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Study of Pauli exchange symmetry in atomic spin-exchange collisions

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Abstract

The following work considers a possible violation of fermionic statistics, in other words, the violation of Pauli's exclusion principle.

We begin by laying the mathematical foundation of the violation, by introducing a ϕ-parameter, so as to quantify the violation. We then introduce an algebra to replace the fermionic one. Combining these, we relate them to already known experimental results.

We finish by establishing a framework, in order to measure ϕ under a new experimental setup and compare to previous work on the problem.

Contents

Chapter 1

Introduction

A rather interesting chapter in physics, is that of atomic spin-exchange collisions. With a plethora of applications, from nuclear physics to medical imaging, the range from experimental to theoretical work, is unbounded.

It does not come as a surprise, the fact that the Pauli exclusion principle, should play an important role in the formulation and evaluation of such scattering processes. For the most part, the existing theoretical work, considers the initial states as uncorrelated, mostly in order to simplify the problem. Hence, we do not, as of yet, have a complete picture of such collisions.

In order for one to study such scattering processes, or any process containing fermions for that matter, a very specific assumption is made. The exclusion principle itself, is assumed to be true. Such a statement might seem to hold as fact, but until now there exists no theoretical framework to fully explain why nature should use either bosons or fermions. It is possible, as we shall discuss below, to have a continuum of representations, apart from the symmetric and antisymmetric, that we are, for the most part, fond of.

On this issue, a number of experiments [1, 2, 6, 3] have been performed, in order to test the principle itself.

In the following work, we begin the process of formulating theoretically the problem, combining and extending existing knowledge on the subject. Our goal is to test the principle, via a mathematical model on atomic spin-exchange collisions. If the principle breaks down, it should slightly change the expected theoretical result of the scattering process between two atoms.

In our study, we focus on systems with one external electron, also known as a valence electron. We will also be focusing on initially uncorrelated scattering states. Both of these simplifications can be generalized, with the latter being a rather hard problem. Therefore, the hydrogen atom suffices as the atom of choice, to formulate the theoretical background, so as to be able to extend the theory in later works.

The final part of such a work, should be the comparison between this and existing

experimental data on the violation of the Pauli exclusion principle. On this front, we provide the mathematical correspondence between the to be performed experiment from our work and the aforementioned existing results.

Chapter 2

The ϕ-parameter

Consider a Hilbert space :

$$\mathbb{H} = \mathbb{H}_{\mathrm{A}} \otimes \mathbb{H}_{\mathrm{B}}$$

with $|\psi\rangle \in \mathbb{H}$ an element of the vector space, such that :

$$|\psi\rangle = |\psi_{\mathrm{A}}\rangle \otimes |\psi_{\mathrm{A}}\rangle \tag{2.1}$$

, where $|\psi_{\mathrm{A}}\rangle \in \mathbb{H}_{\mathrm{A}}$,$|\psi_{\mathrm{B}}\rangle \in \mathbb{H}_{\mathrm{B}}$.

Let $\mathcal{B}(\mathbb{H})$ be a vector space acting on $\mathbb{H}$. Consider an element $\mathrm{P} \in \mathcal{B}(\mathbb{H})$, defined by the action :

$$\mathrm{P} : \mathcal{B}(\mathbb{H}) \times \mathbb{H} \to \mathbb{H} \tag{2.2}$$

$$\mathrm{P} : |\psi_{\mathrm{A}}\rangle \otimes |\psi_{\mathrm{B}}\rangle \to |\psi_{\mathrm{B}}\rangle \otimes |\psi_{\mathrm{A}}\rangle + \phi\, |\psi_{\mathrm{A}}\rangle \otimes |\psi_{\mathrm{B}}\rangle \tag{2.3}$$

, where $\phi \in \mathbb{R}$ is a small parameter, $|\phi| \ll 1$.
It is convenient to deconstruct P, by defining $\mathrm{Q} \in \mathcal{B}(\mathbb{H})$ such that :

$$\mathrm{Q} : \mathcal{B}(\mathbb{H}) \times \mathbb{H} \to \mathbb{H} \tag{2.4}$$

$$\mathrm{Q} : |\psi_{\mathrm{A}}\rangle \otimes |\psi_{\mathrm{B}}\rangle \to |\psi_{\mathrm{B}}\rangle \otimes |\psi_{\mathrm{A}}\rangle \tag{2.5}$$

and thus write P as follows :

$$\mathrm{P} = \mathrm{Q} + \phi \mathbb{1} \tag{2.6}$$

with $\mathbb{1}$ being the identity element of $\mathcal{B}(\mathbb{H})$. We now provide a few useful identities :

$$\mathrm{Q}^\dagger = \mathrm{Q} \quad , \quad \mathrm{P}^\dagger = \mathrm{P}$$
$$\mathrm{P}^\dagger \mathrm{P} = \mathrm{P}^2 = (1+\phi^2)\mathbb{1} + 2\phi \mathrm{Q}$$
$$(\mathbb{1} - \mathrm{P})(\mathbb{1} - \mathrm{P})^\dagger = (\mathbb{1} - \mathrm{P})^2 = 2(\frac{\phi^2}{2} - \phi + 1)\mathbb{1} + 2(\phi - 1)\mathrm{Q}$$

Suppose for a moment that $\phi = 0$, then by use of (2.3) we can write down an anti-symmetric element of $\mathbb{H}$, by the action of the operator $\frac{1}{\sqrt{2}}(\mathbb{1} - \mathrm{P})$ on $\mathbb{H}$. Naturally, this is equivalent to saying that we are considering some fermion in the theory. Therefore the addition of the ϕ-parameter via (2.3), changes the fermionic algebra.

Consider the algebra[1].

$$a_i a_j^\dagger - q a_j^\dagger a_i = \delta_{ij} \tag{2.7}$$

This is a generalization of the classical Bose and Fermi algebras (CCR and CAR) corresponding to $q = 1$ and $q = -1$ respectively. In Appendix A, we show that relation (2.7) has a Hilbert space realization for $q \in (-1, 1)$, providing a positive norm. Here we are specifically interested in $q + 1 \approx 0$, meaning a small violation of the anticommutation algebra, which in turn means that a small violation of the Pauli exclusion principle (PEP) exists.

The parameter ϕ, which represents the aforementioned small violation of the fermionic statistics, can be written in terms of q as :

$$q = -2(\frac{1}{2} - \phi) \quad , \quad \phi \ll 1 \tag{2.8}$$

$$\phi = \frac{1}{2}(1 + q) \tag{2.9}$$

Consider two identical q-particles and the vectors $|\psi_a\rangle, |\psi_s\rangle$[2]. Then we write the density operator :

$$\rho = \frac{1+q}{2} |\psi_s\rangle \langle\psi_s| + \frac{1-q}{2} |\psi_a\rangle \langle\psi_a| \tag{2.10}$$

Hence, if no violation exists, $\phi = 0$, the density operator is of the usual fermionic type.

