The effective number of electrons for DNA and liquid water which is a function to the energy that contributes in the excitations of the target using the dielectric formalism which has been calculated in present work. The electronic response of DNA and liquid water is described by the MELF-GOS model, in which the outer electron excitations of the target are accounted by Mermin-type energy loss functions, whereas the inner-shell electron excitations are modeled by the generalized oscillator strengths of the constituent atoms. The mathematical equations have been program by writing a Fortran-90 program for numerical calculations.

Keywords: MELF-GOS, Effective number of electrons, DNA target, Liquid water, dielectric function, valance shell, inner shell.

1. INTRODUCTION

The study of interaction ion beams with biological materials is very important for predicting the effects of radiation in living tissues [1-3]. Since the amount of energy deposited by the ionizing radiation to tumor cells will determine the outcome of the treatment [1, 4]. Using energetic ion beams for radiation therapy has become a promising technique because high doses can be deposited locally at tumor sites, reducing the damage to the surrounding critical organs and the selection of ion beam energies and the determination of ion ranges are crucial for the calculation of the delivered dose [5]. Research on the effects of radiation on DNA, the most important biological material, is very active, because determining the relationship between the energy deposited by fast particles in the target and the damage they cause is important to radiation biophysics [6, 7]. DNA damage can be produced by direct ionization and excitation of DNA electrons [8] or by indirect chemical reactions of water radiolysis products with DNA [9]. Even electrons with subionizing energies can cause lethal lesions in DNA [10, 11]. An effort to study the interaction of energetic ion beams with liquid water at intermediate energies has been carried out recently, since water represents over 80% of the content of the cells of soft tissues [12, 13]. Therefore, a detailed study of the energy loss of ions in biological targets (such as DNA or liquid water) is desirable to improve our understanding and modeling capabilities of the action of radiation in ion-beam cancer therapy [7, 14, 15].

2. THEORETICAL BACKGROUND

Energy loss function for valance electron and inner shell

The dielectric formulation is one of the most used methods to describe the interaction of swift ions and other charged particles with matter [16]. The dielectric function is the basic of many applications and because it is applicable to only a limited number of so-called nearly-free-electron materials like aluminum [17]. Mermin derived an expression to the dielectric function, in terms of the Lindhard dielectric function by replacing the frequency  into a complex frequency  by using Random Phase Approximation dielectric function (RPA) dielectric function and the result is Mermin dielectric function  which can be written in terms of  as follows [18, 19]:

$$\epsilon_M (k, \omega) = 1 + \frac{(1 + i\gamma / \omega)\epsilon_L (k, \omega + i\gamma) - 1}{1 + (i\gamma / \omega)\epsilon_L (k, \omega + i\gamma) - 1\epsilon_L (k, \omega) - 1}$$ (1)

Where:  is Lindhard dielectric function [16]. The key parameter to obtain reliable results for the energy losses is the energy-loss function (ELF) of the material [17] $\epsilon(k, \omega)$, since it contains all the information about the electron excitation spectrum of the target. Thus it is essential to use a good description of the target ELF for the whole k-ω plane (that is, the Bethe surface) [5]. In present work the Mermin-Energy-Loss-Function-Generalized-Oscillator-Strength (MELF-GOS) method [20, 21] applied to describe the energy-loss function of DNA and liquid water since it has been successfully used to describe the ELF of materials with a complex electronic spectrum [22-24]. Here the target electron excitations are split into two parts, one indicates to excitations of the inner-shell electrons, and the other produce from excitations of the outer (weakly bound) electrons, namely.
The excitations of the outer electrons of the solid, including both collective and single-particle excitations, are described by Mermin type ELF,

$$\text{Im} \left[ \frac{-1}{\varepsilon(k,\omega)} \right] = \text{Im} \left[ \frac{-1}{\varepsilon(k,\omega)} \right]_{\text{outer}} + \text{Im} \left[ \frac{-1}{\varepsilon(k,\omega)} \right]_{\text{inter}}$$

The suitable parameter $A_i$ and $\gamma_i$ are represented position and width, respectively, of the Mermin-type ELF, while the coefficients $A_i$ are the corresponding weights. While $\omega_{th,i}$ is the threshold energy [25]. The parameters for DNA and liquid water are shown in table (1).

**Table (1)** Parameters used to fit the outer electron excitations contribution to the ELF (See Eq. 3) of DNA and liquid water

<table>
<thead>
<tr>
<th>Target</th>
<th>$A_i$</th>
<th>$\gamma_i$</th>
<th>$\omega_{th,i}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DNA</td>
<td>0.159</td>
<td>0.397</td>
<td>35</td>
</tr>
<tr>
<td></td>
<td>0.0707</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liquid Water</td>
<td>0.23</td>
<td>1.15</td>
<td></td>
</tr>
</tbody>
</table>

On the other hand, inner-shell electrons keep their atomic character since they have large binding energies; thus, they are designed in terms of the generalized oscillator strengths (GOS). The connection between the ELF and the GOS model is given by

$$\text{Im} \left[ \frac{-1}{\varepsilon(k,\omega)} \right]_{\text{inner}} = \frac{2\pi^3 N}{\omega} \sum_{nl} \frac{df_{nl}(k,\omega)}{d\omega},$$

Where $df_{nl}(k,\omega)$ is the GOS of the $(n,l)$ sub-shell and $N$ is the molecular density of the target. In the present work the hydrogenic approach is used to get the GOS because it is analytical and describes the contribution of the K-shell ionization corresponding to C, N, O and P atoms well [20]. A one electron atom modelled by a harmonically bound electron. A formula for generalized oscillator strengths (GOS) derived from harmonic oscillator as follows [26]:

$$f_{n0} = \frac{1}{(n-1)!} \left( \frac{\hbar \omega_o}{Q} \right)^{n-2} e^{-Q/\hbar \omega_o},$$

For $n = 1, 2, \ldots$. This represents a Poisson distribution.

