Emergence of Spacetime in Quantum Shape Dynamics

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Abstract

We study kinematics of atoms and molecules in quantum shape dynamics. We analyzed a model universe where there is only electrical force between protons and electrons. In ref. [2] a similar model where there is only gravitational attraction between masses is investigated. Our results is an expansion of the ideas there. We found that hydrogen atoms can form when they are entangled in singlet pairs. On the other hand if there is single hydrogen atom in the universe, it occupies the entire universe. What is more, in the investigation of hydrogen molecule, we found that absolute spacetime emerges by coarse graining the quantum degrees of freedom. It may be that spacetime only exists because of the presence of quantum degrees of freedom. This is especially important from the quantum gravity perspective.

1 Introduction

Shape dynamics is a fully relational theory of gravitation. In the case of N body problem, it states that only the relative distances and angles between them are dynamical [1]. In this scenario universe cannot have a nonvanishing angular momentum otherwise it would define an absolute space in which the universe is rotating [2]. Similarly nonvanishing total energy implies an external absolute time according to which the universe evolves, therefore we require total energy to vanish [2]. Another constraint comes from working in the center of mass frame, the total momentum should be zero. Some works [3] also put another constraint on the system, the vanishing of the dilational momentum: $\sum_a \mathbf{r}^a \cdot \mathbf{p}^a = 0$. This is required for scale invariance [3] however we will not impose it. Overall, we have three constraints:

- $\mathrm{H} = \sum_a E^a = 0$
- $\mathbf{P} = \sum_a \mathbf{p}^a = 0$
- $\mathbf{L} = \sum_a \mathbf{r}^a \times \mathbf{p}^a = 0$

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2 Analysis of Constraints

In this section we consider a universe populated by N_p protons and N_e electrons with masses m_p and m_e and with charges $-e$ and e. The total energy is:

$$H = \sum_a \frac{\mathbf{p}_a^2}{2m_a} + \frac{1}{2}\sum_{a\neq b} \frac{kq_a q_b}{|\mathbf{r}^a - \mathbf{r}^b|}, \tag{1}$$

where $k = 1/4\pi\epsilon_0$. We need to calculate Poisson brackets of commutators with each other in order to classify them. This distinction will be important when we quantize the theory. We do calculations in Appendix A and we list the results here:

$$\{P_i, P_j\} = 0, \tag{2}$$
$$\{L_i, L_j\} = \varepsilon^{ijk} L_k, \tag{3}$$
$$\{L_i, P_j\} = \varepsilon^{ijk} P_k, \tag{4}$$
$$\{H, P_i\} = 0, \tag{5}$$
$$\{H, L_i\} = 0. \tag{6}$$

The results of these commmutators are either zero or another constraint. Hence they vanish weakly. Therefore all the constraints are first class in the terminology of Dirac [4].

3 Quantization of the Model

We quantize the model by promoting positions and momenta to quantum operators. The Poission bracket $\{\cdot,\cdot\}$ is mapped to $i\hbar[\cdot,\cdot]$. Between position and momenta we now have:

$$[\hat{r}_i^a, \hat{p}_j^b] = i\hbar\delta_b^a\delta_j^i. \tag{7}$$

Momenta are represented by operators, $\hat{p}_i^a = -i\hbar\partial/\partial r_i^a$. It is time to consider what happens to constraints in this case. As the readers can verify easily, the constraint algebra survives the quantization. In particular there is no anomaly. In the presence of dilational momentum constraint ref. [3] reports the existence of scale anomaly. It is then argued in [3] that this anomaly may give rise to a gravitational arrow of time.

At the quantum level the constraints become operators acting on the quantum state of the system. For example the Hamiltonian constraint becomes:

$$H\psi = \sum_a -\frac{\hbar^2}{2m}\nabla_a^2\psi + V\psi = 0, \tag{8}$$

where ∇_a stands for gradient with respect to particle a: $(\partial/\partial r_x^a, \partial/\partial r_y^a, \partial/\partial r_z^a)$. We see that we have obtained a time independent Schrödinger equation. Wavefunctions do not evolve in time and are static. This is similar to what happens with the Wheeler-DeWitt equation.

