

Terrestrial ^7Be decay rate and ^8B solar neutrino flux

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The decay rate of ^7Be has always been measured by either forming a beryllium compound or implanting ^7Be in a medium. We can quantitatively understand the measured changes of ^7Be decay rates in different environments as well as its L/K orbital electron capture ratio using tight-binding linear muffin-tin orbital method calculations. We find that ^7Be loses a very substantial fraction of its $2s$ electrons in a medium. As a result of this loss of $2s$ electrons, the extracted nuclear matrix element of the ^7Be electron capture reaction from terrestrial decay rate measurements should increase by 2–2.7%, thus decreasing the calculated ^8B solar neutrino flux from the Standard Solar Model by 2–2.7%.

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I. INTRODUCTION

Recently, the Sudbery Neutrino Observatory (SNO) collaboration [1] measured the ^8B solar neutrino flux within about 5% uncertainty using their neutral current detector, making it now very important to improve upon the accuracy of the ^8B solar neutrino calculation from the Standard Solar Model (SSM) [2] for a precise comparison between theory and experiment. Unfortunately, the uncertainty of the calculated ^8B solar neutrino flux from the SSM is still around 20% [3] and comprises numerous uncertainties (each one ranging from 2% to 7%) from various sources in addition to a large uncertainty regarding the composition of the solar atmosphere. Efforts are ongoing [4] to reduce the uncertainties from different sources and to estimate carefully all uncertainties at a few-percent level.

The nuclear matrix element of the ^7Be electron capture process ($^7\text{Be} + e^- \rightarrow ^7\text{Li} + \nu_e$) is required to calculate the electron capture rate of ^7Be in the solar core using the SSM [5]. This nuclear matrix element was extracted from terrestrial ^7Be decay rate measurements assuming that ^7Be retained both its $2s$ electrons [6]. However, in all terrestrial measurements, the decay rate of ^7Be has always been measured by either forming a beryllium compound or implanting ^7Be in a medium. In such situations, beryllium should lose a substantial fraction of its valence $2s$ electrons, thus reducing the electron density at the nucleus. In this paper, we discuss the correction that should be incorporated in the extraction of the nuclear matrix element of the ^7Be electron capture process because of the loss of $2s$ electrons of ^7Be when it forms a compound or is implanted in a medium.

Usually the valence electrons of an atom can be affected by the surrounding environment and the overlap of electronic wave functions at the nucleus becomes progressively smaller for outer shell electrons. So only for low- Z elements can valence electrons have a measurable overlap at the atomic nucleus. Hence, Segrè and Daudel [7] pointed out that the decay rate of low- Z elements undergoing electron capture decay would be most susceptible to changes of the surrounding environment. Since ^7Be is the lightest radioactive nucleus that decays by electron capture, it was considered the most suitable candidate for studying the change of decay rate in

different environments. The change of decay rate of ^7Be in different beryllium compounds was measured [8] and a maximum change of up to 0.2% was observed. However, relatively large changes [9–13] in the decay rate of ^7Be were observed recently for ^7Be nuclei implanted in different media. All these results can be qualitatively understood in terms of the electron affinities of neighboring host atoms. A beryllium atom forming a compound with an element of high electron affinity or implanted in a medium having high electron affinity generally loses a larger fraction of its $2s$ electrons compared to a beryllium atom interacting with an element of low electron affinity. The loss of $2s$ electrons of ^7Be should also depend on the average distance between the implanted ^7Be and neighboring host atoms. Consequently, the dimensions and structure of the host lattice should also be considered to determine the loss of $2s$ electrons of ^7Be implanted in the host medium. As ^7Be loses more $2s$ electrons, the overlap of the $2s$ electronic wave function at the nucleus is reduced and hence the electron capture rate would be lower. So we expect that the half-life of ^7Be in a high-electron-affinity medium would be longer compared to that of ^7Be in a low-electron-affinity medium.

II. QUALITATIVE DISCUSSION

Let us first discuss whether the available data on ^7Be decay rates in different environments (for both compounds and implantations) can be qualitatively understood in terms of the electron affinities. Table I lists the differences among the decay rates of ^7Be implanted in gold and other media as well as the corresponding electron affinities of the host media. The electron affinity of beryllium is zero to slightly negative and so there is no bound state of an extra electron to the ground state of a beryllium atom. A beryllium atom implanted in a high-electron-affinity medium such as Au should lose a significant fraction of its valence $2s$ electrons. Since the loss of $2s$ electrons would reduce the electron density at the nucleus, the electron capture rate of ^7Be in a high-electron-affinity medium such as Au is expected to be lower. In contrast, ^7Be implanted in a low-electron-affinity medium such as Al should lose a comparatively smaller fraction of its $2s$ electrons and

TABLE I. ^7Be decay rate difference and electron affinity.