Where the quantity $Q = h^2 q_{fi}^2 / 2m$, with $(q_{fi})$ is the momentum transfer [26].

We use the MELF-GOS method to getting the $f$-sum rule at any transferred momentum [27] because one of the advantages of the MELF-GOS method is that the fit of the ELF in the optical limit is analytically and automatically extended to $(k \rightarrow 0)$ through the properties of the Mermin dielectric function and the GOS model [20, 28]; therefore, it is not necessary to assume a particular ELF dependence on the momentum transfer. For the materials where experimental data are available for the ELF at $(k \rightarrow 0)$, the MELF-GOS reproduces the experimental ELF well [28, 29, 30, 31]. Therefore, we use the procedure described previously to extend the optical ELF to the whole Bethe surface. The resulting ELF should satisfy the $f$-sum rule for any wave number $k$[27].

The effective number of electrons is defined as the number of electrons per atom or per molecule share in optical transfers [32]. Where the effective number of electrons in the optical processes is a function of transferred energy ($\omega$) $N_{eff}(\omega)$ could be defined in three clear ways, a situation which had led to massive confusion. This is a result of the fact that oscillator-strength sums may be structure from the imaginary part of the dielectric function $\varepsilon_{im}(\omega)$ and the
refractive index $n(\omega)$ or the energy-loss function $Im[\frac{1}{\varepsilon(\omega)}]$, these quantities are studied for an electronic system embedded in a polarizable medium of dielectric constant $\varepsilon_0$. Optical constants of materials presenting different rules, the $f$-sum rule may be written in three forms for the analysis of optical spectra and this includes the imaginary part of dielectric function $\varepsilon_2(\omega)$ and the imaginary part of the refractive index $n(\omega)$ and the energy-loss function $Im[\frac{1}{\varepsilon(\omega)}]$. The three forms are [27]:

$$\int_0^\infty \omega \varepsilon_2(\omega) d\omega = \frac{\pi}{2} \omega_0^2$$  \hspace{1cm} (6)

$$\int_0^\infty \omega k(\omega) d\omega = \frac{\pi}{4} \omega_0^2$$  \hspace{1cm} (7)

$$\int_0^\infty \omega Im[\varepsilon^{-1}(\omega)] d\omega = -\frac{\pi}{2} \omega_0^2$$  \hspace{1cm} (8)

So, the previous rules indicate to define the effective number of electrons which contributing to the optical properties up to energy $\omega$ and writes in terms of $Im[\frac{1}{\varepsilon^{-1}(\omega)}], k(\omega), \varepsilon(\omega)][3,3]$. 

$$N_{eff}(\omega)|_e = B \int_0^\omega d\omega' \omega' \varepsilon_2(\omega')$$  \hspace{1cm} (9)

$$N_{eff}(\omega)|_k = B \int_0^\omega d\omega' \omega' k(\omega')$$  \hspace{1cm} (10)

$$N_{eff}(\omega)|_{e-1} = -B \int_0^\omega d\omega' \omega' Im[\varepsilon^{-1}(\omega')]$$  \hspace{1cm} (11)

Where: $B$ is a constant and equal to $\frac{m}{2\pi^2 e^2} \frac{A}{\rho N_a}$. In the present work Eq. (11) used to calculate the effective number of electron that may be excited up to a maximum transferred energy ($\hbar \omega$) from an incident projectile.

### 3. RESULTS AND DISCUSSION

The calculation of the previous magnitudes requires the description of its energy-loss function (ELF), $Im[\frac{1}{\varepsilon(\omega)}]$. So the calculation of the energy loss function (ELF) as a function of the transferred energy ($\omega$) based on Eq. (3, 4) is shown in figures (1, 2) in 2 and 3-dimensions plot and by using (MELF-GOS) method for DNA and liquid water. The calculation of the effective number of electrons of DNA and liquid water as a function of the transferred energy based on the energy loss function (ELF) of the outer and inner shell is shown in Figures (3).
Figure (1) Mermin’s energy loss function (ELF) of (a) DNA and (b) liquid water at $k = 0$ as a function of wave number ($k$) and the transferred energy ($\omega$) in 2-dimension.

Figure (2) Mermin’s energy loss function (ELF) of (a) DNA and (b) liquid water as a function of wave number ($k$) and the transferred energy ($\omega$) in 3-dimension.
Figure (3) the effective number of electrons of (a) DNA and (b) liquid water as a function of the transferred energy \( h\omega \).

4. CONCLUSIONS

In the present work the excitation spectrum of the DNA and liquid water target has been described accurately by means of the MELF-GOS method [20, 34], which uses Mermin-type energy-loss functions for the outer electron excitations and generalized oscillator strengths for the inner-shell excitations and the effective number of electrons and the energy loss function had been programmed in Fortran-90. As we can see, the maximum value of the effective number is about \( N_{eff} \approx 205 \) for DNA and \( N_{eff} \approx 6 \) for \( H_2O \) when the transferred energy is about 100 ev and when \( (h\omega \to \infty) \) the effective number of electrons tends to the total number of targets electrons. \( N_{eff} \) doesn’t depend on \( K \) allow \( (h\omega \to \infty) \) and high \( (h\omega \to \infty) \) energy transfer.

REFERENCES
