The Decay Q Value of Neutrinoless Double Beta Decay Revisited

D.-M. Mei$^1$,* and W.-Z. Wei$^1$

$^1$Department of Physics, The University of South Dakota, Vermillion, SD 57069, USA
(Dated: February 8, 2023)

An earlier publication "The implication of the atomic effects in neutrinoless double beta (0νββ) decay" written by Mei and Wei has motivated us to compare the decay Q value ($Q_{ββ}$) derived from the decay of the parent nucleus to the daughter nucleus with the two ejected beta particles in the final state to the $Q_{ββ}$ directly derived from the decay of the initial neutral atom to the final state of double-ionized daughter ion with the two ejected beta particles in the final state. We show that the results are the same, which is the mass-energy difference ($ΔMc^2$) subtracted by the total difference of the atomic electron binding energy ($ΔE_b$) between the ground states of initial and final neutral atoms. We demonstrate that $ΔMc^2$ is the sum of $Q_{ββ}$ and the atomic relaxation energy ($ΔE_b$) of the atomic structure after the decay. Depending on the atomic relaxation time, the release of the atomic binding energy may not come together with the energy deposition of the two ejected beta particles.

Neutrinos take a key role in understanding the universe [1]. The discovery of neutrino oscillation indicates that neutrinos have mass [2]. This has motivated physicists to postulate new properties of neutrinos [3], which have created a possible connection between the observed asymmetry of matter over antimatter in our universe [4]. If neutrinos are Majorana particles [5], this means that neutrinos are their own anti-particles. This Majorana nature of neutrinos, if confirmed, might offer an explanation of the prevalence of matter over anti-matter [6].

The only experimentally feasible way to answer whether neutrinos are Majorana particles [5], this means that neutrinos have mass [2]. This has motivated physicists to postulate new properties of neutrinos [3], which have created a possible connection between the observed asymmetry of matter over antimatter in our universe [4].

In an earlier paper [13], Mei and Wei derived the decay Q value from the decay of the parent nucleus to the daughter nucleus with the two ejected beta particles in the final state. In this case, a $0νββ$ decay process can be described as below [7]:

$$\frac{A}{Z}X_N \rightarrow \frac{A}{Z+2}X_{N-2} + e^- + e^-,$$  \hspace{1cm} (1)

where $\frac{A}{Z}X_N$ is the mother nucleus in the initial state while $\frac{A}{Z+2}X_{N-2}$ is the daughter nucleus in the final state. The two electrons in the final state are the two ejected beta particles as the result of this nuclear decay process. The decay Q value, which is defined as the available kinetic energy for the two ejected beta particles, for this nuclear decay process can be calculated using the mass difference in the rest frame between the initial and final products [13]:

$$Q_{ββ} = |m_N(\frac{A}{Z}X) - m_{N-2}(\frac{A}{Z+2}X')|c^2,$$  \hspace{1cm} (2)

where $m_N(\frac{A}{Z}X)$ stands for the mass of the mother nucleus in the rest frame while $m_{N-2}(\frac{A}{Z+2}X')$ represents the mass of the daughter nucleus in the rest frame. $m_e$ is the mass of electron in the rest frame. $c$ is the speed of light. The mass of a nucleus is related to the corresponding mass of the neutral atom, which is denoted as $M(\frac{A}{Z}X)$, through the following relation:

$$M(\frac{A}{Z}X)c^2 = m_N(\frac{A}{Z}X)c^2 + Zm_ec^2 - \sum_{i=1}^{Z} B_i,$$  \hspace{1cm} (3)

where $B_i$ stands for the atomic binding energy of the $i$th electron. Note that the sign of the binding energies in Eq. 3 must be taken as positive values. Therefore, the atomic binding energies are all positive values in this work and the previous work by Mei and Wei [13]. Replacing the masses of the mother and daughter nuclei in Eq. 2 using the corresponding atomic masses in the neutral form expressed in Eq. 3, by rearranging the terms, $Q_{ββ}$ is found to be:

$$Q_{ββ} = [M(\frac{A}{Z}X) - M(\frac{A}{Z+2}X')]c^2 - \sum_{i=1}^{Z+2} B_i - \sum_{i=1}^{Z} B_i].$$  \hspace{1cm} (4)