Decay rate difference	Electron affinity (eV) [29]		Observed change in decay rate ($\Delta\lambda/\lambda$)	Reference
	First medium	Second medium		
(a) Between ^7Be implanted in				
Al and Au	0.441	2.308	$(0.27 \pm 0.15)\%$	[9,10]
Ta and Au	0.322	2.308	$(0.22 \pm 0.13)\%$	[10]
C (graphite) and Au	1.25	2.308	$(0.38 \pm 0.09)\%$	[10]
LiF and Au	—	2.308	$(0.36 \pm 0.15)\%$	[10,11]
Al_2O_3 and Au	—	2.308	$(0.72 \pm 0.07)\%$	[12]
C (graphite) and Ta	1.25	0.322	$(0.17 \pm 0.11)\%$	[10]
Natural Be and Au	~ 0	2.308	$(0.02 \pm 0.06)\%$	[10,13]
(b) Between ^7Be compounds				
^7BeO and $^7\text{BeF}_2$	Electron affinity	Electron affinity	$(0.1375 \pm 0.0053)\%$	[14]
	of O is 1.46	of F is 3.40	$(0.0609 \pm 0.0053)\%$	[15]
			$(0.1130 \pm 0.0058)\%$	[16]

so the electron capture rate would be relatively higher. The electron affinities of compounds are not known very well and are usually considered as the average of the electron affinities of the constituent elements. Hence the electron affinities of Al_2O_3 and LiF are expected to be substantially lower than that of gold. In Table I, we find consistently that the measured decay rate of ^7Be is lower in Au compared to that in other media with lower electron affinities. These observations support our qualitative understanding of the ^7Be decay rate change in different media according to the electron affinities of the host media.

However, the lattice structure and dimensions of the host lattice also affect the decay rate of ^7Be . If the dimensions of the host lattice are small, host atoms would sit very close to the implanted ^7Be atoms and thus the nearby host atoms would take away a relatively larger fraction of $2s$ electrons from implanted ^7Be even if the electron affinity of the host atom is small. It is observed that the decay rate of ^7Be in Ta is comparable to that of ^7Be in graphite, although the electron affinity of Ta (0.322 eV) is much lower compared to that of graphite (1.25 eV). This result can be understood on the basis of the lattice structure and dimensions of the host lattices. The lattice structures and dimensions of Au, Al, Ta, graphite, LiF, Al_2O_3 , and natural Be have been obtained from the *CRC Handbook* [29]. We find that tantalum has a small body-centered lattice structure with lattice parameter 3.51 Å, whereas the lattice structure of graphite is hexagonal with lattice parameters $a = 2.46$ Å and $c = 6.709$ Å. Then, the average distance between an implanted ^7Be atom and nearby tantalum host atoms is 1.76 Å, whereas for a graphite lattice, the corresponding distance is 2.04 Å. So, because of the shorter average distance between an implanted ^7Be atom and nearby host atoms, ^7Be in tantalum loses more $2s$ electrons and the observed decay rate of ^7Be in tantalum would be less than expected on the basis of electron affinity only. Similarly, natural beryllium has a hexagonal lattice structure with smaller lattice parameters $a = 2.29$ Å and $c = 3.58$ Å compared to the lattice parameter (4.08 Å) of a face-centered cubic gold lattice. In the case of implantation of ^7Be in natural beryllium, the average distance between an implanted ^7Be atom and

nearby beryllium host atoms is 1.6 Å, whereas in the case of implantation in gold, the corresponding average distance is 2.04 Å. Hence the decay rates of ^7Be implanted in gold and natural beryllium are comparable even though the electron affinity of gold is much higher than that of beryllium. Thus, qualitatively, we may say that a combination of electron affinity and lattice geometry of the host medium determines the change in decay rate of ^7Be nuclei in different media.

