1,2}} + \epsilon_{1,2}\right]\psi(\mathbf{x}_{1}, \mathbf{x}_{2}) = 0$$
(1)

In this equation  $\nabla_1^2 = \frac{\partial^2}{\partial \mathbf{x}_1^2}$ , with,  $\mathbf{x}_1 = (x_{1,1}, x_{1,2}, x_{1,3})$ . Similarly for  $\nabla_2^2$  with,  $\mathbf{x}_2 = (x_{2,1}, x_{2,2}, x_{2,3})$ . Further-

more,  $r_{1,2}^{-1} = ||\mathbf{x}_1 - \mathbf{x}_2||^{-1}$  and  $\alpha' = \frac{2e^2m}{4\pi\hbar^2}$  and *e* the unit of charge.  $\varepsilon_{1,2}$  is 2m/n2 times the energy eigenvalue [9, page 182] if n is not in units giving n is unity.

To our mind, the generated plus and minus charged particle participate in a meso-scale Hamiltonian. This Hamiltonian corresponds to the Schrödinger equation that Einstein and Schrödinger were discussing in their friendly exchange of letters. This corresponds to the Positronium form but it is a multiparticle equation where K plus and K minus particles form virtual particles. K must not be too large because of the  $O(m^2)$  approximation. We note that this kind of virtual particles we have in mind are clusters of real particles. This is not the same thing as e.g. the phonon virtualparticle.

#### 2.1 Unexpected independence

Here we ask can there be a transformation of the approximate Schrödinger equation such that, despite the presence and validity of the Coulomb force, we have mutual independence between distant particles? Of course temperature effects are here crucial to the question [19].

In the experiment (see the description Appendix A.1) we have a number of subsequent stages. Each stage is described by a stationary Schrodinger equation. This is what is intended by a steps-in-time change.

First we have the situation where interacting particles are in a micelle. Then, secondly, the initial separation sets in. Here  $\xi = (x_{1,2} + x_{2,1})/2$  is, momentarily, a constant despite changes in respectively,  $x_{1,1}$  and  $x_{2,1}$ . This can be accomplished when e.g.  $x_{1,1} \rightarrow x_{1,1} + \Delta x$  and  $x_{2,1} \rightarrow x_{2,1} - \Delta x$ . In the third next stage in time, we freeze  $x_{1,1}$  and let  $y = x_{1,2}$  and  $z = x_{1,3}$  vary on the particle 1 side. On the particle 2 side we let  $x_{2,1}$  increase. The  $\xi$  in that stage or moment of time is no longer a constant because  $x_{1,1}$  is "freezed". The mathematics below makes things clear about the arrangement of the experiment for "free" but within Coulombrange NMCZ<sup>•®</sup> and TCNB<sup>•®</sup> radical pairs. The cluster of virtual particles, K NMCZ<sup>•®</sup> together with K TCNB<sup>•®</sup>, mimic the  $\psi_A$  and  $\psi_B$  of the Einstein Schrödinger debate.

In order to study this we first look at the Coulomb potential function itself. Now suppose that there is a  $\xi \in \mathbb{R}$  and the  $(x_{1,1}-x_{21})^2$  dominate the  $\sum_{k=2}^{3}(x_{1,k}-x_{2,k})^2$  such that  $r_{1,2} = \sqrt{(x_{1,1}-x_{21})^2 + \epsilon^2}$ . If we then subsequently arrange it such that  $x_{1,1} > \xi$  and  $x_{2,1} < \xi$  we approximate  $r_{1,2}^{-1}$  with a  $0 < \beta$  using

$$r_{1,2}^{-1} \approx 2^{-\beta-1} \{ (x_{1,1} - \xi)^{-\beta} + (\xi - x_{2,1})^{-\beta} \}$$
(2)

If we take e.g.  $\xi = (x_{1,1} + x_{2,1})/2$ , then  $r_{1,2}^{-1} \approx (x_{1,1} - x_{2,1})^{-\beta}$ . This amounts to an approximation of the Coulomb potential in the "amount of space and time" where a Coulomb potential rightfully may be employed. We have

$$\frac{\alpha'}{r_{1,2}} \approx 2^{-\beta - 1} \frac{2e^2 m}{4\pi\hbar^2} \left\{ (x_{1,1} - \xi)^{-\beta} + (\xi - x_{2,1})^{-\beta} \right\}$$
(3)