The momentum and angular momentum constraints become:

$$\mathbf{P}\psi = -i\hbar \sum_a \nabla_a \psi = 0, \tag{9}$$

$$\mathbf{L}\psi = -i\hbar \sum_a \mathbf{r}^a \times \nabla_a \psi = 0. \tag{10}$$

We interpret equations (8) (9) and (10) as operator equations that determines the allowed kinematic states of the system. They do not determine the dynamics.

4 Formation of a Single Hydrogen Atom

In this section we suppose there is only one proton and electron in the universe. Classically, with the constraints in mind, shape dynamics tells us that proton and electron collide head-on with no angular momentum. Let us see if this description changes once the quantum mechanics is taken into account.

Rather than using $\mathbf{r}^1$ and $\mathbf{r}^2$ let us use the center of mass vector $\mathbf{R}$ and $\mathbf{r} = \mathbf{r}^2 - \mathbf{r}^1$ as coordinates. Here the first and second indices refer to proton and electron respectively. In this variables the Hamiltonian becomes:

$$H = \frac{\mathbf{p}_R^2}{2M} + \frac{\mathbf{p}_r^2}{2\mu} - \frac{ke^2}{r}, \tag{11}$$

where $M = m_p + m_e$ is the total mass and $1/\mu = 1/m_p + 1/m_e$ is the reduced mass. Center of mass degree of freedom is decoupled from the relative degrees of freedom. Because we work in the center of mass frame $\mathbf{R} = 0$. The rest of the Hamiltonian give rise to a hydrogen atom. The solutions of the hydrogen atom is well known in the literature. Readers may see [5].

However the eigenfunctions of the Hamiltonian produces an energy $-13.6\ \mathrm{eV}/n^2$ where $n = 1, 2, \ldots$ In order to satisfy the Hamiltonian constraint $H\psi = 0$ it is seen that n must approach to infinity: $n \to \infty$. On the other hand the angular momentum constraint requires $\mathbf{R} \times \mathbf{p}_R\psi + \mathbf{r} \times \mathbf{p}_r\psi = 0$. The first term vanishes because $\mathbf{R} = 0$. The other term vanishes only if the electron occupies an $l = 0$ state.

Moreover we have the momentum constraint. By the Ehrenfest theorem for the momenta of proton and electron we have $d\langle p_r^1\rangle/dt = \langle \partial V/\partial r\rangle$ and $d\langle p_r^2\rangle/dt = \langle -\partial V/\partial r\rangle$. The other components of momenta are zero. By integrating the sum of these two we reach $\langle p_r^1 + p_r^2\rangle = C$ where C is some constant. However because we are in the center of mass reference frame C must be equal to zero. We conclude that one proton and one electron in the universe forms a hydrogen atom occupying the entire universe.

5 Formation of Two Hydrogen Atoms

Let us suppose now there are two protons and two electrons in the universe. Because there are more degrees of freedom, we suspect there are many ways to satisfy the shape dynamics constraints. First we suppose hydrogen atoms are far from each other so that each of them can be regarded as isolated systems. Then we will focus on the possibility of hydrogen molecule.

This case is more interesting because the part of the Hamiltonian that describes each atom can take negative energy eigenvalues. These eigenvalues is then compensated by nonzero atomic momentum, hence the Hamiltonian constraint is satisfied. At maximum the total kinetic energy of atoms will be 27.2 eV. Atoms do form.

By arranging the motion of atoms there is a way to satisfy the Hamiltonian and momentum constraints. However the angular momentum constraint is more involved. If both electrons occupy $l = 0$ states there is nothing to do. However when at least one of them occupies a $l \neq 0$ or $m \neq 0$ angular momentum state we need a way to solve the problem. The solution comes from the addition of angular momenta. When two atoms where electrons occupy l, l' angular momentum states we find the possible *holistic* states by adding the angular momenta appropriately. In general the sum of l and l' gives states of angular momentum ranging from $|l - l'|$ to $l + l'$. However the theory allows only the zero angular momentum state. Therefore the l number of the angular momentum states occupied by the two electrons must be the same. On the other hand if one atom has $m \neq 0$ state the other should have an $m' \neq m$ state. What is more the atoms must become *entangled* in order to give a zero angular momentum overall state. This is a novel prediction of shape dynamics on atoms. In particular if $|\psi_1\rangle$ and $|\psi_2\rangle$ are the states of two atoms the state of the universe is given by the following equation:

