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Use the Heavy Alpha Particles in Simulation Experiments to Find Energy Appropriate for Destruction Cancer Cells

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Abstract: The importance of using the heavy alpha particles in simulation experiments to find the appropriate energy for destruction cancer cells has multiple applications in physics and medical physics. It is found that the probability of destruction of cancer cells increased at energies lower than few 20 MeV and exponentially decreasing at high energies larger than 20 MeV. The programming language FORTRAN - 90 was used for a required calculation. Different kinetic energies of the incident alpha particle (T = 0.05, 1, 2, 2.5 MeV / u) to destroy cancer cells were employed. The energy loss of incident particle was calculated by dielectric formalism using model Plasmon pole approximation (PPA) model in two target , which are Liquid water and DNA , which more than one wavelength of the incident particle (Brandt and Kitagawa Model) and (Kaneko Model) Good agreement is with previous work was achieved.

Key words: Energy-loss Function; Dielectric Formalism; Liquid Water; DNA Target and Energy loss; alpha particle.

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Introduction

Studying the interaction of ionizing radiation (*X-rays ,electrons, positrons, protons or heavier ions*) with living tissues has a paramount importance in cancer therapy, since the amount of energy deposited by the ionizing radiation to tumors cells will determine the outcome of the treatment (1,2). Space radiation health is another area where research on alpha and heavier ion effects on human tissues is important for the radiological protection of human crew in long-duration deep space missions (3). The cure of tambours with hadrons (mainly protons and carbon ions) presents, with respect to the conventional *X-ray* and electron therapy, some advantages, from both the biological and physical point of view. The pattern of energy deposition by hadrons, called the Bragg peak, is characterized by most of the projectile energy deposited at the end of its range. In this way the damage to healthy cells, surrounding the malignant ones to be destroyed, can be strongly reduced (4, 5). The secondary electrons produced by ionizations induced in the living tissues by the projectile also contribute to the

cellular damage. These electrons are able to travel and produce further ionizations in the DNA, eventually leading to the cellular death (6). The lethal efficiency of each secondary electron depends on its energy (7, 8), therefore it is very important to have information about the number and energy of the electrons generated by the projectile in the target.
Even electrons with sub-ionizing energy were shown to produce lethal damage in DNA (7, 9, 10).

Materials and Methods

Energy Transfer

When a swift projectile with mass M_1, atomic number Z_1, kinetic energy T and charge q moves inside a solid, it induces electronic excitations in the material, losing energy in the process. This energy loss mechanism is the dominant one. These electronic excitations can correspond to excitations or ionizations of individual electrons or even excitations of collective modes in the target electron gas.
The dielectric formalism (11) provides a way of studying the response of the electronic system of the target to the perturbation represented by the projectile. The key parameter of the problem is a correct description of the dielectric function of the material $\epsilon = (k, \omega)$, which contains all the information about the electronic excitations that the material can sustain.
Within this framework the probability per unit path length $P_q = (T, E)$ that a projectile with charge state q and energy T produces in the target an excitation of energy $E_{es} = \hbar\omega$ irrespective of its momentum, atomic units (a.u) $\hbar = 1$, is given by

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

Where:

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

e: is the absolute value of the electron charge .

$\rho_q(k)$: is the Fourier transform of the projectile charge density.
Hence, the mean energy lost by the projectile per unit path length (the so called stopping power or stopping force) can be calculated integrating over all possible energy transfer E

$$\frac{dT}{dX} = \int_0^{\infty} \omega . d\omega . P_q(T_{ke}, \omega) \qquad (2)$$

The mean energy of the electronic excitations $\langle E_q(T)\rangle$ induced by the projectile can be written as:

$$\langle E_q(T)\rangle = \frac{\int_0^{\infty} dEEP_q(T,E)}{\int_0^{\infty} dEP_q(T,E)} \qquad (3)$$

If q is the ionization function,
$(q = 1 - \frac{N}{Z_1})$
Where:
N : is the number of bounds electrons.