Let us define  $\gamma = 2^{-\beta - 1} \frac{2e^2m}{4\pi\hbar^2}$ . If we then accept that at a certain point in time the stationary Schrödinger equation (1) for a product wave function  $\psi(\mathbf{x}_1, \mathbf{x}_2) = \psi_1(\mathbf{x}_1)\psi_2(\mathbf{x}_2)$  can be written

$$\left[\nabla_{1}^{2} + \nabla_{2}^{2} + \gamma \left\{\frac{1}{(x_{1,1} - \xi)^{\beta}} + \frac{1}{(\xi - x_{2,1})^{\beta}}\right\} + \epsilon_{1,2}\right]\psi_{1}(\mathbf{x}_{1}|\xi)\psi_{2}(\mathbf{x}_{2}|\xi) = 0$$
(4)

The A and B indices are replaced with indices 1 and 3. This equation (4) can be split into two equations given below. The step-in-time development of the experiment Appendix A.1, allows us to momentarily take  $\xi$  is constanc  $x_{1,1} \rightarrow x_{1,1} + \Delta x$  and  $x_{2,1} \rightarrow x_{2,1} - \Delta x$ . Both the  $x_{,1}$  coordinates change but  $\xi$  does not. The idea is to separate the particles with the use of "dipole radiation" such as described by Wigner [11, around equation (46) of Wigner's lecture]. This appears in principle to be possible with the charged radicals NMCZ<sup>\*®</sup> and TCNB<sup>\*®</sup>. See Appendix A.1. Hence,

$$\psi_2(\mathbf{x}_2|\xi) \left\{ \nabla_1^2 + \frac{\gamma}{(x_{1,1} - \xi)^\beta} + \epsilon_1 \right\} \psi_1(\mathbf{x}_1|\xi) = 0$$
(5)

and

$$\psi_1(\mathbf{x}_1|\xi) \left\{ \nabla_2^2 + \frac{\gamma}{(\xi - x_{2,1})^{\beta}} + \epsilon_2 \right\} \psi_2(\mathbf{x}_2|\xi) = 0$$
(6)

with,  $\varepsilon_{1,2} = \varepsilon_1 + \varepsilon_2$ . It is supposed that the two separate equations describe the situation in a stationary form just after the separation split. Then one may imagine that in experiment it is possible to restrict the stationary description of particle one with wave function  $\psi_1(\mathbf{x}_1)$  to the directions  $x_{1,2} = y$  and  $x_{1,3} = z$ . The *y* and *z* notation are introduced for ease of the presenta- tion of computation.

If we then introduce the transformation of  $\psi_1$  with

$$\varphi_1(\mathbf{x}_1,\xi) = \left(\frac{\partial}{\partial\xi} + \chi(\mathbf{x}_1,\xi)\right)\psi_1(\mathbf{x}_1|\xi) = D\psi_1(\mathbf{x}_1|\xi)$$
(7)

the question can be asked if it is possible to find a transformation (7) such that  $\phi_1$  does not depend on  $\xi$ .

The symmetric propagation where  $x_{1,1} \rightarrow x_{1,1} + \Delta x$ and  $x_{2,1} \rightarrow x_{2,1} - \Delta x$  and the  $x_{.1}$  coordinates change but  $\xi$  does not, is broken in that step in time of the experiment (Appendix A.1). In turn  $\xi$  depends on the  $x_{2,1}$  coordinate of particle 2. It is assumed that the value of  $\xi$  with fixed  $x_{1,1}$  can vary with  $x_{2,1}$ .

Of course, in experiment one can fix  $x_{1,1}$  without fixing  $x_{2,1}$ . Inaddition  $\xi$  can vary because nobody knows exactly where we are allowed to start talking about two separate particles / particle groups. At the "split" the  $\xi$ is approximatedly fixed when looking at e.g.  $x_{1,1}$  for the equation of particle 1. Similar case for particle 2. But when the stationary equations for particle 1 and 2 evolve for later steps in time,  $\xi$ varies.

