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Study of the effect of irradiation with Proton beams on RNA

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Abstract

Radiation causes damage in chromosomes (which are mainly responsible for the transmission of genetic traits from cell to cell and from generation to generation) by directly affecting the hereditary material (DNA and RNA), which in turn leads to physical or mental deformities in children from birth resulting from exposure to one Parent or both of them to ionizing radiation (perhaps during pregnancy for the mother). However, irradiation has many applications in the field of medicine through radiation therapy for cancer patients, and one of its types is proton therapy, which uses beams of protons directed at the cancerous tumor. In this research, the special effects on RNA, which is short for Ribonucleic Acid, or RNA, were studied by knowing the energy loss of proton beams and calculating the stopping power to reach an accurate understanding of how radiation affects RNA compounds and knowing the energy loss by determining the Bragg peak of these compounds. The current work employs the dielectric formalism, Quantum Oscillator (QO) was utilized to evaluate the chance of an energetic proton producing electronic excitations in a high biological interest sample, RNA, that was used to assess the probability that an active proton would produce electronic excitations in a sample. Where the Fortran 90 language (Fortran PowerStation 4.0.) was used to program all mathematical equations.

Keywords: Quantum Oscillator, RNA, Irradiation, Dielectric function, Proton.

دراسة تأثير التشعيع بالبروتونات على RNA

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الخلاصة

يؤثر الإشعاع على إحداث تغيرات تشوهيه في بنية الكروموسومات حيث هي المسؤولة عن انتقال الصفات الوراثية بشكل اساسي من خلية إلى خلية ومن جيل إلى جيل, من خلال التأثير المباشر على المادة الوراثية DNA و RNA التي بدورها تؤدي إلى تشوهات جسمانية أو عقلية لدى الأطفال منذ الولادة ناتجة عن تعرض أحد الوالدين أو كلاهما للإشعاع المؤين (وقد يحدث اثناء فترة الحمل) الا ان للشعيع تطبيقات كثيرة في مجال الطب من خلال العلاج الاشعاعي لمرضى السرطان ومن انواعه العلاج البروتوني الذي يستخدم حزم من البروتونات المسلطة على الورم السرطاني. في هذه البحث تمت دراسة التأثيرات الخاصة على الـ RNA وهو اختصارًا الـRibonucleic Acid أو الحمض النووي الريبوزي، من خلال معرفة فقدان الطاقة للحزم البروتونية وحساب قدرة الايقاف للتوصل الى فهم دقيق لكيفية تأثير الاشعاع على مركبات ال RNA ومعرفة فقدان الطاقة من خلال تحديد Bragg peak لهذه المركبات، العمل الحالي يستخدم صيغة دالة العازلة, المذبذب الكمي (QO) لتقييم امكانية البروتون النشط لإنتاج لإثارة إلكترونية في عينة ذات أهمية بيولوجية عالية هي RNA ، والتي تم استخدامها لتقييم احتمال أن ينتج البروتون النشط إثارة إلكترونية في العينة. حيث تم استخدام لغة فورتران 90 (Fortran PowerStation 4.0.) لبرمجة جميع المعادلات الرياضية.

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1. Introduction

A key step in the mechanism of ion impact-induced radiation damage to bimolecular systems is secondary electron emission. The fact that the ionization yield peaks close to the accuracy and that there is minimal energy deposition in deep-seated tumours while limiting radiation are only a few examples of how ion beam cancer therapy makes use of the special qualities of ion tracks. Damage on healthy surrounding tissues is made possible by the peak at which the particles' trajectories come to a halt (the Bragg peak) [1].