For us to be able to compare our results with the rest of the community on PEP violations, we note the usual convention made to experimentally test the principle. Usually the parameter $\frac{\beta^2}{2}$ is used, so as to relate it to the probability of violating the fermi statistics. Specifically, according to (2.10), by use of $\frac{\beta^2}{2}$, we expect a density operator of the form :

$$\rho = \frac{\beta^2}{2} |\psi_s\rangle \langle\psi_s| + \frac{1}{2}(1 - \beta^2) |\psi_a\rangle \langle\psi_a| \tag{2.11}$$

Equating to (2.10), we conclude that :

$$\frac{\beta^2}{2} = \frac{1}{2}(1 + q) = \phi \tag{2.12}$$

We make use of the Ramberg-Snow bound[4], stating that :

$$0 \leq \frac{\beta^2}{2} \leq 1,7 \cdot 10^{-26}$$

[1] In appendix A we formulate the necessary mathematical framework of the q-algebra.

[2] s for symmetric and a for antisymmetric.

, which in turn implies :

$$0 \leq \phi \leq 1,7 \cdot 10^{-26} \tag{2.13}$$

Concluding, in the following chapter we lay down the necessary theoretical framework, so as to follow up with an experiment to determine ϕ and compare the result to (2.13).

Chapter 3

Mathematical Formulation

Consider two atoms, each formed by a nucleus n_i and an electron e_i, $i = 1, 2$, respectively. Assume, in the context of this work, that both atoms are in the ground state. Both nuclei have the isospin degrees of freedom, apart from the usual spin degrees of freedom, carried by the electrons. In the following work, we denote as m_s the spin projection of each electron and m_I the isospin projection of either nucleus. We also write the ket :

$$|e_i, n_j\rangle \quad , \quad i, j = 1, 2$$

, to denote on which nucleus is either electron bounded to. Additionally, the vector :

$$|n_i, \vec{k}_i\rangle \quad , \quad i = 1, 2$$

denotes the momentum of the center of mass of either bound state, as we take the mass of the nuclei to be much larger than that of the electrons.

3.1 Total Density Operator

Let $\mathbb{H}$ be a Hilbert space, containing the vectors describing the states in our problem. Assume $\mathcal{B}(\mathbb{H})$ to be an acting space on $\mathbb{H}$, containing the operators we are interested in. Let $\mathbb{H}_\mathrm{A}$ and $\mathbb{H}_\mathrm{B}$ be subspaces of $\mathbb{H}$, such that :

$$\mathbb{H} = \mathbb{H}_\mathrm{A} \otimes \mathbb{H}_\mathrm{B}$$

$$\mathcal{B}(\mathbb{H}) = \mathcal{B}(\mathbb{H}_\mathrm{A}) \otimes \mathcal{B}(\mathbb{H}_\mathrm{B})$$

Consider $|e_i, n_j\rangle \in \mathbb{H}_\mathrm{A}$ and $|e_k, n_l\rangle \in \mathbb{H}_\mathrm{B}$, with $i, j, k, l = 1, 2$, $i \neq k$, $j \neq l$. We assume that $\nexists W_q^{(1)}, W_q^{(2)}, W_q^{(3)}, W_q^{(4)} \in \mathbb{C}$ such that :

$$|e_i, n_j\rangle = \sum_{q_1, q_2} W_{q_1}^{(1)} W_{q_2}^{(2)} \, |\epsilon_{i,q_1}\rangle \otimes |\epsilon_{j,q_2}\rangle$$

$$|e_k, n_l\rangle = \sum_{q_1,q_2} W^{(3)}_{q_1} W^{(4)}_{q_2} \, |\epsilon_{k,q_1}\rangle \otimes |\epsilon_{l,q_2}\rangle$$

, with $|\epsilon_{i,q_1}\rangle \in \mathbb{H}_{\mathrm{A},e}$, $|\epsilon_{j,q_2}\rangle \in \mathbb{H}_{\mathrm{A},n}$, $|\epsilon_{k,q_1}\rangle \in \mathbb{H}_{\mathrm{B},e}$, $|\epsilon_{l,q_2}\rangle \in \mathbb{H}_{\mathrm{B},n}$, where

$$\mathbb{H}_{\mathrm{A}} = \mathbb{H}_{\mathrm{A},e} \otimes \mathbb{H}_{\mathrm{A},n}$$

$$\mathbb{H}_{\mathrm{B}} = \mathbb{H}_{\mathrm{B},e} \otimes \mathbb{H}_{\mathrm{B},n}$$

We now have the foundations to define the system's density operator. Let $\sigma_{\mathrm{init}} \in \mathcal{B}(\mathbb{H})$ be defined as :

$$\begin{aligned}\sigma_{\mathrm{init}} \equiv \int \mathrm{d}^3k_i \, \mathrm{d}^3k'_i u(\vec{k}_i) u^*(\vec{k'}_i)(\, |n_1, \vec{k}_i; n_2, -\vec{k}_i\rangle \, \langle n_1, \vec{k'}_i; n_2, -\vec{k'}_i|) \otimes (|e_1, n_1\rangle \langle e_1, n_1|) \\ \otimes (|e_2, n_2\rangle \langle e_2, n_2|) \otimes \rho(n_1, e_1, n_2, e_2)\end{aligned} \tag{3.1}$$

, with the integrals over the initial momenta and $u(\vec{k}_i), u^*(\vec{k'}_i) \in \mathbb{C}$.
For our purposes, we assume that a vector $\in \mathbb{H}_{\mathrm{A}} \otimes \mathbb{H}_{\mathrm{B}}$, is separable, therefore the particle density operator, $\rho(n_1, e_1, n_2, e_2) \in \mathcal{B}(\mathbb{H})$, is separable :

$$\rho(n_1, e_1, n_2, e_2) = \rho_{\mathrm{A}}(n_1, e_1) \otimes \rho_{\mathrm{B}}(n_2, e_2) \tag{3.2}$$

, with $\rho(n_1, e_1) \in \mathcal{B}(\mathbb{H}_{\mathrm{A}})$ and $\rho(n_2, e_2) \in \mathcal{B}(\mathbb{H}_{\mathrm{B}})$. Hence, the system's density operator assumes the form :

$$\begin{aligned}\sigma_{\mathrm{init}} \equiv \int \mathrm{d}^3k_i \, \mathrm{d}^3k'_i u(\vec{k}_i) u^*(\vec{k'}_i)(\, |n_1, \vec{k}_i; n_2, -\vec{k}_i\rangle \, \langle n_1, \vec{k'}_i; n_2, -\vec{k'}_i|) \otimes (|e_1, n_1\rangle \langle e_1, n_1|) \\ \otimes (|e_2, n_2\rangle \langle e_2, n_2|) \otimes \rho_{\mathrm{A}}(n_1, e_1) \otimes \rho_{\mathrm{B}}(n_2, e_2)\end{aligned} \tag{3.3}$$

In addition, we will be imposing the normalization conditions :

$$\int \mathrm{d}^3k_i \, u^*(\vec{k}_i) u^(\vec{k}_i) = 1$$

$$\mathrm{Tr}\{\rho_{\mathrm{A}}\} = 1 \quad \mathrm{Tr}\{\rho_{\mathrm{B}}\} = 1$$

3.2 Indistinguishable Electrons

The transformation law of σ_{init}, to some σ_{fin}, is :

$$\sigma_{\mathrm{init}} \to \frac{(\mathbb{1}_e - \mathrm{P}_e)}{\sqrt{2}} \mathrm{S} \frac{(\mathbb{1}_e - \mathrm{P}_e)^\dagger}{\sqrt{2}} \sigma_{\mathrm{init}} \frac{(\mathbb{1}_e - \mathrm{P}_e)^\dagger}{\sqrt{2}} \mathrm{S}^\dagger \frac{(\mathbb{1}_e - \mathrm{P}_e)}{\sqrt{2}} \tag{3.4}$$