Given equation (5) we then may have

$$\left(\operatorname{div}_{2,3}\operatorname{grad}_{2,3} + \frac{\gamma}{(x-\xi)^{\beta}} + \epsilon_1\right)\psi_1(\mathbf{x}|\xi) = 0$$
(8)

with  $\mathbf{x} = (x, y, z) = (x_{1,1}, x_{1,2}, x_{1,3})$  and  $x = x_{1,1}$  fixed. For ease of notaton denote  $\operatorname{grad}_{2,3}$  for the gradient  $(\frac{\partial}{\partial y}, \frac{\partial}{\partial z})$ . Therefore,  $\operatorname{div}_{2,3} \operatorname{grad}_{2,3} = \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ . This is the nabla squuared in two dimensional (y, z) space. Obviously we also have,

$$D\left(\operatorname{div}_{2,3}\operatorname{grad}_{2,3} + \frac{\gamma}{(x-\xi)^{\beta}} + \epsilon_1\right)\psi_1(\mathbf{x}|\xi) = 0$$
(9)

#### 2.2 Transformation

Let us first look at the term  $D\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi_1$  in (8) Subsequently observe div<sub>2,3</sub> grad<sub>2,3</sub>  $\phi_1 = \operatorname{div}_{2,3} \operatorname{grad}_{2,3}$  $\left\{\left(\frac{\partial}{\partial \xi} + \chi\right)\psi_1\right\}$ .Hence,

$$\operatorname{div}_{2,3} \operatorname{grad}_{2,3} \left( \frac{\partial}{\partial \xi} + \chi \right) \psi_1 = \\ \left( \frac{\partial}{\partial \xi} \operatorname{div}_{2,3} \operatorname{grad}_{2,3} \psi_1 + \chi \operatorname{div}_{2,3} \operatorname{grad}_{2,3} \psi_1 \right) \\ + \psi_1 \operatorname{div}_{2,3} \operatorname{grad}_{2,3} \chi + 2 \operatorname{grad}_{2,3} \psi_1 \cdot \operatorname{grad}_{2,3} \chi = \\ \left( \frac{\partial}{\partial \xi} + \chi \right) \operatorname{div}_{2,3} \operatorname{grad}_{2,3} \psi_1 + \psi_1 \operatorname{div}_{2,3} \operatorname{grad}_{2,3} \chi + 2 \operatorname{grad}_{2,3} \psi_1 \cdot \operatorname{grad}_{2,3} \chi$$
(10)

Therefore the first term in the differential equation (8) transforms like

$$D \operatorname{div}_{2,3} \operatorname{grad}_{2,3} \psi_1 =$$
(11)  
 
$$\operatorname{div}_{2,3} \operatorname{grad}_{2,3} \phi_1 - \psi_1 \operatorname{div}_{2,3} \operatorname{grad}_{2,3} \chi - 2 \operatorname{grad}_{2,3} \psi_1 \cdot \operatorname{grad}_{2,3} \chi$$

The second term contains a  $\xi$ . We have

$$D\frac{\gamma}{(x-\xi)^{\beta}}\psi_1 = \frac{\partial}{\partial\xi}\left(\frac{\gamma}{(x-\xi)^{\beta}}\psi_1\right) + \frac{\gamma}{(x-\xi)^{\beta}}\chi\psi_1$$
(12)

Or, the second term can be written down as,

$$D\frac{\gamma}{(x-\xi)^{\beta}}\psi_1 = \frac{\beta\gamma}{(x-\xi)^{\beta+1}}\psi_1 + \frac{\gamma}{(x-\xi)^{\beta}}\varphi_1$$
(13)

For completeness,

$$\frac{\partial}{\partial \xi} \left( x - \xi \right)^{-\beta} = (-\beta)(-1) \left( x - \xi \right)^{-\beta - 1}$$