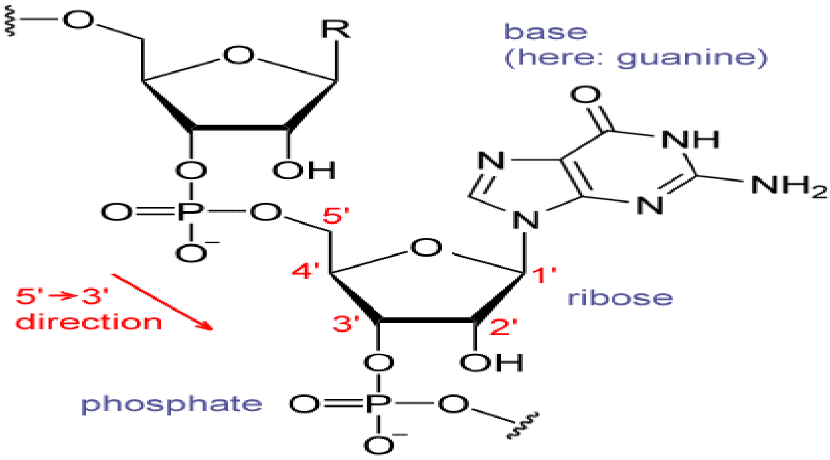

Figure -1 Chemical structure of RNA [3].

Additional ionisations and an onslaught of RNA or proteins could result from the liberated electrons. The sample's response to an external perturbation in terms of its dielectric properties is determined by the energy loss function (ELF) of the target, which computes the probability that an inelastic event with momentum transfer and energy transfer occurs in the target and offers information on the kinds of excitations the material can withstand [2].

The term "RNA" refers to ribonucleic acid, a very complex molecule with a high molecular the substance that cells utilise to produce proteins and that certain viruses use to replace DNA, or deoxyribonucleic acid, the genetic information carrier. The fundamental building blocks of RNA are ribose nucleotides, which are nitrogenous bases added to a ribose sugar and joined by phosphodiester bonds to form strands of various lengths. Adenine, guanine, cytosine, and uracil are nitrogenous bases present in RNA that act as thymine in DNA. The ribose sugar found in RNA has a cyclical structure with five carbons and one oxygen. RNA is susceptible to hydrolysis because the second carbon group of the ribose sugar molecule is linked to a hydroxyl (OH) group that is chemically reactive. It is hypothesised that DNA evolved to become the preferred carrier of genetic information in the majority of animals because RNA is less chemically stable than DNA, which does not contain a reactive OH group in the same place as the sugar moiety (deoxyribose). Additionally, it is assumed that DNA is more stable chemically than RNA. The RNA molecule's structure was first revealed by R.W. Holley in 1965 [4].

RNA is typically a single-stranded biopolymer. The RNA strand has self-complementary patterns with bulges and helices, and the ribonucleotide chain is folded into complex structural formations. Cellular enzymes that attach chemical groups (for example, methyl groups) to the chain can alter the ribose sugar and nitrogenous bases in a number of ways, which is made possible by the three-dimensional structure of RNA, which is crucial to its stability and function. These modifications allow the RNA strand to chemically interact with distant areas, enabling the chain of RNA to twist intricately and further solidifying the RNA structure. The fundamental formula of the structure of RNA is $\mathbf{C_{10}H_{12}O_7N_5P}$ [5].

Ionising radiation (such as X-rays, electrons, positrons, protons, or heavier ions) must interact with biological tissues in order to successfully cure cancer [6]. This is because the amount of energy that the radiation deposits on tumour cells affect how well the treatment works.

Space radiation health is a different field where research on the effects of alpha and heavier ions on human tissues is essential for the radiological safety of human personnel on long-duration deep space missions [6].

Treatment of cancers with hadrons Compared to traditional X-ray and electron therapy, (primarily protons and carbon ions) has a lot of benefits, both medically and physically. The Bragg peak is a pattern of hadronic energy deposition where most of the energy of the projectile is deposited near to the end of its range. The damage to healthy cells surrounding the cancer cells to be removed is considerably reduced by this technique [7-9]. Determine the likelihood and cross-section of proton interaction with the test material, RNA.