, where the index e indicates that the corresponding operator acts on the subspace of $\mathbb{H}$ concerning electrons. Moreover, the S operator, as seen in (3.4) is simply the evolution operator. Defining the parameters :

$$\alpha \equiv \frac{\phi^2}{2} - \gamma \quad , \quad \gamma \equiv \phi - 1 \tag{3.5}$$

, somewhat simplifies the relations. Trivially (3.4), takes the form :

$$\sigma_{\text{init}} \to (\alpha \mathbb{1}_e - \gamma \mathrm{Q}_e)\mathrm{S}\sigma_{\text{init}}\mathrm{S}^\dagger(\alpha \mathbb{1}_e - \gamma \mathrm{Q}_e) \tag{3.6}$$

We now begin the procedure of integrating over the n_2 degrees of freedom, so as to find $\sigma_{\text{fin}}(e, n_1)$, meaning the density operator for distinguishable nuclei :

$$\begin{aligned}\left\langle m_I m_s \middle| \sigma_{\text{fin}}(n_1, e) \middle| m'_I m'_s \right\rangle = \sum_{m''_I, m''_s} \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k'_i \, u(\vec{k}_i) u^*(\vec{k'}_i) \, \langle n_1, m_I, \vec{k}_f, e_1, m_s; n_2, m''_I, -\vec{k}_f, e_2, m''_s| \\ (\alpha \mathbb{1}_e - \gamma \mathrm{Q}_e)\mathrm{S}\sigma\mathrm{S}^\dagger(\alpha \mathbb{1}_e - \gamma \mathrm{Q}_e) \, |n_1, m'_I, \vec{k}_f, e_1, m'_s; n_2, m''_I, -\vec{k}_f, e_2, m''_s\rangle\end{aligned} \tag{3.7}$$

In order to make the calculations simpler, we define the integrals:

$$(\mathrm{I}) \equiv \alpha^2 \sum_{m''_I, m''_s} \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k'_i \, u(\vec{k}_i) u^*(\vec{k'}_i) \langle \mathrm{S}\sigma\mathrm{S}^\dagger \rangle \tag{3.8}$$

$$(\mathrm{II}) \equiv \gamma^2 \sum_{m''_I, m''_s} \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k'_i \, u(\vec{k}_i) u^*(\vec{k'}_i) \langle \mathrm{QS}\sigma\mathrm{S}^\dagger\mathrm{Q} \rangle \tag{3.9}$$

$$(\mathrm{III}) \equiv -\alpha\gamma \sum_{m''_I, m''_s} \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k'_i \, u(\vec{k}_i) u^*(\vec{k'}_i) \langle [\mathrm{QS}\sigma\mathrm{S}^\dagger + \mathrm{S}\sigma\mathrm{S}^\dagger\mathrm{Q}] \rangle \tag{3.10}$$

Therefore (3.7) becomes :

$$\left\langle m_I m_s \middle| \sigma_{\text{fin}}(n_1, e) \middle| m'_I m'_s \right\rangle = (\mathrm{I}) + (\mathrm{II}) + (\mathrm{III}) \tag{3.11}$$

We proceed, by calculating relations (3.8)-(3.10).

Substituting (3.1) into (3.8), we get :

$$(\mathrm{I}) = \alpha^2 \sum_{m''_I, m''_s} \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k'_i \, u(\vec{k}_i) u^*(\vec{k'}_i) S_d(\vec{k}_f, \vec{k}_i) S_d^*(\vec{k}_f, \vec{k'}_i) \left\langle m_I m_s \middle| \rho_{\mathrm{A}} \middle| m'_I m'_s \right\rangle \left\langle m''_I m''_s \middle| \rho_{\mathrm{B}} \middle| m''_I m''_s \right\rangle \tag{3.12}$$

, where we have defined the S-matrix element :

$$S_d(\vec{k}_f, \vec{k}_i) \equiv \langle n_1, \vec{k}_f, e_2; n_2, -\vec{k}_f, e_1| \, S \, |n_1, \vec{k}_i, e_2; n_2, -\vec{k}_i, e_1\rangle \tag{3.13}$$

The integral term of (3.12) is related to a scattering amplitude, as many that will follow in the work, via the phase shift method of scattering theory[9]. For now we simply state this fact[1] and define :

$$\mathcal{A}_d = \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k_i' \, u(\vec{k}_i) u^*(\vec{k'}_i) S_d(\vec{k}_f, \vec{k}_i) S_d^*(\vec{k}_f, \vec{k'}_i) \tag{3.14}$$

, with $\mathcal{A}_d$ describing the scattering procedure, where no electron exchange takes place between the nuclei. Then (3.12) reduces to :

$$\text{(I)} = \alpha^2 \mathcal{A}_d \left\langle m_I m_s \middle| \rho_{\mathrm{A}} \middle| m_I' m_s' \right\rangle \tag{3.15}$$

, where we have used the normalization condition of ρ_{B}.
Similarly relation (3.9), by defining the following :

$$S_t(\vec{k}_f, \vec{k}_i) \equiv \langle n_1, \vec{k}_f, e_2; n_2, -\vec{k}_f, e_1 | \, S \, | n_1, \vec{k}_i, e_1; n_2, -\vec{k}_i, e_2 \rangle \tag{3.16}$$

$$\mathcal{A}_t = \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k_i' \, u(\vec{k}_i) u^*(\vec{k'}_i) S_t(\vec{k}_f, \vec{k}_i) S_t^*(\vec{k}_f, \vec{k'}_i) \tag{3.17}$$

, with $\mathcal{A}_t$ describing the scattering procedure, where electron exchange takes place between the nuclei, can be written as :

$$\text{(II)} = \gamma^2 \mathcal{A}_t \sum_{m_I'', m_s''} \left\langle m_I m_s'' \middle| \rho_{\mathrm{A}} \middle| m_I' m_s'' \right\rangle \left\langle m_I'' m_s \middle| \rho_{\mathrm{B}} \middle| m_I'' m_s' \right\rangle$$

$$\text{(II)} = \gamma^2 \mathcal{A}_t \left\langle m_I m_s \middle| \mathrm{Tr}_s\{\rho_{\mathrm{A}}\} \otimes \mathrm{Tr}_I\{\rho_{\mathrm{B}}\} \middle| m_I' m's \right\rangle \tag{3.18}$$

Finally, in order to tackle (3.10), we define the coefficient :

$$\mathcal{A}_s = \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k_i' \, u(\vec{k}_i) u^*(\vec{k'}_i) S_d(\vec{k}_f, \vec{k}_i) S_t^*(\vec{k}_f, \vec{k'}_i) \tag{3.19}$$

Hence (3.10) takes the form :

$$\begin{aligned} \text{(III)} = -\alpha\gamma [& \mathcal{A}_s \sum_{m_I'', m_s''} \left\langle m_I m_s \middle| \rho_{\mathrm{A}} \middle| m_I' m_s'' \right\rangle \left\langle m_I'' m_s'' \middle| \rho_{\mathrm{B}} \middle| m_I'' m_s' \right\rangle + \\ & \mathcal{A}_s^* \sum_{m_I'', m_s''} \left\langle m_I m_s'' \middle| \rho_{\mathrm{A}} \middle| m_I' m_s' \right\rangle \left\langle m_I'' m_s \middle| \rho_{\mathrm{B}} \middle| m_I'' m_s'' \right\rangle] \end{aligned} \tag{3.20}$$

In Appendix B, we prove that :

$$\mathcal{A}_t + \mathcal{A}_d = 1$$

$$\mathcal{A}_s + \mathcal{A}_s^* = 0$$

[1] In Appendix B, we show exactly that relation.

