Rapid Note

Restoring entanglement in atomic collisions: A gedanken experiment

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Abstract. A new type of collision experiments is discussed, where observations of two successive collisions of *the same pair* of particles would be possible. When such technology is available, a surprising restoring of entanglement, normally considered broken in usual collision experiments, could be observed. As an illustration the collision partners He^+ and He^{++} in a collision regime where the resonant charge transfer is dominating are considered. In the analysis it is shown that in such experiments, two spatially widely separated ion paths, corresponding in fact to two different charge states, would contribute coherently to the final amplitudes, describing which of the ions emerges as singly charged, *i.e.* which carries the single electron involved. The double collision experiments are not trivial, since their overall cross-sections are extremely small. Development of relevant experimental techniques will decide if the proposed phenomena remain in the field of gedanken experiments or enter the world of real experimental physics.

PACS. 34.50.-s Scattering of atoms, molecules, and ions – 34.70.+e Charge transfer – 03.75.-b Matter waves – 03.65.Bz Foundations, theory of measurement, miscellaneous theories (including Aharonov-Bohm effect, Bell inequalities, Berry's phase)

The atoms and ions in atomic collisions are prototypes of entangled systems, as originally defined by Schrödinger [1], see also Zeilinger [2]. Yet the entanglement in atomic collisions is not easy to observe, and as we shall discuss, in many cases the entanglement seems to be broken by the experimental arrangement.

Consider a collision between two atomic systems. The wavefunction may be written as

$$\Psi(\xi_1, \xi_2, \mathbf{R}) = \sum \Phi_{ij}(\mathbf{R}) \, \varphi_i^P(\xi_1) \, \varphi_j^T(\xi_2) \qquad (1)$$

where ξ_1 and ξ_1 are internal coordinates of the colliding partners and $\mathbf{R}$ is the relative distance.

We shall in this note mainly consider atomic collisions where the conditions for a semiclassical description are fulfilled, *i.e.* the motion of each of the atomic systems can be described by a classical trajectory, see *e.g.* [3] or [4]. In a semiclassical description one can alternatively write

$$\Psi(\xi_1, \xi_2, t) = \sum c_{ij}(t) \, \varphi_i^P(\xi_1) \, \varphi_j^T(\xi_2) \qquad (2)$$

where the time dependence is represented by the relative motion of the collision partners described by a classical trajectory $\mathbf{R}(t)$. (The centre of mass motion can be eliminated in such collisions as it corresponds to a free particle motion). The wavefunctions (1, 2) of the collision system

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clearly describe a highly entangled state. If the accessible atomic states have different energies, which will most often be the case, no entanglement can be observed in a typical experiment. This is so because the kinetic energy available for the relative motion in the various reaction channels (i, j)

$$E - \varepsilon_i^P - \varepsilon_j^T$$

is different in each case (here E is the total energy and the symbols ε_i^P, ε_j^T denote the internal atomic state energies of the projectile and target). This implies that the corresponding wavepackets arrive at different times to the detection areas. This is in fact the basis of the energy loss methods, recently being most powerfully demonstrated (*e.g.* [5]) in the cold target recoil ion momentum spectroscopy (COLTRIMS). One can thus well ask where or when during or after the collision is the entanglement broken, or alternatively stated, when is the wavefunction reduced to a single component. This aspect is even strengthened if some of the wavefunction components correspond to different particle arrangements as in the electron exchange processes.

In the gedanken experiment discussed in this note (see also [6]) we shall illustrate how the entanglement can be restored. This is made possible by special experimental arrangements including a possibility for a second collision and beam optics which will reduce the variations in times
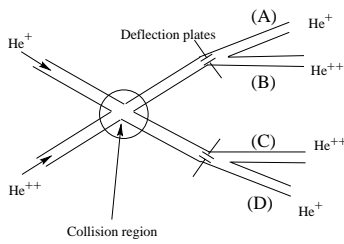
Fig. 1. A simple sketch of a primary crossed beam experiment described in the text.