The observed change in decay rate of ^7Be forming compounds such as $^7\text{BeF}_2$ and ^7BeO can also be understood on the basis of electron affinity of the elements forming the compounds. The difference of decay rates of ^7Be in $^7\text{BeF}_2$ and ^7BeO compounds were measured earlier [14–16]. It was found that the decay rate of ^7Be in $^7\text{BeF}_2$ was lower than that of ^7Be in ^7BeO by about 0.1%. Since fluorine has a higher electron affinity (3.4 eV) than oxygen (1.46 eV) and the dimensions of BeF_2 and BeO lattices are similar, ^7Be should lose more $2s$ electrons in the BeF_2 compound. Hence the decay rate of ^7Be should be lower in a fluoride compound compared to that in an oxide compound. However, significant variations in the measured half-life difference of ^7Be in $^7\text{BeF}_2$ and ^7BeO were observed, as shown in Table I. Since the lattice structures of the beryllium fluoride and oxide compounds produced by different groups [14–16] are not known, we speculate that the observed variations in the measurements are possibly due to the differences in lattice structures of the compounds produced by different groups.

Thus the change of decay rates of ^7Be in different media can be qualitatively understood in terms of electron affinities and lattice geometries of the host media. We discuss in the following a quantitative framework on the basis of tight-binding linear muffin-tin orbital method (cd workTB-LMTO) calculations [17] to estimate the loss of $2s$ electrons of ^7Be implanted in a medium or forming a beryllium compound.

III. THEORETICAL FRAMEWORK

The TB-LMTO method calculation [17] is a first-principles electronic structure calculation using density functional

technique. Following density functional technique, the total energy (electronic plus ionic) of an electron-nucleus system is expressed as a functional of the electron density:

$$E[\rho(r), \{R\}] = E_{\text{el}}[\rho(r), \{R\}] + E_{\text{ion}}[\{R, R'\}] \quad (1)$$

$$= T_s[\rho] + E_{\text{xc}}[\rho] + E_{\text{ES}}[\rho, \{R\}], \quad (2)$$

where $T_s[\rho]$ is the kinetic energy (KE) of the noninteracting electron gas of the same density as that of the actual interacting system; $E_{\text{xc}}[\rho]$ is the exchange-correlation energy, which depends on the relative orientation of the spins of the electrons; and $E_{\text{ES}}[\rho]$ is the total electrostatic energy including energies due to the classical electron-electron Coulomb potential, external potential, and ion-ion Madelung potential. Since the energy functional assumes its minimum value for true ground-state density, the first-order variation in energy density $E[\rho]$ should be zero for the ground state (i.e., $\frac{\delta E[\rho]}{\delta \rho} = 0$). Then, applying the variational principle, one arrives at an Euler equation whose solution yields the Kohn-Sham (KS) equation

$$\{-\nabla^2 + V_{\text{eff}}(r)[\rho]\}\Psi_i(r) = \varepsilon_i \Psi_i(r), \quad (3)$$

where $V_{\text{eff}}(r)[\rho]$ is the effective potential and $\Psi_i(r)$ and ε_i are the wave function and energy, respectively, of the i th electron. The KS equation represents a mapping of the interacting many-electron system onto a system of noninteracting electrons moving in an effective potential resulting from all other electrons and ions. Initially the charge density is assumed to be spherically symmetric around each atomic center and $V_{\text{eff}}(r)[\rho]$ is computed. Then the KS equation is solved self-consistently by minimizing the total energy $E[\rho(r)]$. A periodic boundary condition has been assumed in our calculation. To solve the KS equation the muffin-tin orbital states are used as basis states and are obtained by solving the Schrödinger equation with the muffin-tin potential, which is a superposition of spherically symmetric potentials, truncated outside space-filling atomic spheres.

In the muffin-tin approximation, a sphere called a muffin-tin sphere is inscribed around each atomic nucleus and the potential is assumed to be of the muffin-tin type and written as

$$V_{\text{MT}}(r) = V_i(r_i) + \sum_R V_R(r_R) \equiv V_o + \sum_R v_R(r_R), \quad (4)$$

where $V_R(r_R)$ and $v_R(r_R) - V_o$ are spherically symmetric inside a sphere s_R centered at R . $V_i(r_i)$ takes a constant value V_o (the muffin-tin zero) in the interstitial region and vanishes outside. The Schrödinger equation is solved using the above-mentioned muffin-tin potential. Finally, approximately energy-independent basis states are obtained by using the atomic sphere approximation [18], screening transformation [19], and energy linearization [20].