Note the definition of  $\phi_1$  provided in (7) and used in (13). The third term of (9) is a simple transformation

$$D\varepsilon_1\psi_1 = \varepsilon_1\phi_1 \tag{14}$$

If we then add equations (11), (13) and (14) we are back at (9) and note that

$$\left(\operatorname{div}_{2,3}\operatorname{grad}_{2,3} + \frac{\gamma}{(x-\xi)^{\beta}} + \epsilon_1\right)\varphi_1(\mathbf{x}|\xi) = 0$$
(15)

provided

$$\psi_1 \operatorname{div}_{2,3} \operatorname{grad}_{2,3} \chi + 2 \operatorname{grad}_{2,3} \psi_1 \cdot \operatorname{grad}_{2,3} \chi - \frac{\beta \gamma}{(x-\xi)^{\beta+1}} \psi_1 = 0$$
 (16)

If we observe the previous equation (16), then by construction,  $\phi_1(\mathbf{x}|\boldsymbol{\xi})$  is a solution to (8) operator equationas is  $\psi_1(\mathbf{x}|\boldsymbol{\xi})$ .

#### 2.3 A transformation that allows $\phi$ 1independent of $\xi$

We start with the assumption that the experiment is such that, after the split. Remembering,  $\operatorname{div}_{2,3} \operatorname{grad}_{2,3} = \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial z^2}$ 

$$\left\{ \operatorname{div}_{2,3} \operatorname{grad}_{2,3} + \frac{\gamma}{(x-\xi)^{\beta}} + \epsilon_1 \right\} \psi_1(x, y, z|\xi) = 0$$
(17)

Let us assume an  $O(m^2)$  approximation theory for *m* from  $\gamma$  in the potential function and take

$$\psi_1(x, y, z|\xi) = g(y, z) \ (x - \xi)^{\beta + 1} \tag{18}$$

As an aside please note that this wave function is intended as the inter- molecular one for the K ensemble of radical molecules denoted with the index 1 in the experiment with the other cluster consisting of K molecules denoted with index 2. The equation (17) results into

$$(\operatorname{div}_{2,3}\operatorname{grad}_{2,3}g)(x-\xi)^{\beta+1} + \gamma g(x-\xi) + \varepsilon_1 g(x-\xi)^{\beta+1} = 0 \quad (19)$$

or

$$(\operatorname{div}_{2,3} \operatorname{grad}_{2,3} g) (x-\xi)^{\beta} + \gamma g + \varepsilon_1 g (x-\xi)^{\beta} = 0$$
(20)

Now because we approximate in  $O(m^2)$  it is possible to e.g. have g(y, z) = mh(y, z) and so,  $\gamma g = O(m^2)$ . The possibility to have a function with only g = g(y, z) is there with acknowledged and this is what is needed to have a  $\phi_1$  that, according to our aim, does not in  $O(m^2)$  approximation depend on  $\xi$ . The equation (20) then turns into

$$\operatorname{div}_{2,3} \operatorname{grad}_{2,3} g(y,z) + \varepsilon_1 g(y,z) = 0 \tag{21}$$

in  $O(m^2)$ . Subsequently we can have a look at

$$\psi_{1}(x,y,z|\xi) = g(y,z)(x-\xi)^{\beta+1}$$

$$\chi(x,y,z|\xi) = \frac{f(y,z) + (\beta+1)(x-\xi)^{\beta}}{(x-\xi)^{\beta+1}}$$
(22)

The first of the equations obeys the Schrödinger equation (19) and holds a g = g(y, z) which is independent of  $\xi$ . The second of the equations in (22) is not trivial even though we can multiply nominator and denominator with g(y, z) to, obviously,obtain

$$\chi = \frac{fg - \frac{\partial}{\partial \xi}\psi_1}{\psi_1}$$

It is a part of *D* transformation and combines with the  $\psi_1$ , for convenience again given in the first of (22), to form a  $\phi_1$  as

$$\varphi_1 = \left(\frac{\partial}{\partial\xi} + \chi\right)\psi_1 = -(\beta+1)g(y,z)(x-\xi)^{\beta} + f(y,z)g(y,z) + (\beta+1)g(y,z)(x-\xi)^{\beta}$$
(23)

Hence,  $\phi_1 = g(y, z) f(y, z)$  and  $\phi_1$  is, clearly, independent of  $\xi$ . For completeness,

$$\frac{\partial}{\partial \xi} \psi_1(\mathbf{x}|\xi) = -g(y,z)(\beta+1) \left(x-\xi\right)^{\beta}$$

and

 $\chi(\mathbf{x}|\xi) \ \psi_1 \ (\mathbf{x}|\xi) = g(y,z) \ f(y,z) + g(y,z) \ (\beta+1) \ (x-\xi)^{\beta}$ 