Fig. 2. The crossed beam experiment with two collision regions. The four alternative paths are arranged such that the time of flight through all of them is very nearly equal, due to the acceleration/deceleration areas.

of flight so that the wavepackets in the detection areas could travel together. The problem of time correlated arrivals in somewhat similar context is discussed *e.g.* in [7].

Up to now, most of the studies of entanglement have been performed with photons [2]. Experiments where a single atom is prepared in an entangled state between its position and its internal state have been discussed [8,9]. Entangled states of two atoms which successively interact with a cavity have been studied in [10]. These involve inelasticity, but the exchanged energies are so minute that the time of flight arguments above are not relevant. An entangled state of two atoms from laser induced dissociation, which corresponds to "half a collision", has been discussed in [11], but there the atomic states involved do not differ in energy. All these studies of entanglement and coherence have recently attracted considerable attention [2,12,13], but to our knowledge the aspects of atomic collisions discussed here were not considered previously.

Our gedanken experiment involves collisions with particle exchange. Here, the reaction channels differ by electric charge and mass instead of the differing channel energy discussed above. To demonstrate the persisting entanglement after the collision, we consider a second collision of the same collision partners, which in each of the channels would follow widely different trajectories between the two collisions. The phenomenon of coherence in such subsequent collisions, if observed, would clearly demonstrate that the state of the collision system is not reduced to a single reaction channel. The particle exchange possibility adds new hitherto unnoticed aspects of the entanglement, and is perhaps relevant for understanding of the old problem of "wavefunction collapse".

For the presentation, we discuss the experiment in a crossed beam arrangement, though such realization would probably not be possible in practice due to very low intensity of the events.

A crossed beam experiment is schematically depicted in Figure 1. The two beams consist of He^+ and He^{++} ions. The relative collision velocities are assumed to be such that the cross-section for resonant capture from He^+ ion to the He^{++} ion dominates over all the other excitation and ionisation channels, so that we may assume the two ground states on the two helium nuclei to be the only states necessary for a satisfactory description [14,15]. It should be remarked that these simplifying conditions are not necessary conditions in principle. The discussed type of entanglement would appear also for nonresonant capture and also in the presence of more than two reaction channels. However, the design of the experiment, especially in the case of several channels, will become more complicated.
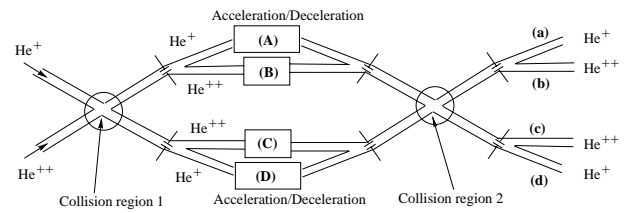
In conventional scattering analysis we can consider the wavefunction of the collision system to be "collapsed" straight after the collision region since the process will be described in terms of cross-sections and not amplitudes. Irrespective how close to that collision we would place our detection system, there would never be any possibility to observe coherence, since the two ion species are entirely different particles.

Our gedanken experiment consists in adding to the arrangement of Figure 1 a similar second part (Fig. 2), containing in addition acceleration-deceleration parts which assure that the paths are traversed in equal times. We would thus have a situation known as "welcher Weg" [16] and thus possibility for interference of amplitudes corresponding to the alternative paths, as discussed below. The distances between the paths of the particles can be meters or more, as far as the precision of the time of flight tuning is high enough.

The reason for choosing the He^+ and He^{++} ions as the colliding partners is that both ions can be manipulated by the electrostatic and electromagnetic fields, unlike cases where one of the collision partners would be a neutral atom.