Let Ψ_{total} be the complete electronic wave function and $\Psi_{\text{Be}2s}$ be the beryllium $2s$ state wave function. Then the square of the overlap of Ψ_{total} with $\Psi_{\text{Be}2s}$ (i.e., $|\langle \Psi_{\text{total}} | \Psi_{\text{Be}2s} \rangle|^2$) represents the average number of $2s$ electrons in a beryllium atom when it is in a medium. All relevant atomic physics calculations have been done by solving the relativistic Dirac equation assuming a point nucleus. In our calculation we placed beryllium at different empty sites available in a host

lattice and calculated the average number of $2s$ electrons of beryllium in that medium using the TB-LMTO method.

IV. APPLICATION

The TB-LMTO code [21] of O. Jepsen and O. K. Andersen was used to calculate the number of $2s$ electrons of ^7Be implanted in different media and forming different compounds. Let us consider the case when ^7Be is implanted in Au. The required inputs to the code are the space group number of the host lattice, dimensions of the lattice, atomic numbers and positions of the constituent host atoms in the lattice, and the electronic structure of each of these atoms. Since Au is a face-centered cubic lattice, an implanted beryllium atom can occupy its empty octahedral or tetrahedral site. Calculations were performed by placing a beryllium atom at an octahedral or a tetrahedral site with a periodic boundary condition. To obtain close packing, empty spheres were placed at interstitial sites of the gold lattice. The overlaps between a beryllium atom and the nearest host atomic sphere are 15% and 16% when beryllium occupies octahedral and tetrahedral sites of gold lattice, respectively. Since this overlap parameter is used as a perturbation term in TB-LMTO calculations, it is not usually taken to be larger than 16%. From physical considerations also, Coulomb repulsion between electronic shells prevents the atoms from coming too close to each other. The total energy convergence limit was set at 10^{-4} Ry for these calculations. The average number of $2s$ electrons ($|\langle \Psi_{\text{total}} | \Psi_{\text{Be}2s} \rangle|^2$) was found to be 0.54 and 0.36 for ^7Be occupying octahedral and tetrahedral positions of gold lattice, respectively. We expect that, as a result of random implantations, the number of ^7Be atoms occupying tetrahedral sites would be twice that occupying octahedral sites, because the number of tetrahedral sites are twice that of octahedral sites in a face-centered cubic lattice. Hence, taking a weighted average, we found ^7Be would have 0.42 electrons in its $2s$ orbital when implanted in Au. There is no free parameter in these calculations except the input radius parameter of the implanted beryllium atom, which is taken to be 1.1 Å. The calculated charge of the implanted beryllium atom does not change by more than 2% by varying the initial input radius parameter up to 20%.

Because the aluminum lattice also has a face-centered cubic structure with lattice parameter 4.05 Å, ^7Be implanted in aluminum would also occupy octahedral and tetrahedral sites. Similar self-consistent TB-LMTO calculations were performed for ^7Be implanted at octahedral and tetrahedral sites of the aluminum lattice. We obtained 0.63 for the average number of $2s$ electrons of ^7Be implanted in aluminum. Hence according to TB-LMTO calculations, beryllium implanted in gold would lose more electrons from its $2s$ orbital compared to that implanted in aluminum, in agreement with our earlier qualitative discussion based on electron affinity.

We also performed TB-LMTO calculations for ^7Be implanted in tantalum, lithium fluoride, natural beryllium, graphite, and aluminum oxide. Tantalum has a small body-centered lattice structure with lattice parameter 3.51 Å. We found only one available interstitial site at the face-center position of this lattice. According to our calculations, there would be

0.60 electrons in the $2s$ shell of beryllium occupying this interstitial site of the tantalum lattice.

The lithium fluoride lattice comprises two cubic lattices of lithium and fluorine displaced by one-quarter of a body diagonal with respect to each other. In this case, an implanted ^7Be atom can occupy any of the three equivalent interstitial sites. TB-LMTO calculations were performed (taking the lattice parameter of the LiF lattice to equal 4.1 \AA) and the average number of electrons in the $2s$ orbital of ^7Be occupying any of the available interstitial sites was found to be 0.73.

The lattice structure of natural beryllium (^9Be) is hexagonal close-packed with lattice parameters $a = 2.2866 \text{ \AA}$ and $c = 3.5833 \text{ \AA}$. Four interstitial sites were found, and an implanted ^7Be atom can go to any of these sites. TB-LMTO calculations were performed by placing a ^7Be atom at each of these interstitial sites. Assuming that an implanted ^7Be can occupy any of these interstitial sites with equal probability, we determined that the average number of $2s$ electrons of an implanted ^7Be atom in natural beryllium is 0.39.