The interaction of charged particles such as protons with compounds of complex chemical composition such as RNA is a complex interaction that results in the liberation of many free radicals or oxides and ions that spread randomly within the sample, which will lead to their union with other compounds, producing many compounds, most of which may be harmful. In the end, it leads to poisoning and cellular death in the irradiated tissue or material. In the event that the proton interacts with RNA, it will lead to the occurrence of large and permanent distortions in the chains of its bases and compounds, which in turn leads to the occurrence of genetic mutations that are transmitted from generation to generation. In the case of radiation therapy, the damage will be large within the tissue, which results in cell death due to high doses of radiation [4].

2. Theoretical Consideration

2.1 Quantum Oscillator dielectric function, QO

The theoretical study has supplied the Dielectric function, which is marked by its reliance on the quantum levels n of linear oscillators in quantum treatment.[1]

$$\in(\vec{k},\omega) = 1 + \frac{\omega_p^2}{2\omega_k}\, e^{-\omega_k/\omega_0} \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{\omega_k}{\omega_0}\right)^n \times \left\{\frac{1}{n\omega_0-\omega-i\gamma} + \frac{1}{n\omega_0+\omega+i\gamma}\right\} \tag{1}$$

Where:

$\omega_k = {\hbar k^2}/{2m}$, $\omega_p^2 = {4\pi n' e^2}/{m}$, ω_0 is Oscillator frequency, n' atomic density and k is wave vector.

The Pauli principle is not strictly followed here, unlike in the Fermi gas, because the set of oscillator wave functions for randomly distributed is not orthogonal. This means that the zero-point motion in a high-density medium will almost always be underestimated. This challenge was solved in a numerical study with a slightly different goal by generating a collection of orthogonal zed wave functions.

A hyper geometric series [9] can be used to describe Eq. (1) rewrite this equation as follows:

$$\in(k,\omega) = 1 + \in_1 . \in_z(\omega) = 1 + \in_1 (\in_x + i \in_y) \tag{2}$$

Where:

$$\in_1 = \frac{\omega_p^2}{2\omega_k} e^{-\omega_k/\omega_0} \sum_{n=1}^{\infty} \frac{1}{n!} (\frac{\omega_k}{\omega_0})^n \tag{3}$$

$$\in_z(\omega) = \frac{1}{n\omega_0 - \omega - i\gamma} + \frac{1}{n\omega_0 + \omega - i\gamma} \tag{4}$$

$$\in_x(\omega) = \frac{(n\omega_0 - \omega)}{(n\omega_0 - \omega)^2 + \gamma^2} + \frac{(n\omega_0 + \omega)}{(n\omega_0 + \omega)^2 + \gamma^2} \tag{5}$$

$$\in_y(\omega) = \frac{\gamma}{(n\omega_0 - \omega)^2 + \gamma^2} + \frac{\gamma}{(n\omega_0 + \omega)^2 + \gamma^2} \tag{6}$$

$$\frac{1}{\in(k,\omega)} = \frac{1}{(1+\in_1\in_x) + i\in_1\in_y} \tag{7}$$

$$\frac{1}{\in(k,\omega)} = [\frac{1+\in_1\in_x}{(1+\in_1\in_x)^2 + (\in_1\in_y)^2}] + i[\frac{-\in_1\in_y}{(1+\in_1\in_x)^2 + (\in_1\in_y)^2}] \tag{8}$$

Therefore, the loss function:

$$Im[\frac{-1}{\in(k,\omega)}] = \frac{\in_1\in_y}{(1+\in_1\in_x)^2 + (\in_1\in_y)^2} \tag{9}$$

2.2 Calculation Methodology

This approximation is employed in the well-known Lind hard function [14] to generate the dielectric function or loss function $Im[\frac{-1}{\in(k,\omega)}]$ at low frequency. This function precisely describes the dielectric function for a low-velocity ion in a non-relativistic free electron plasma with a high density at absolute zero [10].