Z_1 : is the atom number of ions.

$$\rho(k) = z_1 \frac{q + (k\Lambda)^2}{1 + (k\Lambda)^2} \qquad (4)$$

Where:
Λ: is the screening length (12).
The charge state q of the projectile inside the target can vary through capture and loss processes and depends on its energy (T). However, when

charge equilibrium is reached, the probability $\phi_q(T)$ of finding the projectile in a charge state remains constant for each incident energy (T). Here we obtain the values of $\phi_q(T)$ for α-Particle in liquid water or DNA using the parameterization provided by the *CasP* code (13)

Bragg's additively rule has been compound for compound targets. Like H_2O *and DNA* $(C_{20}H_{27}N_7O_{13}P_2)$ .We average over all possible charge states (*q=0 and 1 for α-Particle*) in order to obtain the energy distribution, $P(T,E)$ and the mean energy,$\langle E(T)\rangle$ of the electronic excitations produced in the target as:

$$P(T,E) = \sum_{q=0}^{1} \emptyset_q(T) P_q(T,E) \qquad (5)$$

$$\langle E_q(T)\rangle = \frac{\int_0^\infty dEE \sum_{q=0}^{1} \emptyset_q(T) P_q(T,E)}{\int_0^\infty dE \sum_{q=0}^{1} \emptyset_q(T) P_q(T,E)} \qquad (6)$$

The calculation of the previous magnitudes requires the description of the projectile charge density through $\rho_q(k)$ and of the target excitation spectrum by means of its energy-loss function *(ELF),* $\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]$ .The former is accounted for with the model proposed by Brandt and Kitagawa (14) because it is reliable and provides analytical expressions for $\rho_q(k)$.The stopping power of a singly charged projectile can be expressed (14) by:

$$S = \frac{2}{\pi v^2} \int_0^\infty \frac{dk}{k} |\rho(k)|^2 \int_0^{kv} d\omega\, \omega\, \mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]$$
(7)

Where:v is the projectile velocity and $\rho(k)$ is the Fourier transform of the spatial charge density $\rho(r)$ (total of nuclear and electronic charge densities) in the rest frame of the projectile. A spherically symmetric charge distribution was assumed in a statistical approximation (15).

$$\rho(r) = Z_1\delta(r) - \frac{N_e}{4\pi{\Lambda_0}^3} \frac{\Lambda_0}{r} e^{-\frac{r}{\Lambda_0}}$$
(8)

When:

N_e: is the number of electrons still bound to the projectile nucleus.

The screening Length

Brandt and Kitagawa (BK)(Λ_0)

(Brandt and Kitagawa1982) have supposed that the medium is a valence electrons , thus BK have derived the stopping power effective charge of an electron gas in a dielectric-response approximation for anion of ionization $q(v_r)$ .The projectile in condensed matter can be written as suggested by (14)

$$\Lambda_o = \frac{2aN_e^{2/3}}{\left(Z_1 - \lambda N_e/4\right)} \qquad (9)$$

$$= \frac{2a(1-q)^{2/3}}{Z_1^{1/3}\left[1 - \frac{1}{7}(1-q)\right]} a_0 \qquad (10)$$

Where a =0.240 and a_0=1 a.u. = $0.529A^0$ is the Bohr radius. For the k-shell electrons, *BK* suggested $\Lambda_0 = a_0/Z_{1k}$with $Z_{1k} = Z_1$for $N_e = 1$and $Z_{1k} = Z_1 - 0.3$ for $N_e = 2$.

Kaneko-Model (Λ_k)

Yang (1994) has derived the stopping power and energy straggling effective charge for a projectile in an electron gas by taking into account the static screening effect of conduction electrons in the medium, the projectile screening length in condensed matter was improved to be (12).

$$\Lambda = \Lambda_0 / \left(1 - \frac{2}{3} k_{TF}^2 \Lambda_0^2\right) \qquad (11)$$

Where:

$k_{TF} = (\frac{4k_F}{\pi})^{1/2}$: is the Thomas-Fermi (TF) screening wave number $k_F = (3\pi^2 n)^{1/3}$: is the Fermi wave number with the conduction-electron density. $n = 3/4\pi r_s^3$: is the one-electron radius r_s is the radius of the average volume occupied by each conduction electron of the medium.