Crystalline graphite consists of hexagonal sheets of carbon atoms separated by 3.35 \AA . The lattice parameters are $a = 2.46 \text{ \AA}$ and $c = 6.709 \text{ \AA}$. An implanted ^7Be atom can occupy any of the interstitial sites between the sheets of carbon atoms. Four interstitial sites were found, and TB-LMTO calculations were performed by placing a ^7Be atom at each of these sites one by one. Assuming equal probability of occupying any of these sites during implantation, we determined that the average number of $2s$ electrons of implanted ^7Be atom in graphite is equal to 0.68.

Aluminum oxide has a complicated corundum structure with lattice parameters $a = 4.758 \text{ \AA}$ and $c = 12.99 \text{ \AA}$. The space group number and the position coordinates of constituent atoms of Al_2O_3 are known from the literature [22,29] and were used in our calculations. We determined from our TB-LMTO calculations that the average number of $2s$ electrons of ^7Be implanted in Al_2O_3 was 0.79.

We also performed similar TB-LMTO calculations for several ^7Be compounds to determine the average number of $2s$ electrons of ^7Be forming those compounds. However, the lattice structures of these beryllium compounds are complicated and in most cases a compound can have several possible structures depending on the method of preparation. We have done calculations for two relatively simple beryllium compounds— ^7BeO and $^7\text{BeF}_2$. Johlige *et al.* [16] measured the

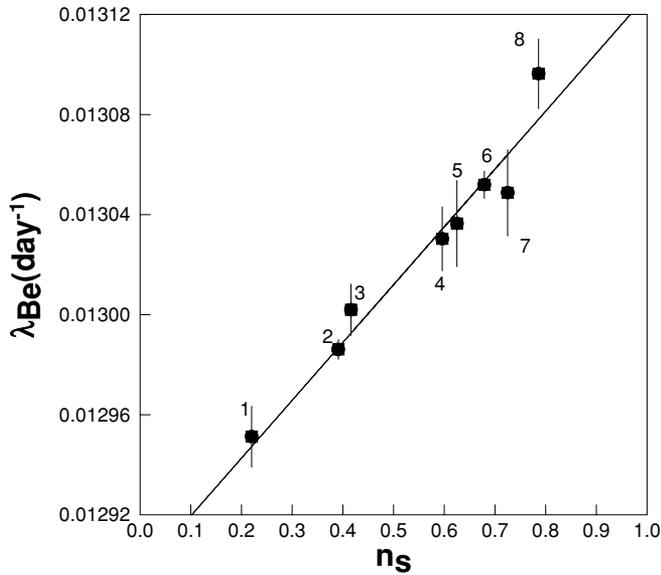
change of decay rate of ^7Be in ^7BeO and $^7\text{BeF}_2$ compounds. They [16] used beryllium oxide having a wurtzite structure in which a beryllium was surrounded by four oxygen atoms at a distance of 1.64 \AA . A beryllium oxide crystal having a wurtzite structure has lattice parameters $a = 2.698 \text{ \AA}$ and $c = 4.380 \text{ \AA}$ and partial coordinates of beryllium and oxygen in the lattice are $(1/3, 2/3, 1/2)$ and $(1/3, 2/3, u+1/2)$ with $u = 0.378$, respectively [22]. The lattice structure, dimension, positions of constituent atoms, and space group of beryllium oxide were given as inputs to the TB-LMTO calculations. We found from our calculations that the average number of $2s$ electrons of ^7Be in ^7BeO was 0.26.

The structure of $^7\text{BeF}_2$ produced by Johlige *et al.* [16] had ^7Be atoms surrounded tetrahedrally by four fluorine atoms at a distance of 1.60 \AA . The BeF_2 lattice has a hexagonal structure with lattice parameters $a = 4.72 \text{ \AA}$ and $c = 5.18 \text{ \AA}$ [15]. Its lattice structure is almost identical to that of SiO_2 [22]. In this structure, three inequivalent beryllium atoms are positioned at $(u, u, 1/3)$, $(u, 0, 0)$, and $(0, u, 2/3)$. However, parameter u is not known for BeF_2 . Since the lattice structures of SiO_2 and BeF_2 are almost identical and the value of the u parameter for SiO_2 , is known and equal to 0.465, the same value of the u parameter was taken for the BeF_2 lattice calculation also. We found from our TB-LMTO calculations that the average number of $2s$ electrons of ^7Be in BeF_2 was 0.19.