, which goes to show that we can write the matrix element as :

$$\mathcal{A}_s = i\mathcal{A}_{s,\text{exch}} \tag{3.21}$$

, with $\mathcal{A}_{s,\text{exch}}$ describing spin exchange. Accordingly (3.20) simplifies to :

$$\text{(III)} = -i\alpha\gamma\mathcal{A}_{s,\text{exch}} \left\langle m_I m_s \right| \rho_\text{A}(\mathbb{1}_I \otimes \text{Tr}_I\{\rho_\text{B}\}) - (\mathbb{1}_I \otimes \text{Tr}_I\{\rho_\text{B}\})\rho_\text{A} \left| m'_I m'_s \right\rangle$$

$$\text{(III)} = -i\alpha\gamma\mathcal{A}_{s,\text{exch}} \left\langle m_I m_s \right| [\rho_\text{A}, \mathbb{1}_I \otimes \text{Tr}_I\{\rho_\text{B}\}] \left| m'_I m'_s \right\rangle \tag{3.22}$$

We are now in a position to put everything back together in (3.11) :

$$\begin{aligned}\left\langle m_I m_s \right| \sigma_\text{fin}(n_1, e) \left| m'_I m'_s \right\rangle =& \alpha^2 \mathcal{A}_d \left\langle m_I m_s \right| \rho_\text{A} \left| m'_I m'_s \right\rangle + \gamma^2 \mathcal{A}_t \left\langle m_I m_s \right| \text{Tr}_s\{\rho_\text{A}\} \otimes \text{Tr}_I\{\rho_\text{B}\} \left| m'_I m' s \right\rangle \\ & - i\alpha\gamma\mathcal{A}_{s,\text{exch}} \left\langle m_I m_s \right| [\rho_\text{A}, \mathbb{1}_I \otimes \text{Tr}_I\{\rho_\text{B}\}] \left| m'_I m'_s \right\rangle\end{aligned}$$

Simply by focusing on the density operators we get the final result, for indistinguishable electrons and distinguishable nuclei, after integrating out the n_2 degrees of freedom [2]:

$$\sigma_\text{fin}(n_1, e) = \alpha^2(1 - \mathcal{A}_t)\rho_\text{A} + \gamma^2 \mathcal{A}_t \, \text{Tr}_s\{\rho_\text{A}\} \otimes \text{Tr}_I\{\rho_\text{B}\} - i\alpha\gamma\mathcal{A}_{s,\text{exch}}[\rho_\text{A}, \mathbb{1}_I \otimes \text{Tr}_I\{\rho_\text{B}\}]$$

Since we are considering $\phi \ll 1$ we can approximate α to first order in ϕ as : $\alpha \sim -\gamma$. Consequently :

$$\sigma_\text{fin}(n_1, e) = \gamma^2(1 - \mathcal{A}_t)\rho_\text{A} + \gamma^2 \mathcal{A}_t \, \text{Tr}_s\{\rho_\text{A}\} \otimes \text{Tr}_I\{\rho_\text{B}\} + i\gamma^2 \mathcal{A}_{s,\text{exch}}[\rho_\text{A}, \mathbb{1}_I \otimes \text{Tr}_I\{\rho_\text{B}\}] \tag{3.23}$$

3.3 Indistinguishable Nuclei - Electrons

This time the transformation law of σ_init, to some $\sigma_\text{fin}(n, e)$, assumes the form :

$$\sigma_\text{init} \to \frac{1}{8}(\mathbb{1}_e - \text{P}_e)^2(\mathbb{1}_n - \text{P}_n)^2 \text{S}\sigma_\text{init}\text{S}^\dagger(\mathbb{1}_e - \text{P}_e)^2(\mathbb{1}_n - \text{P}_n)^2$$

$$\sigma_\text{init} \to (\alpha\mathbb{1}_e - \gamma\text{Q}_e)(\alpha\mathbb{1}_n - \gamma\text{Q}_n)\text{S}\sigma_\text{init}\text{S}^\dagger(\alpha\mathbb{1}_e - \gamma\text{Q}_e)(\alpha\mathbb{1}_n - \gamma\text{Q}_n) \tag{3.24}$$

We now separate (3.25) in three parts :

$$\text{(I)} \equiv \alpha^2[\mathbb{1}_n(\alpha\mathbb{1}_e - \gamma\text{Q}_e)\text{S}\sigma\text{S}^\dagger(\alpha\mathbb{1}_e - \gamma\text{Q}_e)\mathbb{1}_n] \tag{3.25}$$

$$\text{(II)} \equiv \gamma^2[\text{Q}_n(\alpha\mathbb{1}_e - \gamma\text{Q}_e)\text{S}\sigma\text{S}^\dagger(\alpha\mathbb{1}_e - \gamma\text{Q}_e)\text{Q}_n] \tag{3.26}$$

$$\begin{aligned}\text{(III)} \equiv -\alpha\gamma[&\text{Q}_n(\alpha\mathbb{1}_e - \gamma\text{Q}_e)\text{S}\sigma\text{S}^\dagger(\alpha\mathbb{1}_e - \gamma\text{Q}_e)\mathbb{1}_n + \\ &\mathbb{1}_n(\alpha\mathbb{1}_e - \gamma\text{Q}_e)\text{S}\sigma\text{S}^\dagger(\alpha\mathbb{1}_e - \gamma\text{Q}_e)\text{Q}_n]\end{aligned} \tag{3.27}$$

[2] Following a similar calculation, we get a similar result by integrating over the n_1 degrees of freedom.

Notice that (3.25) is relation (3.23) multiplied by a factor of α^2, while (3.26) is that after integrating over n_1 instead of n_2, times a γ^2 factor. We therefore only need to calculate (3.27).

$$\langle m_I m_s|\sigma_{\text{fin}}(n,e)|m'_I m'_s\rangle = \frac{1}{2}\sum_{m''_I,m''_s}\int \mathrm{d}^3k_f\,\mathrm{d}^3k_i\,\mathrm{d}^3k'_i\,u(\vec{k}_i)u^*(\vec{k'}_i)\langle(\mathrm{I}+\mathrm{II}+\mathrm{III})\rangle \tag{3.28}$$

focusing on the third integral :

$$\mathrm{J} = \frac{1}{2}\sum_{m''_I,m''_s}\int \mathrm{d}^3k_f\,\mathrm{d}^3k_i\,\mathrm{d}^3k'_i\,u(\vec{k}_i)u^*(\vec{k'}_i)\langle\mathrm{III}\rangle \tag{3.29}$$