The energy loss cross section of a single charged projectile with velocity v [7] can be expressed using the dielectric function approach as follows:

$$S_{(q)} = \frac{2}{N\pi v^2} \int_0^{\infty} \frac{dk}{k} |\rho(k)|^2 \int_0^{kv} d\omega . \omega Im\left[\frac{-1}{\epsilon(k,\omega)}\right] \tag{10}$$

$$\rho(k) = z_1 \frac{q + (k\Lambda)^2}{1 + (k\Lambda)^2} \tag{11}$$

If $k \to 1, \rho(k) = 1$, then, the projectile's bare nucleus energy loss:

$$S_{(q=1)} = \frac{2}{N\pi v^2} \int_0^{\infty} \frac{dk}{k} \int_0^{kv} d\omega . \omega Im\left[\frac{-1}{\epsilon(k,\omega)}\right] \tag{12}$$

In this situation, data for a wide variety of incident and expelled effects that enable energy to be transferred to delicate bimolecular targets like energies are needed, as well as ionization data for a wide range of projectile and organic target combinations, to gain an understanding of micro and nanometric features damage to bimolecular systems caused by radiation.

The goal of the purpose of this study is to give a simple theoretical method that may be applied to any situation gives the above-mentioned ionization data as well as, using only a little amount of input data, based on the dielectric physically motivated approximations and formalism [11-14]. Proton impact results are shown here. The method can be used to heavy ions, electrons, and other charged particles right away.

Although there are currently a number of straightforward theoretical and semi-empirical techniques for calculating the energy spectra of secondary electrons, such as the Rudd formula and the semi-classical binary encounter approximation (BEA) [4], they are restricted to specific targets (atomic or small molecules), and it is difficult to extend them to complex biological systems.

Furthermore, they may experience issues as a result of ignoring many particle interactions and target physical state effects.

$P_q = (T_{ke}, E)$ that an energy excitation is produced in the target by a projectile with a charge state (q) and energy (T).$E_{es} = \hbar\omega$ irrespective of its momentum, in a.u $\hbar = 1$, is given by,

$$P_q(T,E) = \frac{m_1 e^2}{\pi\,\hbar^2 T}\int_{k_{min}}^{\infty}\frac{dk}{k}\rho_q^2(k) Im\left[\frac{-1}{\epsilon(k,\omega)}\right] \tag{13}$$

Where:

$$K_{min} = \omega/\sqrt{2T_{ke}/m_1}\,,$$

As a result, by integrating over all possible energy transfers, It is possible to calculate the projectile's average energy loss per unit route length (also known as stopping power or stopping force). [11-14]

$$\frac{dT}{dX} = \int_0^{\infty}\omega.d\omega.P_q(T_{ke},\omega) \tag{14}$$

The electronic excitations $\langle E_q(T)\rangle$ caused by the bullet have a mean energy of can be written as [19]:

$$\langle E_q(T)\rangle = \frac{\int_0^{\infty} dEEP_q(T,E)}{\int_0^{\infty} dEP_q(T,E)} \tag{15}$$

2.3 Calculation Methodology

All mathematical equations have been programmed numerically using Fortran 90 software version (Fortran PowerStation 4.0.), it was used to programme the mathematical equations for the analysis of RNA with separation energies between (1, 3) MeV. The chemical make-up of Human tissues is important, as is well recognized [10]. The proton concentration in RNA was also the programming language Matlab was used, in figures, the proton was measured in the RNA inside the cells, and the results are shown in the figures below the measurements in detail. Because it contains all data regarding the electron excitation spectrum of the target.

The material's energy-loss function (ELF) [16, 17]. Because it contains all data regarding the electron excitation spectrum of the target Im $[1-\frac{\omega_p^2}{\omega^2}]$, is the material's energy-loss function (ELF), which is essential for obtaining accurate results for the aforementioned energy losses. Because of this, it's essential to apply an effective target description (ELF) along the entire (k-) plane.

3. Results and Desiccation

As shown in Figure 2, the positively charged particle, such as a proton, will seek to gather electrons from the absorber at low energy, reducing its charge and leading to linear energy loss. At the end of its path, the particle gathers z electrons and becomes a neutral atom. The stopping power rapidly rises with low energies until it reaches its maximum.

The probability per unit route P that a proton projectile generates electronic excitation of energy E in RNA using a quantum oscillator of dielectric function for various incident proton energies T (1, 3) MeV is shown in figure 3 while modelling the energy loss function ELF, in figure 3.