### 3. DISCUSSION AND CONCLUSION

#### 3.1 Verification

We need to verify if the condition in (16) is fulfilled in a way that warrants  $\phi_1$  independence of  $\xi$ . If (22) is substituted in (16) we find, remembering, grad<sub>2,3</sub> =  $\left(\frac{\partial}{\partial u_1}, \frac{\partial}{\partial z}\right)$  and *x*,  $\xi$  constant for grad<sub>2,3</sub>

$$g \operatorname{div}_{2,3} \operatorname{grad}_{2,3} (f + (\beta + 1) (x - \xi)^{\beta} + (24))$$
  
2 grad<sub>2,3</sub> (g)·grad<sub>2,3</sub> (f + (\beta + 1)(x - \xi)^{\beta} - \beta\gamma g = 0)

Therefore,

 $g \operatorname{div}_{2,3} \operatorname{grad}_{2,3}(f) + 2 \operatorname{grad}_{2,3}(g) \cdot \operatorname{grad}_{2,3}(f) - \beta \gamma g = 0 (25)$ with,  $\operatorname{grad}_{2,3} = \left(\frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$  and,  $x - \xi = (x_{1,1} - x_{2,1})/2$ . For  $x = x_{1,1}$  fixed,

 $\operatorname{grad}_{2,3}((\beta+1)(x-\xi)^{\beta}) = (0,0)$  (26)

We also note that it is assumed  $\gamma g = O(m^2)$ . Moreover we note that (25) allows the conclusion that f = f(y,z) is indeed possible. This implies that  $\phi_1 = \phi_1(y,z)$  is a solution of (15) despite the presence of the potential  $\frac{\gamma}{(x-\xi)^{\beta}}$  in that equation. Please also observe that  $\phi_1(y, z) = g(y, z)f(y, z)$  which need not be  $O(m^2)$ . In addition,  $\gamma g(y, z)$  is  $O(m^2)$  but that does also not imply that  $\psi_1$ , defined in (22), is small of  $O(m^2)$  for all cases as well. This so because of the occurence of the  $(x - \xi)^{\beta+1}$  as a factor in  $\psi_1$ .

When  $x_{1,1} - x_{2,1}$  is large, the potential in (15) decreases. But some wave function descriptions of the same particle, like  $\psi_1$ , still "feel" the effect while others  $\phi_1 = D\psi_1$  may become "immune" to it. Observe that the *D* transformation can transform  $\psi(\mathbf{x}|\xi)$ , which is  $\xi$  *dependent*, into  $\phi(\mathbf{x})$ , which is  $\xi$  independent. Both functions in (8) and (15) are a solution to

$$\left(\operatorname{div}_{2,3}\operatorname{grad}_{2,3} + \frac{\gamma}{(x-\xi)^{\beta}} + \epsilon_1\right)\Psi_1 = 0 \tag{27}$$

Here,  $\Psi_1 \in \{\psi_1(\mathbf{x}|\xi), D\psi_1(\mathbf{x}|\xi),...\}$ . As an aside we note that also in 2 instead of 3 spatial dimensions, anyons do not obey the fermion/boson spin statistics [13]. Let us look at the potential  $\frac{\gamma}{(x-\xi)^{\beta}}$  and combine this with the wave function  $\psi_1(x,y,z|\xi) = g(y,z)(x-\xi)^{\beta+1}$ . We note that  $\gamma g(y,z)$  is O(m). This, however, does not make by necessity (5), (27) and the transformation  $\phi_1(y,z) = g(y,z)(x-\xi)^{\beta+1}$ .

 $D\psi_1(x,y,z|\xi) = f(y,z)g(y,z)$ , trivial. For instance,  $\varepsilon_j$ , with j = 1,2, is 2m/n2 times the energy eigenvalue.

#### 3.2 Schrödinger's end of story

A "relatively" large  $|x_{1,1}-x_{2,1}|$ , with fixed  $x_{1,1}$ , maintains the influence of the  $x_{2,1}$  coordinate of the second particle on the  $\psi_1$  function. This must be true despite the  $1/(x_{1,1} - x_{2,1})$  form of the potential function in the Hamiltonian.