Define :

$$\mathcal{A}_I = \int \mathrm{d}^3k_f\,\mathrm{d}^3k_i\,\mathrm{d}^3k'_i\,u(\vec{k}_i)u^*(\vec{k'}_i)S_d(\vec{k}_f,\vec{k}_i)S_t^*(-\vec{k}_f,\vec{k'}_i) \tag{3.30}$$

$$\mathcal{A}^{(1)}_{Is} = \int \mathrm{d}^3k_f\,\mathrm{d}^3k_i\,\mathrm{d}^3k'_i\,u(\vec{k}_i)u^*(\vec{k'}_i)S_d(\vec{k}_f,\vec{k}_i)S_d^*(-\vec{k}_f,\vec{k'}_i) \tag{3.31}$$

$$\mathcal{A}^{(2)}_{Is} = \int \mathrm{d}^3k_f\,\mathrm{d}^3k_i\,\mathrm{d}^3k'_i\,u(\vec{k}_i)u^*(\vec{k'}_i)S_t(\vec{k}_f,\vec{k}_i)S_t^*(-\vec{k}_f,\vec{k'}_i) \tag{3.32}$$

Using (3.30)-(3.32), relation (3.29) expands as :

$$\begin{aligned}
\mathrm{J} =& -\frac{\alpha^3\gamma}{2}\mathcal{A}_I\left\langle m_I m_s\middle|\rho_{\mathrm{A}}(\mathrm{Tr}_s\{\rho_{\mathrm{B}}\}\otimes\mathbb{1}_s)\middle|m'_I m'_s\right\rangle - \frac{\alpha^3\gamma}{2}\mathcal{A}_I^*\left\langle m_I m_s\middle|(\mathrm{Tr}_s\{\rho_{\mathrm{B}}\}\otimes\mathbb{1}_s)\rho_{\mathrm{A}}\middle|m'_I m'_s\right\rangle \\
&-\frac{\alpha\gamma^3}{2}\mathcal{A}_I\left\langle m_I m_s\middle|\rho_{\mathrm{B}}(\mathrm{Tr}_s\{\rho_{\mathrm{A}}\}\otimes\mathbb{1}_s)\middle|m'_I m'_s\right\rangle - \frac{\alpha\gamma^3}{2}\mathcal{A}_I^*\left\langle m_I m_s\middle|(\mathrm{Tr}_s\{\rho_{\mathrm{A}}\}\otimes\mathbb{1}_s)\rho_{\mathrm{B}}\middle|m'_I m'_s\right\rangle \\
&+\frac{\alpha^2\gamma^2}{2}\mathcal{A}^{(1)}_{Is}\left\langle m_I m_s\middle|\rho_{\mathrm{A}}\rho_{\mathrm{B}}\middle|m'_I m'_s\right\rangle + \frac{\alpha^2\gamma^2}{2}\mathcal{A}^{(1)*}_{Is}\left\langle m_I m_s\middle|\rho_{\mathrm{B}}\rho_{\mathrm{A}}\middle|m'_I m'_s\right\rangle \\
&+\frac{\alpha^2\gamma^2}{2}\mathcal{A}^{(2)}_{Is}\left\langle m_I m_s\middle|\mathrm{Tr}_{Is,2}\{\mathrm{P}_e\rho_{\mathrm{A}}\otimes\rho_{\mathrm{B}}\mathrm{P}_n\}\middle|m'_I m'_s\right\rangle \\
&+\frac{\alpha^2\gamma^2}{2}\mathcal{A}^{(2)*}_{Is}\left\langle m_I m_s\middle|\mathrm{Tr}_{Is,2}\{\mathrm{P}_n\rho_{\mathrm{A}}\otimes\rho_{\mathrm{B}}\mathrm{P}_e\}\middle|m'_I m'_s\right\rangle
\end{aligned} \tag{3.33}$$

In Appendix B, we prove that :

$$\mathcal{A}_I + \mathcal{A}_I^* = 0$$
$$\mathcal{A}^{(1)}_{Is} + \mathcal{A}^{(2)}_{Is} = 0$$

Hence (3.33) becomes :

$$\begin{aligned}
\mathrm{J} =& -\frac{\alpha^3\gamma}{2}\mathcal{A}_I\left\langle m_I m_s\middle|[\rho_{\mathrm{A}},\mathrm{Tr}_s\{\rho_{\mathrm{B}}\}\otimes\mathbb{1}_s]\middle|m'_I m'_s\right\rangle - \frac{\alpha\gamma^3}{2}\mathcal{A}_I\left\langle m_I m_s\middle|[\rho_{\mathrm{B}},\mathrm{Tr}_s\{\rho_{\mathrm{A}}\}\otimes\mathbb{1}_s]\middle|m'_I m'_s\right\rangle \\
&-\frac{\alpha^2\gamma^2}{2}\mathcal{A}^{(2)}_{Is}\left\langle m_I m_s\middle|[\rho_{\mathrm{A}}\rho_{\mathrm{B}}+\rho_{\mathrm{B}}\rho_{\mathrm{A}}-\mathrm{Tr}_{Is,2}\{\mathrm{P}_e\rho_{\mathrm{A}}\otimes\rho_{\mathrm{B}}\mathrm{P}_n+\mathrm{P}_n\rho_{\mathrm{A}}\otimes\rho_{\mathrm{B}}\mathrm{P}_e\}]\middle|m'_I m'_s\right\rangle
\end{aligned}$$

Since $\mathcal{A}_I + \mathcal{A}_I^* = 0$, we can write the matrix element as :

$$\mathcal{A}_I = i\mathcal{A}_{I,\text{exch}}$$

, with $\mathcal{A}_{I,\text{exch}}$ describing the isospin exchange. Thus (3.33) is ultimately reduced to :

$$\begin{aligned}\mathrm{J} = &-\frac{\alpha\gamma}{2} i\mathcal{A}_{I,\text{exch}} \left\langle m_I m_s \right| (\alpha^2[\rho_\mathrm{A}, \mathrm{Tr}_s\{\rho_\mathrm{B}\} \otimes \mathbb{1}_s] + \gamma^2[\rho_\mathrm{B}, \mathrm{Tr}_s\{\rho_\mathrm{A}\} \otimes \mathbb{1}_s]) \left| m_I' m_s' \right\rangle \\ &- \frac{\alpha^2\gamma^2}{2} \mathcal{A}_{Is}^{(2)} \left\langle m_I m_s \right| [\rho_\mathrm{A}\rho_\mathrm{B} + \rho_\mathrm{B}\rho_\mathrm{A} - \mathrm{Tr}_{Is,2}\{\mathrm{P}_e\rho_\mathrm{A} \otimes \rho_\mathrm{B}\mathrm{P}_n + \mathrm{P}_n\rho_\mathrm{A} \otimes \rho_\mathrm{B}\mathrm{P}_e\}] \left| m_I' m_s' \right\rangle\end{aligned} \tag{3.34}$$