Plasmon- Pole Approximation (PPA) with Damping

At high velocities, where the projectile can excite Plasmon's in the medium, Brandt Kitagawa (BK) used the Plasmon Pole Approximation (PPA) of the dielectric function (16).

$$\epsilon(k,\omega) = 1 + \frac{w_p^2}{w_p^2 + \beta^2 K^2 + {k^4}/{4} - (w - i\gamma)}$$
(12)

Contributions from single-particle excitations are accounted for through the square of the kinetic energy $k^2/2$ of a free electron of momentum($\vec{K}$). The small constant γ represents damping processes. It follows that in the limit $\gamma \rightarrow 1$, (11).

$$Im\left[\frac{-1}{\epsilon(k,\omega)}\right] = \frac{\pi\, w_p^2}{2A}\,\delta(w - A) \qquad (13)$$

Where:

$$A^2 = \Omega_p^2 + \beta^2 K^2 + {k^4}/{4}$$

The upper and lower integration limits in $\vec{K}$ are the maximum and minimum momentum transfers $\vec{K}_+$ and $\vec{K}_-$ to target electrons.

$$k\pm = \left\{2(\nu_1^2 - \beta^2) \pm 2\left[(\nu_1^2 - \beta^2)^2 - \Omega_p^2\right]^{1/2}\right\}^{1/2} (14)$$

This gives as threshold for ν_1

$$\nu_{thr.} = \left(\beta^2 - \Omega_p^2\right)^{1/2},$$

Below which Plasmon contributions subside. Then

$$S_{(q=1)} = \frac{\omega_p^2 Z_1^2}{\nu_1^2}\int_{k_-}^{k_+}\frac{dk}{k} \qquad (15)$$

Then:

$$S_{(q=1)} = \frac{\omega_p^2 Z_1^2}{\nu_1^2}\,\mathrm{In}\frac{k_+}{k_-} \qquad (16)$$

Is given in Eq. (7) there for the ***(PSPEC)***

$$\zeta = \left[\frac{S_q}{S_{q=1}}\right]^{1/2} \qquad (17)$$

Bragg's additivity rule for $S_{(q)}$,

$$S_{DNA}(q) = \{20S_C(q) + 27S_H(q) + 17S_N(q) + 13\,S_O(q) + 2S_P(q)\} (18)$$

For water:

$$S_{H2O}(q) = 2S_H(q) + S_O(q) \qquad (19)$$

Where:
$S_C(q), S_H(q), S_N(q), S_O(q) and\ S_P(q)$, the stopping cross – section for carbon,

Results and Discussion

A Program ***(DNA.F90)*** has been written using FORTRAN-90 which DNA for the numerical calculations given in previous section and a copy from program is an available (17). Figs (1-4) show the variation of Probability per unit length $P_q(T,E)$ that $\alpha - Particle$ electronic excitation of energy *E* in *liquid water* and *DNA* for ($T = 0.05, 1, 2, 2.5\ Mev/u$) at Λ_o and Λ .

There is a shoulder for incident He-ions with energy $T \approx 0.05$ Mev/u While this shoulder dinappear at $T \geq 1.0$ Mev/u and this is because at low incident He-ions , the time of interaction is large which cause a high Probability of interaction , However there are sizeable differences at intermediate and small *T*. The stopping power of charged particle *S(q)* of individual element given in DNA ($C_{20}H_{27}N_7O_{13}P_2$)has been calculated numerically and used to find the ***(PSPEC)***of DNA(17)

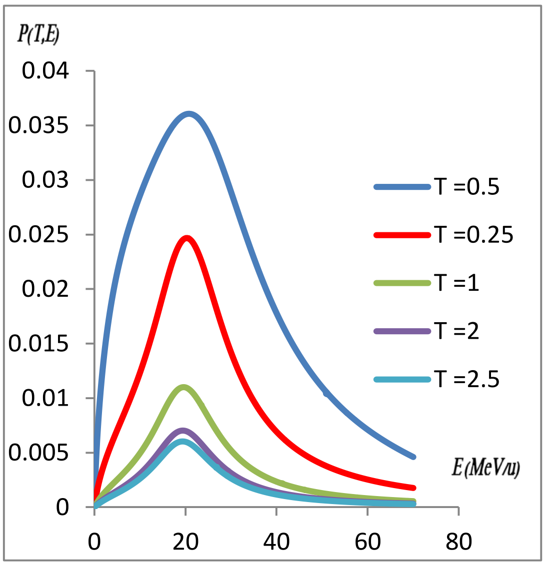


Figure (1): Probability per Unit Path (P a.u.) that Helium Projectile Induces Electronic Excitation of Energy E in DNA for Different T MeV/a.u when modeling the ELF at Brandt and Kitagawa model (Λ_o).