It allows also a transformation to  $\phi_1 = D\psi_1$  which is order  $O(m^2)$  independent of  $\xi$ . Suppose that we in our analysis remain in the distances where Schrödinger implicitly talked about in his letter to Einstein. The  $\xi$ represents the influence, via the Coulomb force, of the coordinate of the second entangled charged molecular radical(s) on the wave function of the first.

Apparently, quantum mechanics allows a transformation of a wave funcion where the inevitable Coulombic interaction (a prehistoric entanglement start equation [3]), according to Schrödinger's end of story, is "immunized".

The use of charged molecular radicals makes the description with theSchrödinger equation more open to experimen: Appendix A.1. Note that the charged radicals are particles with wave functions of their own. The latter intra-molecular wave functions are likely related to the posibility of the inter-molecular wave function in the here discussed Schrödinger equation. Nevertheless, a description of the role of the particle in the experimental environment is aimed for, not the intrinsic molecular wave function. We are looking at a meso-scale, but still quantum, behavior.

The mathematics of the Schrödinger equation implies that one can transform away the Coulombic influence of the second particle on the first. We can also ask the question what it means when not a single "onium" pair can be found. E.g. what does it mean for radical chemistry, when this transformation cannot be accomplished.

A possible explanation for the effect can be a transformation or decoherence to classical levels. But then again Coulomb interaction is basic. Can temperature effects disallow all kinds of "non temperature based" mathematics to be realised in the real world. From [19] we may learn that asymptotic behavior of atom-atom interaction at sufficiently large separation, which is perhaps needed in our present case, are profoundly influenced by excitations in the radiation field. This has the effect that the initial quantum interaction goes over to its classical analogue. On the other hand, working with molecular radicals perhaps lowers the thermal noise that could as well spoil the physical realization of the "non temperature based" mathematics [20]. It is also noted that other forces [19] of the order  $1/r_{1,2}^6$  might play a role as well in the physics of a possible experiment with photon generated micelle based charged radicals.

In any case, the transformation  $\phi_1 = D\psi_1$  appears to open a new chapter in the Schrödinger-Einstein story. One may, firstly, wonder what Einstein would have thought of a description of a particle or small group of particles that can transform itself in such a way that it does not "feel" the Coulomb force anymore. Note that both particle groups are supposed to be in a distance towards each other where Coulomb forces reign. The question may linger if in classical domain the Coulomb force at the distance in the experiment will persist. Secondly, the author believes he is halfway a criticism of the inseparability of the quantum analogue of classical mechanics and a genuine possible discovery in the physical organic chemistry of charged radicals. Perhaps that the "mechanism" in Appendix A.2 and Appendix A.3 allow applications e.g. in synthesis of molecules or the biochemistry of radical molecules[21].

Here we tally the conditions for a phenomenon in physical organic chemistry. They are presented in the form of questions.

- is it possible to create onium for most of the NMCZ<sup>•⊕</sup> and TCNB<sup>•⊖</sup> in the micelle? The situation is described in Appendix A.1.
- is it possible to separate NMCZ<sup>•</sup> and TCNB<sup>•</sup> and to stop one radical group along the x axis but still allow movement along y and z, while the other charged radical group is separated along the x axis in the opposite direction? Again we refer to AppendixA.1.
- is it possible to, initially, orderly x-axis separate NMCZ<sup>•</sup> and TCNB<sup>•</sup> with  $x_{1,1} \rightarrow x_{1,1} + \Delta x$  and  $x_{2,1} \rightarrow x_{2,1} \Delta x$ ?
- is it possible to bring (a number of) either NMCZ<sup>•</sup>θ and TCNB<sup>•</sup>Θ, considered mesoscopic, in a state wave function that can be represented with ψ<sub>1</sub>(x,y,z|ξ) = g(y,z)(x-ξ)<sup>β+1</sup>?
  - what is the influence of the intrinsic wave function on the possibility to arrive at mesoscopic ψ<sub>1</sub>?
  - what does it mean when it is impossible to bring the – or even any – charged radical molecules in mesoscopic ψ<sub>1</sub>. Is this state function, based on Schrödinger equations, unphysical?
- is it possible to find a physical equivalent for  $D = \frac{\partial}{\partial \xi} + \chi(\mathbf{x}|\xi)$  so that the "Coulomb immunity" mesoscopic state wave function actually can be determined? We refer here to Appendix A.2 and Appendix A.3.