Relation (3.29) then takes the form :

$$\begin{aligned}\sigma_{\text{fin}}(n,e) = &\frac{\alpha^4}{2}(1-\mathcal{A}_t)\rho_\mathrm{A} + \frac{\alpha^2\gamma^2}{2}\mathcal{A}_t\,\mathrm{Tr}_s\{\rho_\mathrm{A}\} \otimes \mathrm{Tr}_I\{\rho_\mathrm{B}\} - i\frac{\alpha^3\gamma}{2}\mathcal{A}_{s,\text{exch}}[\rho_\mathrm{A}, \mathbb{1}_I \otimes \mathrm{Tr}_I\{\rho_\mathrm{B}\}] \\ &+ \frac{\gamma^4}{2}(1-\mathcal{A}_t)\rho_\mathrm{B} + \frac{\alpha^2\gamma^2}{2}\mathcal{A}_t\,\mathrm{Tr}_s\{\rho_\mathrm{B}\} \otimes \mathrm{Tr}_I\{\rho_\mathrm{A}\} - i\frac{\alpha\gamma^3}{2}\mathcal{A}_{s,\text{exch}}[\rho_\mathrm{B}, \mathbb{1}_I \otimes \mathrm{Tr}_I\{\rho_\mathrm{A}\}] \\ &- i\frac{\alpha\gamma}{2}\mathcal{A}_{I,\text{exch}}(\alpha^2[\rho_\mathrm{A}, \mathrm{Tr}_s\{\rho_\mathrm{B}\} \otimes \mathbb{1}_s] + \gamma^2[\rho_\mathrm{B}, \mathrm{Tr}_s\{\rho_\mathrm{A}\} \otimes \mathbb{1}_s]) \\ &- \frac{\alpha^2\gamma^2}{2}\mathcal{A}_{Is}^{(2)}[\rho_\mathrm{A}\rho_\mathrm{B} + \rho_\mathrm{B}\rho_\mathrm{A} - \mathrm{Tr}_{Is,2}\{\mathrm{P}_e\rho_\mathrm{A} \otimes \rho_\mathrm{B}\mathrm{P}_n + \mathrm{P}_n\rho_\mathrm{A} \otimes \rho_\mathrm{B}\mathrm{P}_e\}]\end{aligned}$$

Again approximating α to first order in ϕ , $\alpha \sim -\gamma$, we get[3] :

$$\begin{aligned}\sigma_{\text{fin}}(n,e) = &\frac{\gamma^4}{2}(1-\mathcal{A}_t)\rho_\mathrm{A} + \frac{\gamma^4}{2}\mathcal{A}_t\,\mathrm{Tr}_s\{\rho_\mathrm{A}\} \otimes \mathrm{Tr}_I\{\rho_\mathrm{B}\} - i\frac{\gamma^4}{2}\mathcal{A}_{s,\text{exch}}[\rho_\mathrm{A}, \mathbb{1}_I \otimes \mathrm{Tr}_I\{\rho_\mathrm{B}\}] \\ &+ \frac{\gamma^4}{2}(1-\mathcal{A}_t)\rho_\mathrm{B} + \frac{\gamma^4}{2}\mathcal{A}_t\,\mathrm{Tr}_s\{\rho_\mathrm{B}\} \otimes \mathrm{Tr}_I\{\rho_\mathrm{A}\} - i\frac{\gamma^4}{2}\mathcal{A}_{s,\text{exch}}[\rho_\mathrm{B}, \mathbb{1}_I \otimes \mathrm{Tr}_I\{\rho_\mathrm{A}\}] \\ &+ i\frac{\gamma^4}{2}\mathcal{A}_{I,\text{exch}}([\rho_\mathrm{A}, \mathrm{Tr}_s\{\rho_\mathrm{B}\} \otimes \mathbb{1}_s] + [\rho_\mathrm{B}, \mathrm{Tr}_s\{\rho_\mathrm{A}\} \otimes \mathbb{1}_s]) \\ &- \frac{\gamma^4}{2}\mathcal{A}_{Is}^{(2)}[\rho_\mathrm{A}\rho_\mathrm{B} + \rho_\mathrm{B}\rho_\mathrm{A} - \mathrm{Tr}_{Is,2}\{\mathrm{P}_e\rho_\mathrm{A} \otimes \rho_\mathrm{B}\mathrm{P}_n + \mathrm{P}_n\rho_\mathrm{A} \otimes \rho_\mathrm{B}\mathrm{P}_e\}]\end{aligned} \tag{3.35}$$

3.4 Cross-Sections

Concluding our calculation, we take the ratios of cross sections obtained from the $\mathcal{A}$-coefficients we defined, so as to provide a way of experimentally checking the PEP violation we considered.

From Appendix B, we know that :

$$\sigma_t \sim \mathcal{A}_t \tag{3.36}$$

[3] $\mathrm{Tr}_{Is,2}\{\}$runs over the spin and isospin projections of n_2

$$\sigma_{s,\text{exch}} \sim \mathcal{A}_{s,\text{exch}} \tag{3.37}$$

In order to distinguish the cross sections from each calculation, we give the index (D) and (I), for distinguishable and indistinguishable respectively.
Therefore, we compare the first line of (3.35) to result (3.23) :

$$\frac{\sigma_t^D}{\sigma_t^I} \approx \frac{\gamma^2 \mathcal{A}_t}{\frac{1}{2}\gamma^4 \mathcal{A}_t} = \frac{2}{\gamma^2} \implies \frac{\sigma_t^D}{\sigma_t^I} \approx \frac{2}{\gamma^2} \tag{3.38}$$

$$\frac{\sigma_{s,\text{exch}}^D}{\sigma_{s,\text{exch}}^I} \approx \frac{\gamma^2 \mathcal{A}_{s,\text{exch}}}{\frac{1}{2}\gamma^4 \mathcal{A}_{s,\text{exch}}} = \frac{2}{\gamma^2} \implies \frac{\sigma_{s,\text{exch}}^D}{\sigma_{s,\text{exch}}^I} \approx \frac{2}{\gamma^2} \tag{3.39}$$

We now approximate γ^2 to lowest order in ϕ^2, to finally get :

$$\frac{\sigma_t^D}{\sigma_t^I} \approx \frac{2}{1-2\phi} \approx 2(1+2\phi+\mathcal{O}(\phi^2)) \tag{3.40}$$

$$\frac{\sigma_{s,\text{exch}}^D}{\sigma_{s,\text{exch}}^I} \approx \frac{2}{1-2\phi} \approx 2(1+2\phi+\mathcal{O}(\phi^2)) \tag{3.41}$$

Chapter 4

Conclusion

Concluding, we have managed to lay the groundwork to test a possible PEP violation under a future experiment, as well as establish a framework, upon which, one can expand the above work. We see the result obtained in [5], changes by a factor of γ^2, referring to (3.35). We have provided a simple ratio test, between the cross sections of different atoms to atoms of the same kind, so as to measure an upper bound of the $\phi-$parameter violation of the exclusion principle.

An immediate generalization, would be that of disallowing the separation of $\rho(e_1, n_1, e_2, n_2)$, leading to the analysis of a fully entangled problem. Leastwise, it should be noted that in its current form, the q-algebra is valid only at the level of non-relativistic physics. Apart from that, any kind of generalization aims to construct similar $\mathcal{A}$-coefficients, to that of the above work, so as to calculate the ratio of cross-sections and measure the upper bound of ϕ.

Closing, the connection between this work and previous experimental results, has been established, which is valid for any generalization of the work in chapter 3.

Appendices

Appendix A

Hilbert Space realization of q-algebra

[7, 8, 10] **Theorem.** Define a Hilbert space $\mathbb{H}$ embedded with an inner product :

$$\langle \cdot, \cdot \rangle : \mathbb{H} \times \mathbb{H} \to \mathbb{R}$$

Consider an element $\mathcal{M}_q \in \mathbf{GL}(n, \mathbb{R})$. If $q \in (-1, 1)$, the matrix $\mathcal{M}_q$ is positive definite, such that the algebra over $\mathbb{R}$, has a Hilbert space realization for q in this range.