$$|\Psi\rangle = e^{i\mathbf{R}^1\cdot\mathbf{k}^1} e^{i\mathbf{R}^2\cdot\mathbf{k}^2} \frac{|\psi_1\rangle|\psi_2\rangle - |\psi_2\rangle|\psi_1\rangle}{\sqrt{2}}, \tag{12}$$

where $\mathbf{k}^1$ and $\mathbf{k}^2$ are appropriate momenta that are chosen to satisfy the momentum constraint.

6 Formation of Hydrogen Molecules

It is time to consider the formation of a hydrogen molecule. First, we think that there are two hydrogen atoms. Second we will look at the case where there are many atoms in the universe.

If the two atoms are close to one other, we expect they form a hydrogen molecule. This situation is more complex. Because electrons no longer occupy definite angular momentum states. Only the z component of angular momentum is quantized: molecular orbitals are common eigenfunctions of L_z and H.

When the molecule forms the expectation value of $\mathbf{L}$ will be nonzero. In order to satisfy the angular momentum constraint the molecule must rotate in a way to cancel the expectation value of $\mathbf{L}$. However this cannot occur. Because the $\langle\mathbf{L}\rangle$ rotates with the molecule as well. It is true that *time average* of angular momentum may vanish but this is still contrary to shape dynamic constraints. We therefore conclude that if there are two hydrogen atoms in the universe, a hydrogen molecule cannot form.

In a universe with N_p protons and N_e electrons hydrogen atoms and molecules will form possibly with the exception of a few unbound protons and electrons. Hydrogen molecules will form if there is a subsystem of the rest of the system whose angular momentum cancels that of the hydrogen molecule. For example bypassing two hydrogen atom may yield a total angular momentum in the direction of the angular momentum of the molecule. The same is true for $m \neq 0$

states of the hydrogen atom. The rest of the system must compensate for nonzero $\langle \mathbf{L} \rangle$.

This observation is especially striking from the point of view of classical shape dynamics. When considered as point particles, two atoms and one hydrogen molecule cannot rotate in a way to acquire angular momentum because it violates the angular momentum constraint and defines an absolute space in which things can rotate [2]. However when atoms are regarded as having internal structure, we have seen that a two hydrogen atoms can bypass each other in a way to cancel the expectation value of quantum angular momentum of the hydrogen molecule. From this observation we find that absolute spacetime emerges by coarse graining of quantum degrees of freedom. This conclusion is especially important from the quantum gravity perspective. It may be that spacetime only exist because of the presence of quantum degrees of freedom.

If we consider two atoms in the $l = 0$ state, when an electron excited in one atom, an electron of another atom must be excited and the two atoms should form a singlet state. This scenario may also be realized in disintegration of a hydrogen molecule. This is not a local effect. It is a holistic argument that determines the allowed atomic states of the universe. Hence quantum shape dynamics departs from usual quantum mechanics in that aspect.

7 Conclusion

In this paper we analyzed a model universe where there is only electrical force between protons and electrons. In ref. [2] a similar model where there is only gravitational attraction between masses is investigated. Our results are expansions of the ideas there. We found that if there is single hydrogen atom in the universe, it occupies the entire universe. Two hydrogen atoms can form when they are entangled in singlet pairs. Hydrogen molecules can form in bigger systems when a subsystem has angular momentum that cancels the angular momentum expectation value of the molecule.

From the quantum gravity point of view, we have found that when we coarse grain the quantum degrees of freedom absolute spacetime emerges due to rotation of the molecules.

Quantum shape dynamics impose numerous constraints on the quantum system. In order to solve the constraints we only thought about atomic degrees of freedom. However an open problem is to see how the results we found changes when one includes the field energy, momenta and angular momentum. Another problem is to see in a very large system of hydrogen atoms whether the formation of hydrogen molecules imply the existence of curved spacetime.