Table II lists the calculated average number (n_s) of $2s$ electrons of ^7Be implanted in different media and forming different compounds as well as their corresponding measured half-lives. In the first row, we show the calculated average number of $2s$ electrons of ^7Be in BeF_2 , BeO , and $\text{Be}(\text{C}_5\text{H}_5)_2$ compounds and the corresponding decay rate as measured by Johlige *et al.* [16]. TB-LMTO calculations were actually done only for ^7BeO and $^7\text{BeF}_2$ compounds. Using the result of our ^7BeO calculation and Johlige *et al.*'s [16] measurement that the decay rate of ^7Be in BeO decays was greater than that of ^7Be in $\text{Be}(\text{C}_5\text{H}_5)_2$ by $(0.079 \pm 0.0074)\%$ along with Hartree and Hartree's result [12,23] regarding the contribution of $2s$ electrons of ^7Be to the total decay rate, we found that ^7Be in a $^7\text{Be}(\text{C}_5\text{H}_5)_2$ compound would have 0.21 electrons in its $2s$ orbital. Then the average number (n_s) of $2s$ electrons of ^7Be in $^7\text{BeF}_2$, ^7BeO , and $^7\text{Be}(\text{C}_5\text{H}_5)_2$ is 0.22. In the third and fourth columns of the last row of Table II, we show the calculated number of $2s$ electrons of ^7Be in Al_2O_3 , and the decay rate of ^7Be in Al_2O_3 , respectively. The absolute value $(52.927 \pm$

TABLE II. Half-lives of ^7Be and average number of $2s$ electrons of ^7Be in different media.

Serial number	Medium	Calculated average number of $2s$ electrons of ^7Be (n_s)	Measured ^7Be half-life ($\tau_{1/2}$) in days	Reference
1.	Average of BeO , BeF_2 , and $\text{Be}(\text{C}_5\text{H}_5)_2$	0.22	53.520 ± 0.050	[16]
2.	^7Be in natural beryllium	0.39	53.376 ± 0.016	[13]
3.	^7Be in Au	0.42	53.311 ± 0.042	[10]
4.	^7Be in Ta	0.60	53.195 ± 0.052	[10]
5.	^7Be in Al	0.63	53.170 ± 0.070	[9]
6.	^7Be in graphite	0.68	53.107 ± 0.022	[10]
7.	^7Be in LiF	0.73	53.120 ± 0.070	[11]
8.	^7Be in Al_2O_3	0.79	52.927 ± 0.056	[12]


 FIG. 1. Decay rate versus number of $2s$ electrons of ${}^7\text{Be}$.

0.056 days) of the decay rate of ${}^7\text{Be}$ in Al_2O_3 was determined by using the absolute value of the decay rate of ${}^7\text{Be}$ in Au $[(53.311 \pm 0.042)\text{days}]$ as measured by Norman *et al.* [10] and the measured difference of decay rates $(0.72 \pm 0.07)\%$ [12] between the decay rate of ${}^7\text{Be}$ in Au and Al_2O_3 .

In Fig. 1, the decay rate of ${}^7\text{Be}$ ($\lambda_{\text{Be}} = \frac{\ln 2}{\tau_{1/2}}$) in a medium has been plotted against the number (n_s) of $2s$ electrons of ${}^7\text{Be}$ in the corresponding medium, as calculated by the TB-LMTO code. As shown in Fig. 1, a number has been assigned to each point in the plot corresponding to the serial number of the medium as given in Table II. A good linear fit has been obtained, confirming the expected approximate direct proportionality between the decay rate of ${}^7\text{Be}$ and the number of $2s$ electrons of ${}^7\text{Be}$ in that medium. We find from

the extrapolation of the fitted straight line that the decay rate (λ_{Be}) of a neutral and free ${}^7\text{Be}$ having two full $2s$ electrons ($n_s = 2$) is $0.0133585 \text{ days}^{-1}$ and that of a ${}^7\text{Be}^{++}$ ion with no $2s$ electron ($n_s = 0$) is $0.0128964 \text{ days}^{-1}$. So the difference in decay rates of a neutral ${}^7\text{Be}$ atom and ${}^7\text{Be}^{++}$ ion is 3.4% , in good agreement with the calculations of Hartree and Hartree [23]. Using the linear relationship of Fig. 1, we show in Table III the measured and calculated decay rate changes of ${}^7\text{Be}$ in different environments. Reasonable agreement between calculated and measured values has been obtained. We find from the extrapolation of the straight line shown in Fig. 1 that the decay rate of a neutral ${}^7\text{Be}$ atom should be greater than that of a ${}^7\text{Be}$ implanted in a medium or forming a compound by between 2% and 2.7% depending on the medium. In this analysis, we have not considered the effect of exchange and overlap corrections, because their effect on the total decay rate of ${}^7\text{Be}$ is less than 0.1% [24].