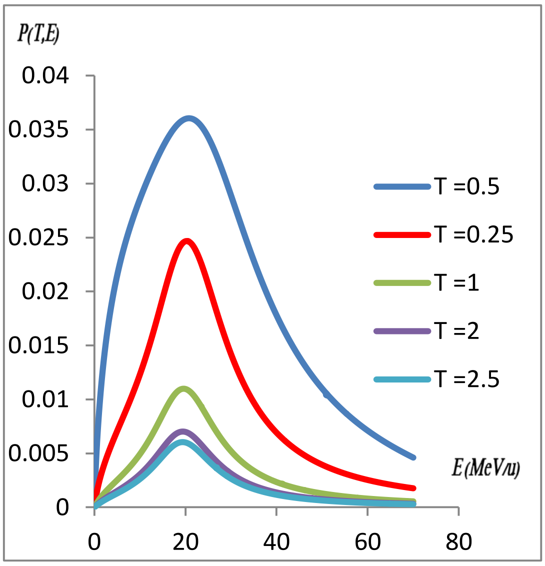


Figure (2): Probability per Unit Path (P a.u.) That Helium Projectile Induces Electronic Excitation of Energy E in DNA for Different T MeV/a.u when modeling the ELF at Kaneko-model (Λ)

When the alpha bombardment of the target $He - H_2O$ the results areas (P)vs. (E) follows :

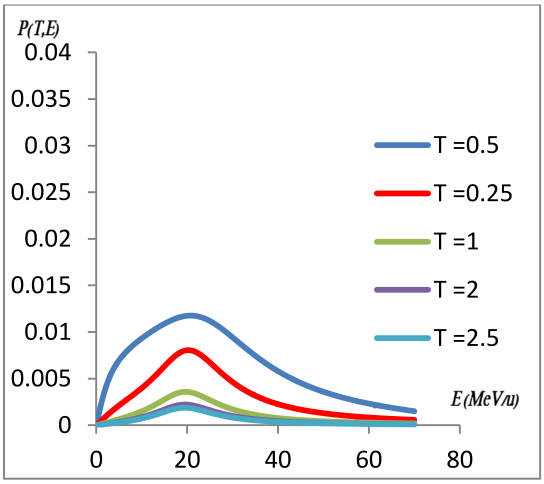


Figure (3): Probability Per Unit Path P that Helium Projectile Induces Electronic Excitation of Energy E in H_2O for Different T when Modeling the ELF at Brandt and Kitagawa model (Λ_o)

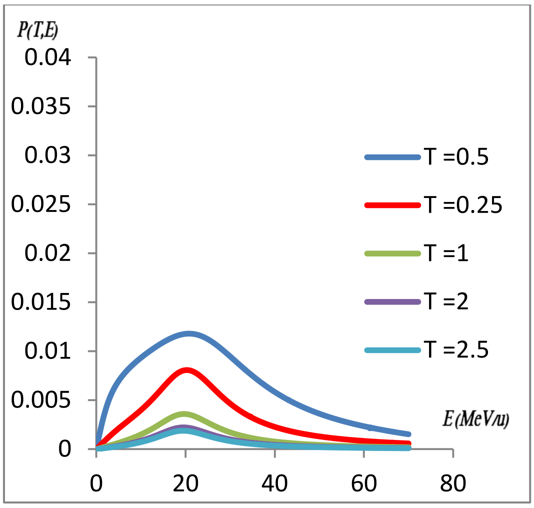
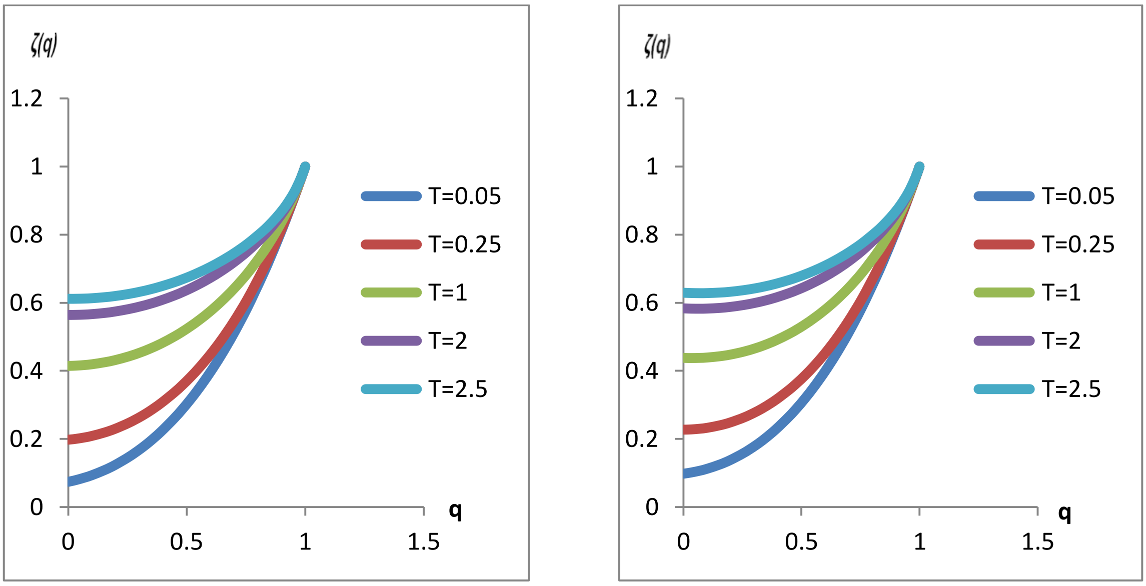