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References

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A Constraint Analysis

Commutation of momentum components:

$$\{P_i, P_j\} = \sum_{ab} \left\{p_i^a, p_j^b\right\} = 0. \tag{13}$$

Commutation of angular momentum components (We adopt Einstein summation convention: repeated indeces are summed over):

$$\{L_i, L_j\} = \left\{\sum_a \varepsilon^{ikl} r_k^a p_l^a, \sum_b \varepsilon^{jmn} r_m^b p_n^b\right\} \tag{14}$$

$$= \sum_{ab} \varepsilon^{ikl} \varepsilon^{jmn} [p_l^a r_m^b \left\{r_k^a, p_n^b\right\} + r_k^a p_n^b \left\{p_l^a, r_m^b\right\}] \tag{15}$$

The Poisson brackets will yield a product of Kronecker deltas: $\delta_b^a \delta_n^k$ and $-\delta_b^a \delta_m^l$

$$= \sum_a \varepsilon^{ikl} \varepsilon^{jmk} r_m^a p_l^a - \sum_a \varepsilon^{ikl} \varepsilon^{jln} r_k^a p_n^a \tag{16}$$

The sum of two Levi-Civita symbols over one index yields two Kronecker deltas: $\varepsilon^{ijk}\varepsilon^{ilm} = \delta_l^j \delta_m^k - \delta_m^j \delta_l^k$.

$$= \sum_a (r_i^a p_j^a - r_j^a p_i^a) \tag{17}$$

$$= \varepsilon^{ijk} L_k \tag{18}$$

Commutation of momentum and angular momentum components:

$$\{L_i, P_j\} = \left\{\sum_a \varepsilon^{ilm} r_l^a p_m^a, \sum_b p_j^b\right\} \tag{19}$$

$$= \sum_{ab} \varepsilon^{ilm} p_m^a \left\{r_l^a, p_j^b\right\} \tag{20}$$

$$= \varepsilon^{ijm} \sum_a p_m^a \tag{21}$$

$$= \varepsilon^{ijk} P_k \tag{22}$$

Commutation of Hamiltonian and momentum:

$$\{H, P_i\} = \left\{\sum_a \frac{(\mathbf{p^a})^2}{2m_a} + V, \sum_b p_i^b\right\} \tag{23}$$
$$= \sum_b \left\{V, p_i^b\right\} \tag{24}$$
$$= \sum_b \frac{\partial V}{\partial r_i^b} \tag{25}$$
$$= 0 \tag{26}$$

This is because V is only a function of interparticle separations. This is expected because the commutator $\{P_i, H\}$ equals the total external force on the system which is zero. Commutation of Hamiltonian and angular momentum:

$$\{H, L_i\} = \left\{\sum_a \frac{(\mathbf{p^a})^2}{2m_a} + V, \sum_b \varepsilon^{ijk} r_k^b p_k^b\right\} \tag{27}$$
$$= \sum_{ab} \frac{p_l^a \left\{p_l^a, r_j^b\right\} p_k^b \varepsilon^{ijk}}{m_a} + \sum_b \varepsilon^{ijk} r_j^b \left\{V, p_k^b\right\} \tag{28}$$

The first term will yield a sum over $\mathbf{p}^a \times \mathbf{p}^a$ which is zero.

$$= \sum_b \varepsilon^{ijk} r_j^b \frac{\partial V}{\partial r_k^b} \tag{29}$$
$$= \sum_b \mathbf{r^b} \times \nabla_b V\Big|_i \tag{30}$$

where ∇_b stands for gradient with respect to particle b: $(\partial/\partial r_x^b, \partial/\partial r_y^b, \partial/\partial r_z^b)$.

$$= 0 \tag{31}$$

It vanishes because V only depends on the interparticle separations. This is a check that the angular momentum constraint is preserved as time goes on.

All in all, we have the following relations:

$$\{P_i, P_j\} = 0, \tag{32}$$
$$\{L_i, L_j\} = \varepsilon^{ijk} L_k, \tag{33}$$
$$\{L_i, P_j\} = \varepsilon^{ijk} P_k, \tag{34}$$
$$\{H, P_i\} = 0, \tag{35}$$
$$\{H, L_i\} = 0. \tag{36}$$