The intensities of the partial beams in each of the lines (A), (B), (C), (D) of Figure 2 are given by cross-sections for charge exchange and can be analyzed by a relatively well known method [17]. The fact that the beams cross twice naturally does not assure that each of the particle pairs meet twice. The mentioned analysis of crossed beams is straightforward, and is built on the concept of cross-section, *i.e.* no coherence between the two possible charge states needs to be considered. It will also assume a complete independence of the collisional processes in collision region 1 and region 2.

If we now for a moment in addition to extremely precise focusing of the beams also consider extremely low intensity to avoid unwanted collisions, the double crossing of the beams would also lead to a possibility of double collisions between each pair of particles, *i.e.* such doubly crossed beam experiment will become a double collision experiment. The elimination of double collisions where the second one is with another particle is a crucial problem of a real experiment where the intensities should be as high as possible, and is shortly discussed below.

In the double collision experiment the collisions in regions 1 and 2 are no longer independent in the framework
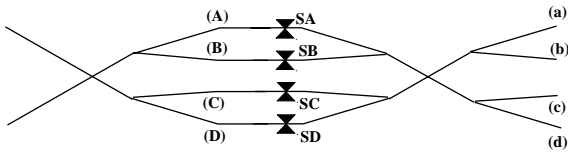
Fig. 3. A simplified diagram of the merged beam experiment with two collision regions as in Figure 2. The shutters on the four alternative ion paths are added, denoted by SA, SB, SC and SD. These shutters can keep closed or open the corresponding ion paths.

of quantal analysis, as follows from the above reference to the "welcher Weg" situation.

To observe the effect of superposition, we must extend the experimental arrangement depicted in Figure 2 by including the possibility to close any of the paths A, B, C and D. This is shown in Figure 3, which is a simplified version of Figure 2 with added shutters SA, SB, SC and SD. It is in fact enough to have just two shutters at two complementary arms, as a simple consideration shows.

Considering design of a crossed beam experiment where it is aimed to assure that the particles will meet at two different spatial positions, we conclude that such requirements cannot be reconciled with the uncertainty relations. Instead, as in all other collision processes, the experimenter prepares the conditions, and then picks up only the suitable events where the double collision actually happened. This is in fact the usual situation in collision physics: if we wish to study scattering to say 45 degrees, we will not be able to assure that all particles really come to the wanted solid angle. The measurement is done by eliminating all the other uninteresting events.

The crossed beam experiment is relatively easy to understand, but in practice nearly impossible to realize, since the particles must come as close as some nanometers to each other twice at two remote places. We outline a different arrangement, which is far less suited for discussions, but which might even be realized experimentally.

1. The crossing of the beams is replaced by passing of two beams with different velocities. Thus the alignment of the two beams provides a better chance for the particles of the two beams to come close.
2. In this case one can pick up only the particles which really came close in the first collision region by selecting a certain small but finite scattering angle. A set of collimating "funnels" can be devised to assure the most optimal arrangement. By such techniques one could also attempt to suppress the background of unwanted double collisions with two different particles of the beam, e.g. by using the "collision plane" as a marking device.
3. Most of the "deflecting plates" can be replaced by magnetic field arrangements, which also separate the beams with respect to velocity.

It is outside of the scope of this paper to discuss detailed experimental arrangements. We only mention that a certain optimistic merged beams scenario with beam currents of about 10 nA and assumption of perfectly overlaping beam areas of 1 μm^2 gave us an estimate of the frequency of one real double collision in about one hour, assuming a collision cross-section $\approx 10^{-15}$ cm^2.

Also other realizations of the outlined mechanism can be considered, e.g. replacing the He ions by ions of Be or Mg, which are quasi two-electron atoms, and might allow manipulations by laser fields before entering the experimental regions (e.g. for cooling the transversal motion or focusing). Another possibility might be larger and slower singly charged systems where the exchanged particle might be a whole atom. The advantage would be that the particle exchange will not change the charge of the colliding systems. Storage rings, ion traps and cool atoms might be considered as parts of scenarios to attempt realization of the outlined phenomena. Storage rings would allow reuse of the beams, a very special ion trap with e.g. just one pair of ions present would allow nearly idealized conditions. The still little known behavior of beams of cold atoms might provide new means to "mark" the desired double collisions on the background of the unwanted collisions with two different particles of the beam.