Proof.

Let $\Psi_{\mathbf{k}} \in \mathbb{H}$, such that $\Psi_{\mathbf{k}} = a^{\dagger}_{k_1} ... a^{\dagger}_{k_n} \Psi_0, \forall n \geq 0$ and each n-tuple of indices $\mathbf{k}$. Then under the normalization condition $\langle \Psi_0, \Psi_0 \rangle = 1$, we have :

$$\langle \Psi_{\mathbf{k}}, \Psi_{\mathbf{k}} \rangle = q \tag{A.1}$$

Now define an element in $\mathbf{GL}(n, \mathbb{R})$ as :

$$\mathcal{M}_q \equiv \langle \Psi_{\mathbf{k}}, \Psi_{\mathbf{r}} \rangle \tag{A.2}$$

Relation (A.2) vanishes if $\mathbf{k}$ is not a permutation of $\mathbf{r}$, therefore $\mathbb{H}$ is the direct sum of infinitely many finite dimensional spaces, indexed by all unordered n-tuples. It therefore, suffices to prove the positive definiteness of these.

Consider an element $\pi \in \mathbf{S}_n$, then according to (A.1), we conclude :

$$\langle \Psi_{\pi(1)...\pi(n)}, \Psi_{1...n} \rangle = q^{i(\pi)} \tag{A.3}$$

, where $i(\pi)$ denotes the number of inversions of π. Therefore for $\sigma, \pi \in \mathbf{S}_n$, we need to prove that :

$$\mathcal{M}_q(\sigma, \pi) = q^{i(\sigma^{-1}\pi)} \tag{A.4}$$

is positive definite for $q \in (-1, 1)$. For this to hold true, it suffices to prove that $\mathcal{M}_q$ is non-singular in $(-1, 1)$. We therefore calculate $\det\{\mathcal{M}_q\}$.

Let $\pi \in \mathbf{S}_n$ and $\sigma \in \mathbf{S}_{n-1}$, then for $1 \leq k \leq n, \exists \rho_k = (1, ..., k-1, n, k, k+1, ..., n-1) \in \mathbf{S}_n$ such that $\pi = \sigma \circ \rho_k$, with $k = \pi^{-1}(n)$. Thus by the work in [10], we define :

$$a_n = \sum_{\pi \in \mathbf{S}_n} q^{i(\pi)} \pi = [\sum_{\sigma \in \mathbf{S}_{n-1}} q^{i(\pi)} \sigma] \circ [\sum_{k=1}^{n} q^{n-k} \rho_k] \tag{A.5}$$

Define :

$$\beta_n = \sum_{k=1}^{n} q^{n-k} \rho_k \tag{A.6}$$

Then combining the two relations we conclude that :

$$a_n = a_{n-1} \beta_n \tag{A.7}$$

Therefore (A.7) in terms of matrices can be written as :

$$\mathrm{A}_{q,n} = (\mathrm{A}_{q,n-1} \otimes \mathbb{1}) \mathrm{B}_{q,n} \tag{A.8}$$

, with $\mathrm{B}_{q,n} = q^{n-k}$, if $\sigma^{-1} \circ \pi = \rho_k$ for some $1 \leq k \leq n$, else it is zero. Taking the determinant, we find :

$$\det\{\mathrm{A}_{q,n}\} = (\det\{\mathrm{A}_{q,n-1}\})^n \det\{\mathrm{B}_{q,n}\} \tag{A.9}$$

This goes to show that we can prove the theorem, by use of induction on $\mathrm{B}_{q,n}$. We also note that :

$$\mathcal{M}_q = \mathrm{A}_{q,n}$$

We write $\beta_n \gamma_n = \delta_{n-1}$, where :[1]

$$\gamma_n = (1 - q^{n-1}\rho_1)(1 - q^{n-2}\rho_2)...(1 - q\rho_{n-1})$$
$$\delta_n = (1 - q^{n+1}\rho_1)(1 - q^{n}\rho_2)...(1 - q^2\rho_{n-1})$$

Therefore :

$$\det\{\mathrm{B}_{q,n}\} = \frac{\det\{\Delta_{q,n-1}\}}{\det\{\Gamma_{q,n}\}} = \frac{\prod_{k=1}^{n-1}(1 - q^{k(k+1)})^{\frac{n!}{k+1}}}{\prod_{k=1}^{n}(1 - q^{k(k+1)})^{\frac{n!}{k}}}$$

$$\det\{\mathrm{B}_{q,n}\} = \prod_{k=1}^{n-1}(1 - q^{k(k+1)})^{\frac{n!}{k(k+1)}} \tag{A.10}$$

By induction, (A.9) and (A.10) provide us with the proof of the theorem :

$$\det\{\mathcal{M}_q\} = \prod_{k=1}^{n-1}(1 - q^{k(k+1)})^{\frac{n!(n-k)}{k(k+1)}} \tag{A.11}$$

Which shows that $\mathcal{M}_q$ is non-singular $\forall q \in \mathbb{C}$, except for the roots of unity $\{n^2 - n\}$, meaning that for $q \in \mathbb{R}$, the algebra has no peculiarities.

[1] For a deeper understanding of the proof the reader should examine [10]

Appendix B

$\mathcal{A}$-coefficients

B.1 $\mathcal{A}-$identities

In this section, we prove some of the relations used in the work. Let :

$$\begin{aligned}\mathbb{1} = \int \mathrm{d}^3k_f \, [\, |n_1, \vec{k}_f; n_2, -\vec{k}_f\rangle \, \langle n_1, \vec{k}_f; n_2, -\vec{k}_f|] \otimes \\ [|e_1, n_1; e_2, n_2\rangle \, \langle e_1, n_1; e_2, n_2| + |e_1, n_2; e_2, n_1\rangle \, \langle e_1, n_2; e_2, n_1|]\end{aligned} \tag{B.1}$$

be the identity element. We begin by proving : $\mathcal{A}_t + \mathcal{A}_d = 1$

$$\begin{aligned}\mathcal{A}_t + \mathcal{A}_d &= \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k'_i \, u(\vec{k}_i) u^*(\vec{k'}_i) S_d(\vec{k}_f, \vec{k}_i) S_d^*(\vec{k}_f, \vec{k'}_i) \\ &\quad + \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k'_i \, u(\vec{k}_i) u^*(\vec{k'}_i) S_t(\vec{k}_f, \vec{k}_i) S_t^*(\vec{k}_f, \vec{k'}_i) \\ &= \int \mathrm{d}^3k_f \, \mathrm{d}^3k_i \, \mathrm{d}^3k'_i \, u(\vec{k}_i) u^*(\vec{k'}_i) [S_d(\vec{k}_f, \vec{k}_i) S_d^*(\vec{k}_f, \vec{k'}_i) + S_t(\vec{k}_f, \vec{k}_i) S_t^*(\vec{k}_f, \vec{k'}_i)] \\ &= \int \mathrm{d}^3k_i \, \mathrm{d}^3k'_i \, u(\vec{k}_i) u^*(\vec{k'}_i) \left\langle n_1, \vec{k}_i, e_2; n_1, -\vec{k}_i, e_1 \middle| \mathrm{S}\mathbb{1}\mathrm{S}^\dagger \middle| n_1, \vec{k}'_i, e_2; n_1, -\vec{k}'_i, e_1 \right\rangle \\ &= \int \mathrm{d}^3k_i \, \mathrm{d}^3k'_i \, u(\vec{k}_i) u^*(\vec{k'}_i) \delta(\vec{k}_i - \vec{k}'_i) \\ &= \int \mathrm{d}^3k_i \, u(\vec{k}_i) u^*(\vec{k}_i) \\ &= 1\end{aligned}$$