If these points can be met in an experiment then, looking at Appendix A.1, there is a Circle *C* in a plane parallel to the *yOz* plane of the experiment where the  $\phi_1$ form of the first radical can move more freely because of "immunity" for the attraction of the second opposite charged particle. The condition must apply that the  $1/|x_{1,1}-x_{2,1}|$  approximation of the Coulomb  $1/r_{1,2}$ is valid for given *x* and  $(y, z) \in C$ . We claim for this experiment that *C* for the *NMCZ* or *TCNB* radical in  $\phi_1$ =  $D\psi_1$  is larger, but still with  $1/|x_{1,1}-x_{2,1}|\approx 1/r_{1,2}$ , than for the *NMCZ* or *TCNB* radical with  $\psi_1$ . It is assumed that either *TCNB* or *NMCZ* can play the part with a wave function  $\psi_1$ .

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## APPENDIX A PICTURE OF A POSSIBLE EXPERIMENT AND A TENTATIVE REACTION PATH GEOMETRY

In Fig A1 below a possible experiment is depicted. We assume that intra-molecular wave functions do not resist mesoscopic inter-molecular Coulomb immunity. This immunity transformation is presently unknown.

In this appendix we look at a transformation via a synthesis of a 1,3,5 triazine ring with substituents (Fig A2) and suggest (Fig A3) that next to internalpi-bon dstorageoftheadditionalelectron, geometry of themolec ule allows external compensations with e.g. a  $N \rightarrow N^{*}$  bond (Fig 3A). One of the participating Ns comes from the 1,3,5 triazine. The other one from a nearby cyanide group in TCNB. This could be a step towards the claimed immunisation.

The whole scheme in Fig 1 Fig 3 is theoretical. Nevertheless the mathematics of the Schrödinger equation presented in the paper suggests that this hiding of charge in the geometry of a molecular structure is perhaps an interesting possibility in physical organic chemistry. In this sense we tried to provide the chemical equivalent of

$$D = \frac{\partial}{\partial \xi} + \chi$$



**Figure Appendix A.1.** Set-up of the experiment described in the main body of paper. The charged radical molecules are generated by light in a micelle. Subsequently they are separated and a transformation of the mesoscopic inter-molecular wave function such that the NMCZ(+) and the TCNB(-) are immune to each others Coulomb field at a mesoscopic scale.

in the paper. We remind the reader, perhaps superfluous, that the chemical transformation equivalent to the wave function D transformation, is speculative. The reader please forgive the author also for yet another (nutty ?) observation.Please note that the synthesis structure in Appendix A.2 below is a rather flat, pi-bond, system of atoms connected to each other. Perhaps this geometry neatly reflects the yOz plane restricted freedom in the wave function represented in the mathematics and holds a chemical expression of (A.1) such as suggested in Appendix A.3.



**Figure Appendix A.2.** Possible reaction path on the TCNB side of the experiment (Fig A1). The R residual is depicted on the left hand upper side of the figure and is presented to provide details. The reaction is among three TCNB radicals. We think this reaction is theoretically possible. CN is the cyanide group. For ease of drawing we omitted the (-) charge in the R of the lower row right hand product.



**Figure Appendix A.3.** Possible formation of N $\rightarrow$ N coordinate bond with CN group and (the lone electron pair) on the N from the triple N ring. A coordinate bond on a lone pair of N generates a plus on the N of the triple N ring. One can compare this to the formation of the plusion NH<sup>⊕</sup><sub>4</sub> or e.g. (CH<sub>3</sub>)<sub>2</sub>N<sup>⊕</sup> = O. In addition to the internal pi-bond storage of the additional electric charge, a plus charge can be formed with a coordinate bond. Perhaps that such a geometric hiding of the charge will contribute to what is claimed in the paper to be a immunization of Coulomb interaction between NMCZ and TCNB. The three joined TCNB molecules are triple negatively charged.