As can be seen in Eq. 4, $Q_{ββ}$ is given by two terms. The first term,

$$ΔMc^2 = [M(\frac{A}{Z}X) - M(\frac{A}{Z+2}X')]c^2,$$  \hspace{1cm} (5)

is the mass-energy difference between the atomic masses of the mother and daughter atoms in the neutral form, and the second term,

$$ΔE_b = [\sum_{i=1}^{Z+2} B_i + \sum_{i=1}^{Z} B_i]$$  \hspace{1cm} (6)

represents the difference of the total atomic binding energy of the mother and daughter atoms in the neutral form. Therefore, $Q_{ββ}$ can be written as:

$$Q_{ββ} = ΔMc^2 - ΔE_b.$$  \hspace{1cm} (7)

* Corresponding author.

Email: Dongming.Mei@usd.edu
It is important to point out that this is a standard definition for the decay Q value, which is similar to a normal beta decay process where the decay Q value is expressed as [15, 16]:

$$Q_{\beta} = [M(\frac{A}{Z} X) - M(\frac{A}{Z+1} X')]c^2 - \left[ \sum_{i=1}^{Z+1} B_i - \sum_{i=1}^{Z} B_i \right], \quad (8)$$

Considering that $0\nu\beta\beta$ decay in a nucleus occurs very fast in a level of picoseconds, the atomic structure may have no time to respond to the change of the nuclear charge right after the decay. The daughter nucleus would be surrounded by the atomic electrons from the mother atom. In this case, the daughter atom is a double-ionized ion. The decay Q value can be directly derived from the decay of the ground state of the mother atom to the double-ionized daughter ion with the two ejected beta particles in the final state. This process can be expressed as:

$$\frac{A}{Z} X \rightarrow \frac{A}{Z} X'''' + e^- + e^-,$$  

(9)

where $\frac{A}{Z} X$ is the parent atom in the neutral form and $\frac{A}{Z} X''''$ is the double-ionized daughter ion in which the daughter nucleus is surrounded by the parent atomic electrons right after the decay. Therefore, the atomic member, Z, is the same as the parent atom when the nuclear charge is altered by two units in the final state of the nucleus. The decay Q value for this decay is calculated as:

$$Q_{\beta\beta} = M(\frac{A}{Z} X)c^2 - M(\frac{A}{Z} X''')c^2 - 2m_ec^2,$$  

(10)

where $M(\frac{A}{Z} X)$ is the mass of the parent atom in the neutral form and $M(\frac{A}{Z} X''')$ is the mass of the double-ionized daughter ion. Note that $M(\frac{A}{Z} X''')$ is related to the mass of the daughter nucleus through the following relation:

$$M(\frac{A}{Z} X''')c^2 = m_{N-2}(\frac{A}{Z+2} X')c^2 + Zm_ec^2 - \sum_{i=1}^{Z} B_i,$$  

(11)

where $m_{N-2}(\frac{A}{Z+2} X')c^2$ is the mass of the daughter nucleus, $Zm_e$ represents the total mass of the orbital electrons from the parent atom and $\sum_{i=1}^{Z} B_i$ stands for the total atomic binding energy from the parent atom. Since the mass of the daughter nucleus can be calculated using the mass of the daughter atom in the neutral form using Eq. 3, thus, $m_{N-2}(\frac{A}{Z+2} X')c^2$ can be expressed as:

$$m_{N-2}(\frac{A}{Z+2} X')c^2 = M(\frac{A}{Z+2} X)c^2 - (Z + 2)m_ec^2 + \sum_{i=1}^{Z+2} B_i,$$  

(12)

where $M(\frac{A}{Z+2} X)c^2$ is the mass of the daughter atom in the neutral form, $(Z + 2)m_ec^2$ is the total mass of the orbital electrons surrounding the daughter nucleus, and $\sum_{i=1}^{Z+2} B_i$ represents the total atomic binding energy of the daughter atom in the neutral form. Putting Eq. 12 into Eq. 11 and rearranging the terms, $M(\frac{A}{Z} X''')c^2$ can be expressed as:

$$M(\frac{A}{Z} X''')c^2 = M(\frac{A}{Z+2} X)c^2 - 2m_ec^2 + \sum_{i=1}^{Z+2} B_i - \sum_{i=1}^{Z} B_i.$$  