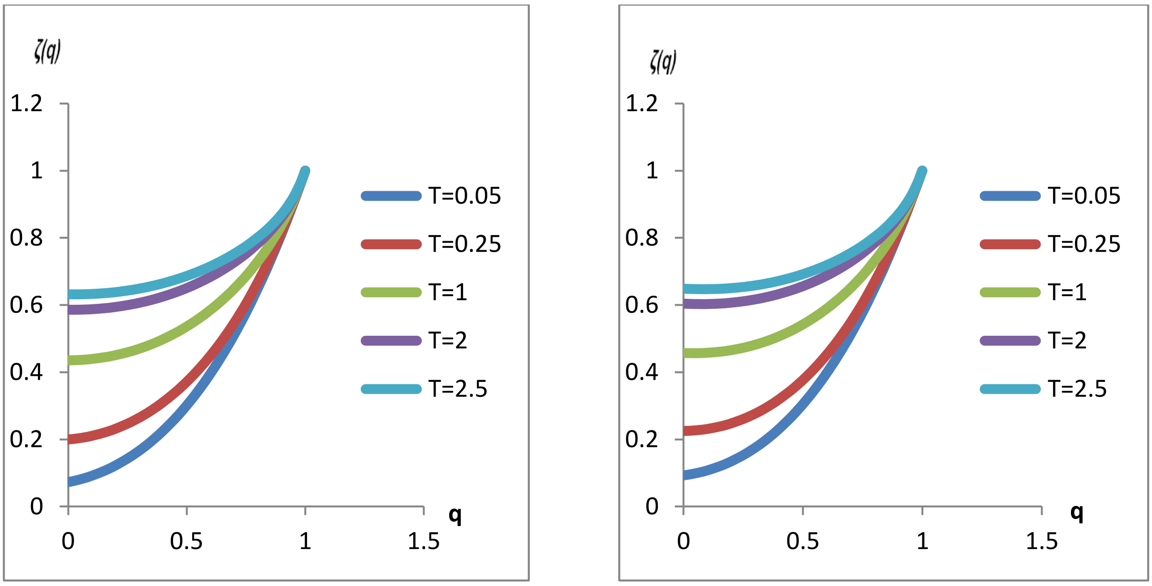
Figure (4): Probability Per Unit Path P that Helium Projectile Induces Electronic Excitation of Energy E in H_2O for Different T when Modeling the ELF at Kaneko-model Λ .

With Eq. (18) and denotes the (PSPEC) of each elements in DNA. For Water with Eq. (19).



(a) (b)

Figure (5): *ζ(q)* for Helium-DNA (q=1) with Energy for (a) Λ_0 (b) Λ



(a) (b)

Figure (6): ζ(q) for Helium-H_2O (q=1) with Energy for (a) Λ_0 (b) Λ

Figure (5-6) show the stopping parameter $\zeta(q)$ with ionization fraction for different incident α-Particle energy *T (0.05, 0.25, 1, 2, 2.5Mev/u)* on DNA, H_2O at Λ_0 *and* Λ . $\zeta(q)$ Strongly dependent on incident $\alpha - Particle$ energy at $(q) \to 0$, while $\zeta(q) \to 1$ at $(q) \to 1$ different incident α-Particle energy. There is minor different between $\zeta(q)$ at Λ_0 *and* Λ $(q) \to 0$, while they are exactly matched at $(q) \to 1$.

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