Although Fig. 1 shows the expected linear relationship between the number of $2s$ electrons (n_s) and the decay rate (λ_{Be}) of ${}^7\text{Be}$, this does not mean that the absolute values of calculated n_s are correct. For example, if all the calculated values of n_s are increased by the same amount (say by 1.0), then we would also get a linear relationship between n_s and λ_{Be} and the slope of the fitted straight line would be the same as before, thus agreeing with Hartree's result [23]. However, in such a situation, the difference between the decay rate of a neutral ${}^7\text{Be}$ and that of an implanted ${}^7\text{Be}$ (in a medium) would be much smaller than 2% . So the absolute value of calculated n_s should be checked by an independent method.

Recently, the L/K electron capture ratio of ${}^7\text{Be}$ in mercury telluride (HgTe) was measured [25]. The measured ratio (0.040 ± 0.006) was found to be less than half of the expected theoretical value (0.09) [26]. This discrepancy can be understood by TB-LMTO calculations [27]. According to TB-LMTO calculations [27], the number of $2s$ electrons of ${}^7\text{Be}$ in HgTe was found to be 1.15. So in the zeroth order, the L-electron capture rate should be reduced by the factor

 TABLE III. Comparison between experimental and calculated values of decay rate difference of ${}^7\text{Be}$.

Decay rate difference	Percentage increase in decay rate of ${}^7\text{Be}$ in first medium compared to that in second medium	
	Experimental value	Calculated value
(a) Between ${}^7\text{Be}$ implanted in		
Al and Au	$(0.27 \pm 0.15)\%$	0.40 %
Ta and Au	$(0.22 \pm 0.13)\%$	0.31%
C (graphite) and Au	$(0.38 \pm 0.09)\%$	0.44 %
LiF and Au	$(0.36 \pm 0.15)\%$	0.53%
Al_2O_3 and Au	$(0.72 \pm 0.07)\%$	0.63%
C (graphite) and Ta	$(0.17 \pm 0.11)\%$	0.14%
Au and ${}^9\text{Be}$	$(0.02 \pm 0.06)\%$	0.02%
(b) Between ${}^7\text{Be}$ compounds		
${}^7\text{BeF}_2$ and ${}^7\text{BeO}$	$(0.1375 \pm 0.0053)\%$	0.12%
	$(0.0609 \pm 0.0053)\%$	
	$(0.1130 \pm 0.0058)\%$	

$1.15/2.0 = 0.576$. Since K electrons essentially remain unaffected by the environment, the theoretical L/K electron capture ratio should be reduced by a factor of 0.576, which would be 0.0518, in reasonable agreement with the experimental result [25]. So the agreement with the measured L/K electron capture ratio of ${}^7\text{Be}$ in a medium (HgTe) provides an independent check on the absolute value of the calculated number (n_s) of 2s electrons of ${}^7\text{Be}$. Hence ${}^7\text{Be}$ indeed loses a considerable fraction of its 2s electrons in a medium and the loss of electrons can be quantitatively estimated using the TB-LMTO code. Therefore, the assumptions made in our calculations seem to be well justified and our results can be considered quite robust.

Instead of determining the average number of valence 2s electrons of ${}^7\text{Be}$, one can, in principle, also extract the total electron density at the ${}^7\text{Be}$ nucleus directly from the TB-LMTO code and plot it against the measured decay rate of ${}^7\text{Be}$ in different media. However, the measured electron capture rate of ${}^7\text{Be}$ in different media varies from about 0.1% to 1% and so there will be similar very small changes of the total electron density at the ${}^7\text{Be}$ nucleus. Hence, a reasonable comparison with the measured changes of the electron capture rate of ${}^7\text{Be}$ in different media requires that the electronic wave function at the ${}^7\text{Be}$ nucleus be known to better than a few tenths of a percent accuracy. The TB-LMTO code calculates energy very accurately, but it is probably very difficult to determine the electronic wave function with such a high accuracy. However, the number of valence 2s electrons of ${}^7\text{Be}$ changes appreciably (about 10% to over 30%) as ${}^7\text{Be}$ is put in different chemical environments. The uncertainty in the calculated number of 2s electrons of ${}^7\text{Be}$ is not more than a few percent. It is already known [6] that the removal of 2s electrons of a beryllium atom does not essentially affect the wave function of 1s electrons at the nucleus. Hence there should be a linear relationship between the electron capture rate of ${}^7\text{Be}$ in different media and the corresponding number of valence 2s electrons of ${}^7\text{Be}$ as shown in Fig. 1.