(13)

Replacing $M(\frac{A}{Z} X''')c^2$ in Eq. 10 using Eq. 13, one obtains the following:

$$Q_{\beta\beta} = M(\frac{A}{Z} X)c^2 - M(\frac{A}{Z} X')c^2 - \left[ \sum_{i=1}^{Z+2} B_i - \sum_{i=1}^{Z} B_i \right].$$  

(14)

Eq. 14 is the decay Q value directly derived from the decay of the ground state of the mother atom in the neutral form to the double-ionized daughter ion as described in Eq. 9. Note that Eq. 14 is exactly the same as Eq. 4, which is the decay Q value derived from the decay of the parent nucleus to the daughter nucleus with the two ejected beta particles in the final state as described in Eq. 1. Since the decay Q value is defined as the mass difference between the initial state and the final state products, the decay Q value is expected to be the same regardless of how it is derived.

From Eq. 7, it is apparent that the decay Q value for $0\nu\beta\beta$ is equal to the mass difference of the neutral atoms in the initial and final states subtracted by the difference of the total atomic electron binding energy between the mother and daughter atoms. This indicates that the calculation of $Q_{\beta\beta}$ must take into account the difference of the total atomic binding energy between the mother and daughter neutral atoms. As long as $Q_{\beta\beta}$ is calculated by using the mass-energy difference between the ground state of mother and daughter neutral atoms, it is required by the energy conservation as shown in Eq. 3 that $Q_{\beta\beta} = \Delta Mc^2 - \Delta E_b$.

To calculate $\Delta E_b$, one must know the total electron binding energy for a given atomic system. Since this quantity cannot be easily measured, a good approximation is given by Lunney, Perrson, and Thibault [14]:

$$B_e(Z) = 14.4381Z^{2.39} + 1.55468 \times 10^{-6}Z^{5.35} \times \text{eV},$$  

(15)

where $B_e(Z)$ represents the total electron binding energy for a given atomic system. Therefore, $\Delta E_b$ can be expressed as:

$$\Delta E_b = B_e(Z + 2) - B_e(Z),$$  

(16)

for any given $0\nu\beta\beta$ decay process. Figures 1, 2, and 3 display the calculated electron binding energy as a function of Z according to Eq. 15 for nine $0\nu\beta\beta$ decay candidates and their corresponding decay daughters. The difference in the total electron binding energy, $\Delta E_b$, is labelled respectively for the nine $0\nu\beta\beta$ decay processes. As can be seen in Figures 1, 2, and 3, the difference in the total electron binding energy, $\Delta E_b$, ranges from a minimum of
tial and the final state atoms in the neutral form. This
is just taken as the mass-energy difference of the ini-
tial state. Therefore, $\Delta E_{\text{b}}$ for $^{48}\text{Ca}\rightarrow^{22}\text{Ti}$, $^{32}\text{Ge}\rightarrow^{34}\text{Se}$, and $^{34}\text{Se}\rightarrow^{36}\text{Kr}$.

![Figure 1](image1.png)

Figure 1. The electron binding energy as a function of atomic number $Z$ and the labelled electron binding energy difference for $^{40}\text{Zr}\rightarrow^{42}\text{Mo}$, $^{42}\text{Mo}\rightarrow^{44}\text{Ru}$, and $^{46}\text{Cd}\rightarrow^{50}\text{Sn}$.

$4.76$ keV for $^{48}\text{Ca}\rightarrow^{22}\text{Ti}$ to a maximum of $21.89$ keV for $^{150}\text{Nd}\rightarrow^{76}\text{Sm}$. This will result in a significant contribution to the calculation of $Q_{\beta\beta}$ for a given $0\nu\beta\beta$ decay process using Eq. 7. Therefore, $\Delta E_{\text{b}}$ cannot be ignored.