The theoretical analysis of successive collisions has to our knowledge not been formulated before, simply because of the experimental difficulties of the corresponding observations, as discussed above. A convenient description of double collisions can be given in terms of classical trajectories of the heavy particles and single particle quantum mechanical treatment of the electron. Such theoretical description is standard in the physics of ion-atom and ion-ion collisions (e.g. Bang and Hansteen [4]).

In the semiclassical picture, the electron shared by the pair of nuclei A and B in question, obeys the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = (T + V(|\mathbf{r} - \mathbf{R}_A|) + V(|\mathbf{r} - \mathbf{R}_B|))\Psi(\mathbf{r},t). \tag{3}$$

The vectors $\mathbf{R}_A$ an $\mathbf{R}_B$ for the trajectories with repeated collisions can then be written as

$$\begin{aligned} \mathbf{R}_A &= 0 & -\infty &< t < \infty \\ \mathbf{R}_B &= \mathbf{b}_1 + \mathbf{v}_1 t & -\infty &< t < t_1 \\ |\mathbf{R}_B| &\gg R_{\text{coll}} & t_1 &< t < t_2 \\ \mathbf{R}_B &= \mathbf{b}_2 + \mathbf{v}_2 t & t_2 &< t < \infty \end{aligned} \tag{4}$$

with impact parameters $\mathbf{b}_1$, $\mathbf{b}_2$ and collision velocities $\mathbf{v}_1$, $\mathbf{v}_2$ where the actual shape of the trajectory between t_1 and t_2 is not important, as far as the distance between the two ions is so large that the couplings causing the particle exchange are negligible.

It might be advantageous to describe the solution of (3) in terms of the time development operator $U(t_2, t_1)$,

$$\Psi(\mathbf{r}, t_2) = U(t_2, t_1)\Psi(\mathbf{r}, t_1)$$

which is known to obey the same equation.

Considering only the two-state description (i.e. electron on nucleus A or nucleus B), all the single collision experiments are described by

$$U_{\mathbf{b},\mathbf{v}}(\infty, -\infty)$$

which can be written as

$$U_0(\infty, t_{\text{coll}})U_{\mathbf{b},\mathbf{v}}(t_{\text{coll}}, -t_{\text{coll}})U_0(-t_{\text{coll}}, -\infty)$$

since outside of the collision region, which is passed in time t_{coll}, there is no coupling between the states.

The independent development of each of the states is described by the "unperturbed" U_0, which will have a very simple form because both the energies in resonant capture are equal

$$U_0(t_2 - t_1) =$$
$$(|\varphi(A)\rangle\langle\varphi(A)| + |\varphi(B)\rangle\langle\varphi(B)|)\, e^{-\mathrm{i}\frac{E}{\hbar}(t_2-t_1)} \quad (5)$$

The state of the electron which is shared by a pair of ions who by chance did undergo the double collision, is obtained from the original state $|\varphi(A)\rangle$ by applying the time development operator

$$U_{\text{double}}(\infty, -\infty) = U_0(\infty, t_2 + 2t_{\text{coll}})U_{\mathbf{b}_2,\mathbf{v}_2}(t_2 + 2t_{\text{coll}}, t_2)$$
$$\times U_0(t_2, t_1)U_{\mathbf{b}_1,\mathbf{v}_1}(t_1, t_1 - 2t_{\text{coll}})U_0(t_1 - 2t_{\text{coll}}, -\infty). \quad (6)$$

Denoting

$$U_{\mathbf{b},\mathbf{v}}(t_{\text{coll}}, -t_{\text{coll}}) \; \rightarrow \; \mathcal{U}_{\mathbf{b},\mathbf{v}} \quad (7)$$

the probability for transfer in the usual single collision process is given as

$$I(\varphi(B) \leftarrow \varphi(A)) = |\langle\varphi(B)|\mathcal{U}_{\mathbf{b},\mathbf{v}}|\, \varphi(A)\,\rangle|^2 = |f_{BA}(\mathbf{b}, \mathbf{v})|^2 \quad (8)$$

where the phases are canceled by the absolute value operation.