V. DISCUSSION AND IMPLICATION ON SOLAR NEUTRINO RESULT

Our observations regarding the substantial loss of 2s electrons of ${}^7\text{Be}$ in a medium and corresponding significant change (2–2.7%) of decay rate with respect to that of a neutral ${}^7\text{Be}$ imply reduction of the calculated ${}^8\text{B}$ solar neutrino flux from the SSM [2]. Bahcall [6] deduced the electron capture rate (λ_{star}) of ${}^7\text{Be}$ from continuum orbits under typical stellar conditions and obtained the following relation:

$$\frac{\lambda_{\text{star}}}{\lambda_{\text{lab}}} = A^{-1} \left(\frac{2}{\pi k T} \right)^{1/2} \alpha Z n_e, \quad (5)$$

where λ_{lab} is the ${}^7\text{Be}$ decay rate measured in a terrestrial experiment, $A = |\Psi_{1s}(r=0)|^2 + |\Psi_{2s}(r=0)|^2$ is the atomic overlap factor for the terrestrial decay, k is the Boltzmann constant, T is the solar core temperature, α is the fine structure constant, Z is the atomic number of ${}^7\text{Be}$, and n_e is the continuum electron density. To calculate the decay rate of ${}^7\text{Be}$

at the solar core, Bahcall initially took Segrè and Wiegand, [28] and Kraushaar *et al.*'s [15] measured decay rate (λ_{lab}) of ${}^7\text{Be}$ in a natural beryllium environment and computed the overlap factor A , assuming ${}^7\text{Be}$ in natural beryllium retained both its 2s electrons. However, we have already seen from Fig. 1 and TB-LMTO calculations that ${}^7\text{Be}$ implanted in a medium or forming a compound loses a substantial fraction of its 2s electrons and, as a result, its decay rate is slowed down. Hence, the atomic overlap factor A should be corrected for the loss of 2s electrons and the correction will clearly depend on the medium where the ${}^7\text{Be}$ decay rate was measured. Since the atomic overlap factor A is inversely proportional to λ_{star} , the decay rate of ${}^7\text{Be}$ in the solar core would increase as a result of this correction. The magnitude of the correction would be the same as the percentage change in the decay rate of ${}^7\text{Be}$ in a medium with respect to that of a free and neutral ${}^7\text{Be}$ atom.

By considering the dynamic equilibrium condition in the solar interior, the ${}^8\text{B}$ solar neutrino flux [$\phi({}^8\text{B})$] is proportional to [5]

$$\phi({}^8\text{B}) \propto \frac{R_p}{R_e + R_p}, \quad (6)$$

where R_e and R_p are the electron capture rate and proton capture rate of ${}^7\text{Be}$ at the center of sun, respectively. Because $R_p \approx 10^{-3} R_e$, approximately

$$\phi({}^8\text{B}) \propto \frac{1}{R_e}. \quad (7)$$

Since the decay rate of ${}^7\text{Be}$ at the solar core (R_e) should increase by 2–2.7% owing to the decrease of the atomic overlap factor A by the same percentage because of the loss of 2s electrons of ${}^7\text{Be}$ in a medium, the ${}^8\text{B}$ solar neutrino flux $\phi({}^8\text{B})$ should also decrease by the same amount owing to the inverse relationship with R_e as shown in Eq. (7). This result is important because the calculation of the ${}^8\text{B}$ solar neutrino flux would need to be refined in the future for a high-precision comparison with the measured flux [1].

It would be interesting to measure a few more cases of large differences of decay rates of ${}^7\text{Be}$ in different media. For example, the decay rate of ${}^7\text{Be}$ in HgTe is expected to be 1.2% higher than that of ${}^7\text{Be}$ in Au and this should be checked experimentally. It would also be interesting to do a few more measurements of L/K electron capture ratios of ${}^7\text{Be}$ in different media such as gold or aluminum. It is expected that the L/K electron capture ratio of ${}^7\text{Be}$ in Au would be much lower ($L/K = 0.0187$) [27] and such measurements would further check our calculations.

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