The decay Q value used by the current experiments [9–12] is just taken as the mass-energy difference of the initial and the final state atoms in the neutral form. This refers to a decay of the following form:

$$^{Z}\text{X} \rightarrow ^{Z+2}\text{X}',$$

where $^{Z}\text{X}$ and $^{Z+2}\text{X}'$ are the neutral atoms from the initial and the final states. This does not represent $0\nu\beta\beta$ decay, which is expected to have two beta particles present in the final state. Therefore, the decay Q value derived from this decay form, $Q_{\beta\beta} = M(\frac{\Delta}{Z}\text{X})c^2 - M(\frac{Z+2}{Z}\text{X}')c^2$, is not the decay Q value for $0\nu\beta\beta$ decay. From Eq. 7, one obtains the following:

$$\Delta Mc^2 = Q_{\beta\beta} + \Delta E_{\text{b}}.$$  

$\Delta Mc^2$ is the sum of the decay Q value for $0\nu\beta\beta$ decay ($Q_{\beta\beta}$) and the relaxation energy ($\Delta E_{\text{b}}$) of the initial atomic structure after the decay. It is critical to distinguish the decay Q value, which is the available energy for the two ejected beta particles in the final state for $0\nu\beta\beta$ decay, and the relaxation energy of the initial atomic structure. The former is the experimental signature for $0\nu\beta\beta$ decay while the latter is the release of the atomic binding energy difference after the decay. The release of the atomic binding energy difference depends on the relaxation time of the atomic structure after the decay. This relaxation time is not well understood for $0\nu\beta\beta$ decay since it has not been observed yet. The atomic relaxation time in Rydberg blockaded-A atoms through spontaneous decay [17] may shed light on the atomic relaxation time of $0\nu\beta\beta$ decay. In the recent paper written by Qiao et al. [17], the atomic relaxation time is calculated using the atomic number and the decay rate as below:

$$t_{\tau} = \frac{2Z}{\gamma_{\text{rd}}} \sqrt{2\pi Z}(1 - \frac{2}{\sqrt{Z}}),$$

where $t_{\tau}$ is the atomic relaxation time, $\gamma_{\text{rd}}$ is the decay rate. If one uses $Z$ (the atomic number) and $\gamma_{\text{rd}}$ (the decay rate) for $0\nu\beta\beta$ decay, the relaxation time of the atomic orbits can be very long. In particular, the lifetime of the double-ionized daughter ion in the final state can be very long. This is because the thermalized two ejected beta particles cannot be easily captured by the double-ionized daughter ion due to the repulsive Coulomb forces from large numbers of electrons surrounding the daughter nucleus. These repulsive forces provide a stabilizing energy balance between the two thermalized electrons and the positively charged daughter nucleus. An indicator of long-lived ions from $\beta$ decay is a good example of the above theory. The $^{42}\text{K}$ ions, which are from the $\beta$ decay of $^{42}\text{Ar}$, produced uniformly throughout the Ar volume, are transported near the detectors by convective flow in the GERDA detector [9], where ion collection onto the detector surfaces is aided by the stray electric fields from the biased detector surface and any unshielded high voltage components. The observed enhancement of $\gamma$ rays from the $\beta$ decay of $^{42}\text{K}$ ion in the GERDA experiment indicates that the lifetime of $^{42}\text{K}$ ions can be very long. Thus, it is
reasonable to assume that the release of the atomic binding energy after the $0\nu\beta\beta$ decay may not come within the detection time window for the energy deposition from the two ejected beta particles.

Even if the release of the atomic binding after the $0\nu\beta\beta$ decay is within the detection time window of the two ejected beta particles, the full relaxation of the atomic orbital structure is a multistep process, which results in a cascade of atomic radiation. Depending on the atomic number, the electron orbital configuration involved, and electron shells, the energy of emitted X-rays and/or Auger electrons is typically in the range from a few eV to a couple of keV. Such low energy X-rays or Auger electrons have a short range (nm to $\mu$m) to lose all energies. Therefore, the linear energy transfer (LET) is very high. A high LET means that the majority of energy loss is converted into the production of phonons. Depending on the detection technology, there is a chance that the majority of the atomic energy released by atomic radiation may not be detected.