The probability for transfer in the double collision process is obtained by using the corresponding amplitude

$$I_{\text{double}}(\varphi(B) \leftarrow \varphi(A)) = \left| f_{BA}^{\text{double}}(\mathbf{b}_2, \mathbf{v}_2; \mathbf{b}_1, \mathbf{v}_1)\right|^2. \quad (9)$$

Evaluating the amplitude from equation (6), inserting in it the equation (5), one obtains

$$f_{BA}^{\text{double}}(\mathbf{b}_2, \mathbf{v}_2; \mathbf{b}_1, \mathbf{v}_1) =$$
$$e^{\mathrm{i}\alpha}\, [\langle\varphi(B)|\mathcal{U}_{\mathbf{b}_2,\mathbf{v}_2}|\varphi(A)\rangle\langle\varphi(A)|\mathcal{U}_{\mathbf{b}_1,\mathbf{v}_1}|\varphi(A)\rangle$$
$$+ \langle\varphi(B)|\mathcal{U}_{\mathbf{b}_2,\mathbf{v}_2}|\varphi(B)\rangle\langle\varphi(B)|\mathcal{U}_{\mathbf{b}_1,\mathbf{v}_1}|\varphi(A)\rangle]. \quad (10)$$

With the notation implied in equation (8)

$$f_{BA}^{\text{double}}(\mathbf{b}_2, \mathbf{v}_2; \mathbf{b}_1, \mathbf{v}_1) = e^{\mathrm{i}\alpha}\, [f_{BA}(\mathbf{b}_2, \mathbf{v}_2)f_{AA}(\mathbf{b}_1, \mathbf{v}_1)$$
$$+ f_{BB}(\mathbf{b}_2, \mathbf{v}_2)f_{BA}(\mathbf{b}_1, \mathbf{v}_1)] \quad (11)$$

where again the common phases are summarized by a phase factor. The analysis based on cross-sections, replaces the present I_{double} of equations (9, 11) by a combination of non-coherent products of probabilities,

$$I_{\text{succ}}(\varphi(B) \leftarrow \varphi(A)) = |f_{BA}(\mathbf{b}_2, \mathbf{v}_2)|^2\; |f_{AA}(\mathbf{b}_1, \mathbf{v}_1)|^2$$
$$+ |f_{BB}(\mathbf{b}_2, \mathbf{v}_2)|^2\; |f_{BA}(\mathbf{b}_1, \mathbf{v}_1)|^2. \quad (12)$$

The difference between I_{double} in equation (9) and I_{succ} in equation (12) could be detected in the experiment. Precisely how this would be done depends on the actual experimental arrangement.

Concluding, we have proposed a gedanken experiment with crossed or merged beams of He^+ and He^{++} ions. In a collision region the ions can exchange an electron. The proposed experimental arrangement is such that the beams can merge once more in a second collision region, and it is assumed that the possibility of a second encounter of the same pair of ions is experimentally enhanced as much as possible. The electron can be exchanged in either of the two collision regions. This leads to observable interference of probability amplitudes. The two interfering histories require that any of the two ions travels through the apparatus in form of two completely different physical systems, *i.e.* either as a bare nucleus or as a singly charged ion. The present phenomenon thus brings one more "reincarnation" of the Schrödinger cat. Unlike for the original cat, which could not decide if it were alive or dead, the two ions cannot "decide" whether to be singly charged or doubly charged. However, their behaviour is not a paradox, but rather a simple prediction of quantum mechanics.

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