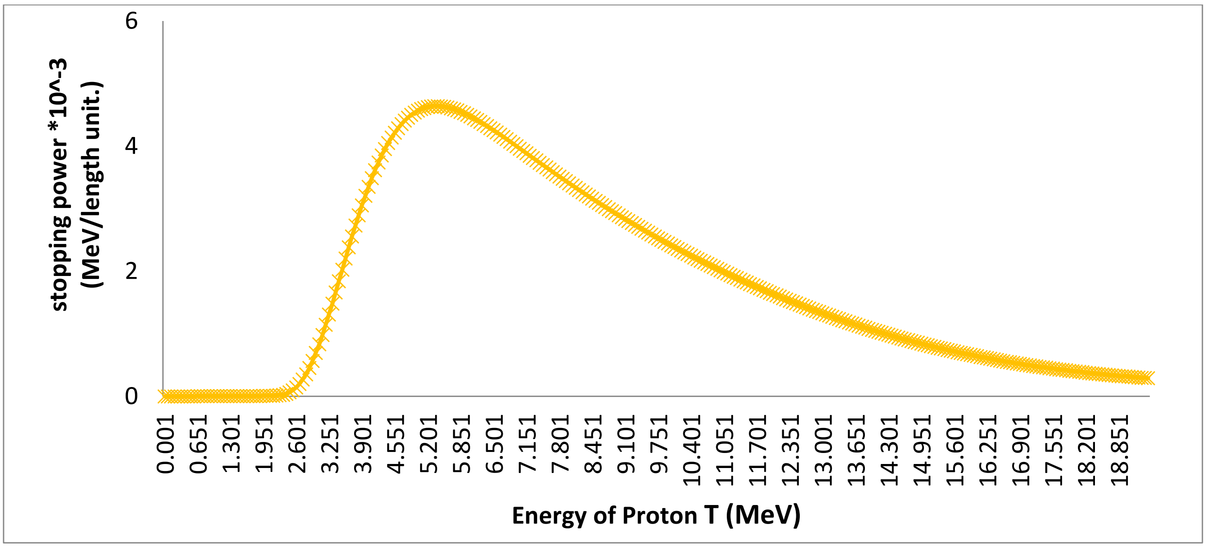

Figure -2 The stopping power as a function of the energy of Proton T of the proton beams.

The stopping power increases when the energy of the particle is low when penetrating the target material, and this is a result of the interaction of the particle with a positive charge, such as the proton, with the electronic fields of the target material, where the maximum value of the electronic irritation can be observed at the energy of 1 MeV, and it remains the same no matter how much it increases Valuable, as seen in the figure 4.