In any case, for calculating $Q_{\beta\beta}$ for $0\nu\beta\beta$ decay, the difference in the total atomic binding energy between the mother and daughter neutral atoms must be taken into account because it is in the level of a few keV to more than 10 keV as also calculated in our earlier publication [13]. This difference in the total atomic binding energy is larger than the detection energy window, which is so called the energy region of interest (ROI), used for several $0\nu\beta\beta$ decay experiments such as GERDA [9], MAJORANA DEMONSTRATOR [10], LEGEND [18], CUORE [12] and CUPID [19]. A narrow energy window can be used by these experiments because they possess excellent energy resolution. A narrow energy window allows these experiments to keep background events especially the $2\nu\beta\beta$ decay events out of the ROI and thus have the potential to discover the $0\nu\beta\beta$ decay process. However, based on the discussions in this work and the previous publication [13], the size of a narrow energy window, which can be used to search for $0\nu\beta\beta$ decay, should be evaluated using the atomic binding energy difference between the mother and daughter atoms in the neutral form. Otherwise, $0\nu\beta\beta$ decay experiments could miss the decay signature because the real decay Q value is out of the ROI, which is determined using $\Delta E^b$, which is different from the current value ($\Delta E^b$) used in the experiments. For example, this difference ($\Delta E^b$) can be as large as 8.97 keV for $0\nu\beta\beta$ decay in $^{76}$Ge, 17.73 keV for $0\nu\beta\beta$ in $^{130}$Te, and 18.74 keV for $0\nu\beta\beta$ in $^{136}$Xe, respectively, as shown in Figures 1, 2, and 3. We emphasize that $\Delta Mc^2$ is not the decay Q value for $0\nu\beta\beta$ decay and is the sum of the decay Q value and the relaxation energy of the total atomic binding energy difference between the mother and daughter atoms in the neutral form. This atomic relaxation after the decay may not come within the detection time window depending on the atomic relaxation time, which is not well understood for $0\nu\beta\beta$ decay since it has not been observed yet. Therefore, it is worth pointing out that the current and planned $0\nu\beta\beta$ decay experiments may need to re-evaluate the ROI, which should be larger than the current ROI, as we suggested in the previous publication [13].

This work was supported in part by NSF OISE 1743790, DE-SC0004768, and a governor’s research center supported by the State of South Dakota. The authors would like to thank Dr. Christina Keller for a careful reading of the manuscript.