We now continue on with the proof of : $\mathcal{A}_s + \mathcal{A}_s^* = 0$

$$\begin{aligned}
\mathcal{A}_s + \mathcal{A}_s^* &= \int \mathrm{d}^3k_f\, \mathrm{d}^3k_i\, \mathrm{d}^3k_i'\, u(\vec{k}_i)u^*(\vec{k'}_i)S_d(\vec{k}_f,\vec{k}_i)S_t^*(\vec{k}_f,\vec{k'}_i) \\
&\quad + [\int \mathrm{d}^3k_f\, \mathrm{d}^3k_i\, \mathrm{d}^3k_i'\, u(\vec{k}_i)u^*(\vec{k'}_i)S_d(\vec{k}_f,\vec{k}_i)S_t^*(\vec{k}_f,\vec{k'}_i)]^* \\
&= \int \mathrm{d}^3k_f\, \mathrm{d}^3k_i\, \mathrm{d}^3k_i'\, u(\vec{k}_i)u^*(\vec{k'}_i)[S_d(\vec{k}_f,\vec{k}_i)S_t^*(\vec{k}_f,\vec{k'}_i) + S_d^*(\vec{k}_f,\vec{k'}_i)S_t(\vec{k}_f,\vec{k}_i)] \\
&= \int \mathrm{d}^3k_i\, \mathrm{d}^3k_i'\, u(\vec{k}_i)u^*(\vec{k'}_i)\, \langle n_1,\vec{k'}_i,e_2;n_2,-\vec{k'}_i,e_1|n_1,\vec{k}_i,e_1;n_2,-\vec{k}_i,e_2\rangle
\end{aligned}$$

Assuming that the initial states have no overlapping, we get :

$$\mathcal{A}_s + \mathcal{A}_s^* = 0$$

In a similar manner we get :

$$\mathcal{A}_I + \mathcal{A}_I^* = 0$$

Now the final proof is :

$$\begin{aligned}
\mathcal{A}_{Is}^{(1)} + \mathcal{A}_{Is}^{(2)} &= \int \mathrm{d}^3k_f\, \mathrm{d}^3k_i\, \mathrm{d}^3k_i'\, u(\vec{k}_i)u^*(\vec{k'}_i)S_d(\vec{k}_f,\vec{k}_i)S_d^*(-\vec{k}_f,\vec{k'}_i) \\
&\quad + \int \mathrm{d}^3k_f\, \mathrm{d}^3k_i\, \mathrm{d}^3k_i'\, u(\vec{k}_i)u^*(\vec{k'}_i)S_t(\vec{k}_f,\vec{k}_i)S_t^*(-\vec{k}_f,\vec{k'}_i) \\
&= \int \mathrm{d}^3k_f\, \mathrm{d}^3k_i\, \mathrm{d}^3k_i'\, u(\vec{k}_i)u^*(\vec{k'}_i)[S_d(\vec{k}_f,\vec{k}_i)S_d^*(-\vec{k}_f,\vec{k'}_i) + S_t(\vec{k}_f,\vec{k}_i)S_t^*(-\vec{k}_f,\vec{k'}_i)] \\
&= \int \mathrm{d}^3k_i\, \mathrm{d}^3k_i'\, u(\vec{k}_i)u^*(\vec{k'}_i)\, \langle n_1,\vec{k'}_i,e_1;n_2,-\vec{k'}_i,e_2|\, \mathrm{S}^\dagger \mathbb{1} \mathrm{S}\, |n_1,\vec{k}_i,e_1;n_2,-\vec{k}_i,e_2\rangle \\
&= \int \mathrm{d}^3k_i\, \mathrm{d}^3k_i'\, u(\vec{k}_i)u^*(\vec{k'}_i)\, \langle n_1,\vec{k'}_i,e_1;n_2,-\vec{k'}_i,e_2|n_1,-\vec{k}_i,e_1;n_2,\vec{k}_i,e_2\rangle \\
&= 0
\end{aligned}$$

Since the nuclear wave packets do not overlap.

B.2 Scattering Process - Phase shifts

In this section, we show how to relate the $\mathcal{A}$-coefficients to the corresponding scattering cross-sections, we are interested in. We will be focusing on $\mathcal{A}_t$, as the work is exactly the same for any of them.

We know, from non-relativistic scattering theory in quantum mechanics that we can expand, the S-matrix elements as [5]:

$$\mathrm{S}_d(\vec{k}_f,\vec{k}_i) = \frac{1}{k_i^2}\delta(|\vec{k}_f| - |\vec{k}_i|\,) \sum_{l,m} e^{i\delta_l}\cos(\delta_l)\mathcal{Y}_l^{m*}(\hat{k}_f)\mathcal{Y}_l^m(\hat{k}_i) \tag{B.2}$$

$$\mathrm{S}_t(\vec{k}_f, \vec{k}_i) = \frac{i}{k_i^2}\delta(|\vec{k}_f| - |\vec{k}_i|)\sum_{l,m} e^{i\delta_l}\sin(\delta_l)\mathcal{Y}_l^{m*}(\hat{k}_f)\mathcal{Y}_l^m(\hat{k}_i) \tag{B.3}$$

Therefore, using (B.2) in the definition of $\mathcal{A}_t$, we get :

$$\int \mathrm{d}^3k_i\,\mathrm{d}^3k_i'\,\frac{u(\vec{k}_i)u^*(\vec{k'}_i)}{k_i k_i'}\delta(k_i - k_i')\sum_{l,m} e^{i\delta_l}\sin^2(\delta_l)\mathcal{Y}_l^{m*}(\hat{k}_f)\mathcal{Y}_l^m(\hat{k}_i) \tag{B.4}$$

Using the rectangular function $\Pi(k)$, we suppose $u(\vec{k})$ to be :

$$u(\vec{k}) = \frac{L}{\pi\sqrt{\epsilon}}\Pi(k_x)\Pi(k_y)\Pi(k_z - k_0) \tag{B.5}$$

, where L is directly proportional to the lateral spread of the wave packet, on the xy-plane, and ϵ is the energy. Using relation (B.5), we provide a closed form for $\mathcal{A}_t$.

By use of the summing theorem of spherical harmonics, as well as (B.5), we conclude that :

$$\mathcal{A}_t = \frac{1}{4\pi^2L^2k_0^2}\sum_l (2l+1)\sin^2(\delta_l) \tag{B.6}$$

But from scattering theory, for example [9], we know that :

$$\sigma_t = \frac{1}{k_0^2}\sum_l (2l+1)\sin^2(\delta_l) \tag{B.7}$$

Concluding, we see that :

$$\sigma_t = 4\pi L^2\mathcal{A}_t \tag{B.8}$$

An equivalent line of reasoning gives us the rest of the cross-sections.

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