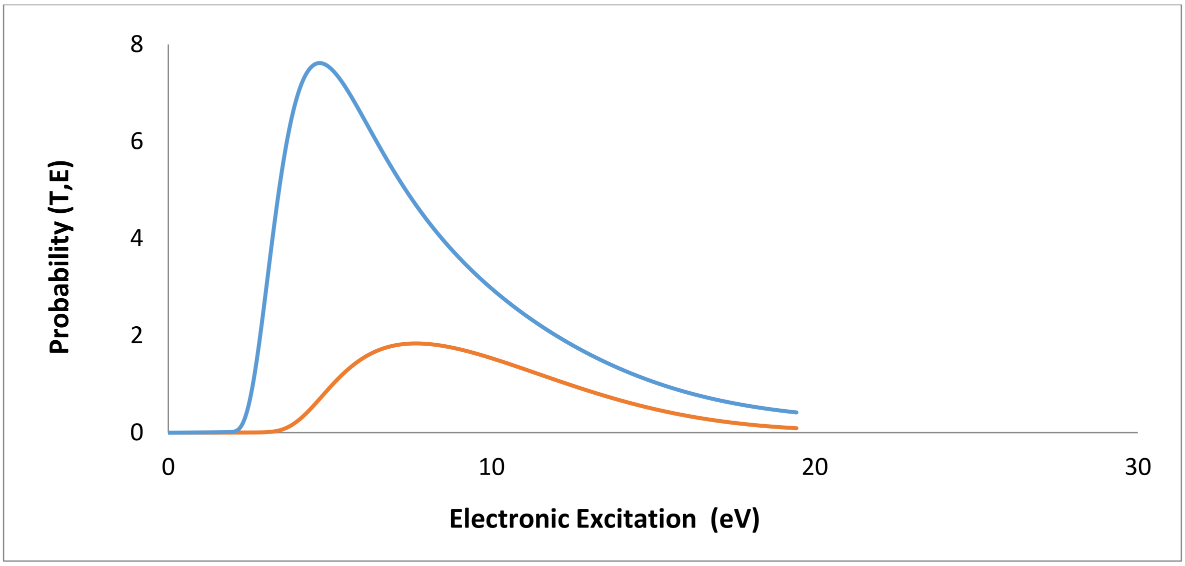

Figure -3 Probability per unit path *P* that a proton-projectile induces electronic excitation of energy E in RNA with the red line value of energy incident proton-projectile T is 3Mev and the blue line is 1Mev of T.

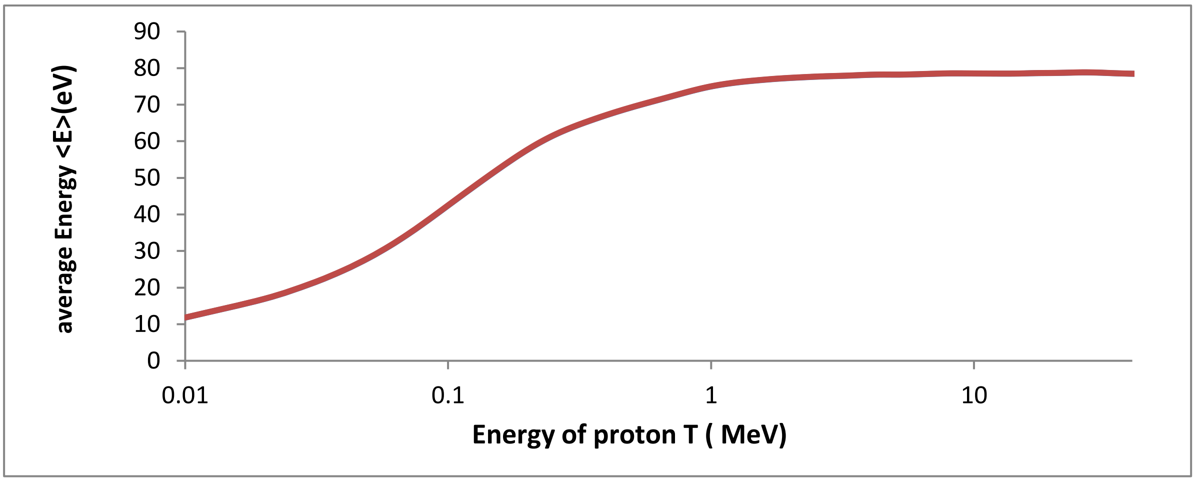

Figure 4: The average Energy <E> for Energy of proton induces in RNA by using (QO) dielectric function.

4. Conclusion

The energy loss of proton particles in that medium is mitigated by stopping power at the very low energy of proton because of the interaction that occurs with electromagnetic fields and electrons in the medium. With rising proton energy, stopping power falls down dramatically. Electronic stopping power is exactly proportional to energy of proton It is noticed that when the energy of the proton bundles is increased, this leads to a rise in the probability of interaction with the medium to a certain extent. Whenever the energy of the protons increases, the interaction will decrease, and the potential for interaction begins to decrease. After that, at very high speeds, the medium will become transparent to charged particles, meaning that the probability of interaction with energy or speed, so the relationship between the energy of proton beams and the probability of interaction becomes inverse. As for the average Energy, it is noticeable that when a certain kinetic energy value begins to rise to a certain value, the average Energy remains constant no matter how much the value of the kinetic energy of the particles (proton beams) increases.

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