[1] A. Atre, T. Han, S. Pascoli, B. Zhang, “The search for heavy Majorana neutrinos,” JHEP 0905:030, 2009, arXiv: 0901.3589.
[2] Y. Fukuda et al. (Super-Kamiokande Collaboration), “Evidence for Oscillation of Atmospheric Neutrinos”, Phys. Rev. Lett. 81 (1998) 1562.
[3] R.N. Mohapatra, G. Senjanovic, ”Neutrino mass and spontaneous parity non-conservation”. Phys. Rev. Lett.
44 (14) (1980) 912–915.
[4] Silvia Pascoli and Jessica Turner, “Matter-antimatter symmetry violated,” Nature 580, 323-324 (2020).
[5] Majorana, Ettore; Maiani, Luciano (2006). "A symmetric theory of electrons and positrons". In Bassani, Giuseppe Franco (ed.). Ettore Majorana Scientific Papers. pp. 201-233. Translated from: Majorana, Ettore (1937). "Teoria simmetrica dell'eletrone e del positrone". Il Nuovo Cimento (in Italian). 14 (4): 171–184. Bibcode:1937NCim...14..171M. doi:10.1007/bf02961314. S2CID 18973190.
[6] Barbieri, Riccardo; Creminelli, Paolo; Strumia, Alessandro; Tetradiis, Nikolaos, "Baryogenesis through leptogenesis". Nuclear Physics B. 575 (1–2)(2000)61–77. arXiv:hep-ph/9911315.
[7] Frank T. Avignone, III, Steven R. Elliott, and Jonathan Engel, "Double beta decay, Majorana neutrinos, and neutrino mass," Rev. Mod. Phys. 80, 481 (2008).
[8] A. Giuliani, A. Poves, "Neutrinoless Double-Beta Decay," Advances in High Energy Physics 2012: 1.
[9] M. Agostini et al. (GERDA Collaboration) “Improved limit on neutrinoless double beta decay of 76Ge from GERDA Phase II,” Phys. Rev. Lett. 120 (2018) 132503.
[10] N. Abgrall et al. (Majorana Collaboration) “The MAJORANA DEMONSTRATOR Neutrinoless Double-Beta Decay Experiment,” Advances in High Energy Physic Volume 2014 (2014), Article ID 365432, 18 pages.
[11] S. Delaquis et al. (EXO Collaboration) “Deep Neutrino Network for Energy and Position Reconstruction in EXO- 200.” 2018 JINST 13 P08023. arXiv:1804.09641.
[12] M. Sisti et al. (CUORE Collaboration) “Status of the CUORE and results from the CUORE-0 neutrinoless double beta decay experiments,” Nuclear and Particle Physics Proceedings 273-275 (2016) 1719 - 1725. arXiv:1502.03653.
[13] D.-M. Mei and W.-Z. Wei, "The implication of the atomic effects in neutrinoless double-beta decay," Modern Physics Letters A. Vol. 37, No. 10 (2022) 2250058.
[14] D. Lunney, J. M. Pearson, C. Thibault, "Recent trends in the determination of nuclear masses," Review of Modern Physics, V 75 (2003) 1021.
[15] S. Gasiorowicz, Quantum Mechanics (Wiley, New York, 1996).
[16] Kenneth S. Krane, Introductory Nuclear Physics, Wiley, New York, 1987) p275.
[17] Chang Qiao et al., "Spontaneous decay induced quantum dynamics in Rydberg blockaded A-type atoms," J. Phys. B 54 (2021)205501.
[18] N. Abfrall et al. (LEGEND Collaboration), "The Large Enriched Germanium Experiment for Neutrinoless Double Beta Decay (LEGEND)", AIP conference proceedings 1894, 020027 (2017). arXiv: 1709.01980.
[19] D. R. Artusa et al., "Enriched TeO₂ bolometers with active particle discrimination: Towards the CUPID experiment”, Phys. Lett. B 767 (2017)321-329.
[20] T. Eronen at al., "JYFLTRAP: A Penning trap for precision mass spectroscopy and isobaric purification”, Eur. Phys. J. A (2012) 48:46.
[21] A. A. Kwiatkowski et al., "New determination of double-β-decay properties in ⁴⁸Ca: high precision Q_{ββ}-value measurement and improved nuclear matrix element calculations", Phys. Rev. C 89 (2014)045502.
[22] Rahaman et al., "Q values of ⁷⁶Ge and ¹⁰⁰Mo double-beta decays,” Physics Letters B 662 (2008) 111-116.
[23] David L. Lincoln et al., “First Direct Double-Beta Decay Q-value Measurement of ³²Se in Support of Understanding the Nature of the Neutrino,” arXiv:1211.5659.
[24] K. Gulyuz et al., "Determination of direct double-β-decay Q value of ⁸⁶Zr and atomic masses of ⁸⁰–⁹²,Zr and ⁹₂–⁹⁶Mo,” Phy. Rev. C 91 (2015)1179712.
[25] A. A. Kwiatkowski et al., "Double-beta decay Q values of ¹¹⁶Cd and ¹⁳⁰Te”, Physics Letters B 703 (2011) 412-416.
[26] Matthew Redshaw et al., "Mass and Double-Beta-Decay Q value of ¹³⁶Xe,” Phys. Rev. Lett. 98 (2007) 053003.
[27] V. S. Kolhinen et al., ”Double-β decay Q value of ¹⁵⁰Nd,” Phys. Rev. C 82 (2010)022501(R).
[28] R. Arnold et al., ”Detailed studies of ¹⁰⁰Mo two-neutrino double beta decay in NEMO-3”, Eur. Phys. J. C (2019) 79:440.