New calculations for phase space factors involved in double-β decay

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(Received 1 July 2013; published 30 September 2013)

We present new results for the phase space factors involved in double-β decay for $\beta^-\beta^-$ transitions to ground states and excited 0_1^+ states for isotopes of experimental interest. The Coulomb distortion of the electron wave functions is treated by solving numerically the Dirac equation with inclusion of the finite nuclear size and electron screening effects and using a Coulomb potential derived from a realistic proton density distribution in the daughter nucleus. Our results are compared with other results from literature, obtained in different approximations, and possible causes that can result in differences are discussed.

DOI: 10.1103/PhysRevC.88.037303 PACS number(s): 23.40.Bw, 21.60.Cs, 14.60.Pq

Introduction. Within the standard model (SM) double-β decay (DBD) can occur through several decay modes, but the only measured one at present is that with the emission of two electrons and two antineutrinos ($2\nu\beta^-\beta^-$) and which conserves the lepton number. However, theories beyond the SM allow this process to occur without emission of neutrinos as well, and this possibility makes DBD a nuclear process of major interest for testing the lepton number conservation (LNC) and for understanding neutrino properties. There are recent excellent reviews, containing also a comprehensive list of references [1–5], where the reader can find complete information on this subject. The DBD lifetimes can be factorized, in a good approximation, as follows:

$$\left(T_{1/2}^{2\nu}\right)^{-1} = G^{2\nu}(E_0, Z)|M^{2\nu}|^2, \quad (1)$$

$$\left(T_{1/2}^{0\nu}\right)^{-1} = G^{0\nu}(E_0, Z)|M^{0\nu}|^2 \left(\langle \eta_l \rangle\right)^2, \quad (2)$$

where $\langle \eta_l \rangle$ is a beyond SM parameter containing information about the properties of the virtual particles involved in the decay within a specific mechanism, $M^{(2\nu,0\nu)}$ are the nuclear matrix elements (NMEs), and $G^{(2\nu,0\nu)}$ are phase space factors (PSFs) for the corresponding decay modes (see, e.g., Ref. [5]). As seen, they are key quantities for estimating the lifetimes and/or for deriving the $\langle \eta_l \rangle$ parameter, so it is very important to calculate them precisely. So far much effort has been put into the accurate calculation of the NMEs. Several methods have been developed for that, the most used being quasi random phase approximation (QRPA)-based method [6–12], the shell-model-based method [13–17], interaction boson approximation (IBA)-2 [18], the energy- density-functional Method [19], and projected Hartree Fock Bogoliubov (PHFB) [20]. The NMEs have been calculated for all the transitions, decay modes, and isotopes of interest, and the uncertainties in their estimation have been largely discussed over time in the literature. The PSFs have been calculated for a long time [21–27] but they have been less discussed, being considered to be computed with enough precision. Recently, they were recalculated within an improved approach by using exact electron Dirac wave functions, taking into account the finite nuclear size and the electron screening effects [28]. The authors found differences between their results and those calculated previously with approximative electron wave functions, especially for heavier nuclei. However, besides the NMEs, it is very important to have values of the PSFs precisely calculated as well, both to improve the DBD lifetime predictions and to extract nuclear model parameters. One example is the extraction of the g_{pp} parameter in the QRPA calculations of the NMEs involved in DBD. In this work we report new results for the PSFs involved in 2ν- and 0ν-$\beta^-\beta^-$ decay modes for transitions to the ground states (g.s.) and excited 0_1^+ states. We developed routines for computing the relativistic (Dirac) electron wave functions, taking into account the nuclear finite size and screening effects. In addition to the previous calculations, we use a Coulomb potential derived from a realistic proton density distribution in the daughter nucleus. We compare our results with other results from the literature, obtained in different approximations, and discuss the causes that result in differences between different calculations.

Formalism. The PSFs have been calculated first in Refs. [21, 22] by using a nonrelativistic approach. The distortion of the wave function by the Coulomb field of the daughter nucleus was considered through Fermi (Coulomb) factors obtained by taking the square of the ratio of the Schrödinger scattering solution for a point charge Z to a plane wave, evaluated at the origin. The use of such a simple expression for the Fermi factors allows us to get analytical formula for the PSFs. In a better approximation, the Fermi factor is defined as the square of the ratio of the values of the Dirac s wave function of the electron at the nuclear surface $R_A = 1.2A^{1/3}$ fm [27]:

$$F_0(Z, \epsilon) = 4(2pR_A)^{2(\gamma_1-1)} \frac{|\Gamma(\gamma_1 + iy)|^2 \exp(\pi y)}{[\Gamma(2\gamma_1 + 1)]^2}, \quad (3)$$

where $y = \pm\alpha Z\epsilon/p, \epsilon$ and $p = |\mathbf{p}|$ are the energy and electron momentum, and $\gamma_1 = [1 - (\alpha Z)^2]^{1/2}$ with $\alpha = 1/137$. In a more rigorous treatment the electron relativistic wave functions are expressed as a superposition of s and p Coulomb-distorted spherical waves. Their radial parts are obtained as solutions of the Dirac equations with a central field [26,28]:

$$\frac{dg_\kappa(\epsilon, r)}{dr} = -\frac{\kappa}{r} g_\kappa(\epsilon, r) + \frac{\epsilon - V + m_e c^2}{c\hbar} f_\kappa(\epsilon, r), \quad (4)$$

$$\frac{df_\kappa(\epsilon, r)}{dr} = -\frac{\epsilon - V - m_e c^2}{c\hbar} g_\kappa(\epsilon, r) + \frac{\kappa}{r} f_\kappa(\epsilon, r), \quad (5)$$

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which depends on the relativistic quantum number $\kappa = (l - j)(2j + 1)$. The quantities $g_\kappa(\epsilon, r)$ and $f_\kappa(\epsilon, r)$ are the small and large components of the solutions that have the following asymptotic behavior:

$$\begin{pmatrix} g_k(\epsilon, r) \\ f_k(\epsilon, r) \end{pmatrix} \sim \frac{\hbar e^{-i\delta_k}}{pr} \begin{pmatrix} \sqrt{\frac{\epsilon + m_e c^2}{2\epsilon}} \sin(kr - l\frac{\pi}{2} - \eta \ln(2kr) + \delta_k) \\ \sqrt{\frac{\epsilon - m_e c^2}{2\epsilon}} \cos(kr - l\frac{\pi}{2} - \eta \ln(2kr) + \delta_k) \end{pmatrix}. \quad (6)$$

Here, c is the velocity of the light, m_e/ϵ is the electron mass/energy, $k = p/\hbar$ is the electron wave number, $\eta = Ze^2/\hbar v$ is the Sommerfeld parameter, δ_κ is the phase shift, and V is the Coulomb potential between the electron and the daughter nucleus. The nuclear size corrections are usually taken into account by considering an unscreened potential V obtained for a uniform charge distribution in a sphere of radius R_A [23,28]:

$$V(r) = \begin{cases} -\frac{Z\alpha\hbar c}{r}, & r \geqslant R_A, \\ -Z(\alpha\hbar c)\left(\frac{3-(r/R_A)^2}{2R}\right), & r < R_A, \end{cases} \quad (7)$$

A further improvement in the calculation is to take into account the screening effect. This can be done by multiplying the above expression of $V(r)$ with a function $\phi(r)$, which is the solution of the Thomas-Fermi equation: $d^2\phi/dx^2 = \phi^{3/2}/\sqrt{x}$, with $x = r/b$, $b \approx 0.8853 a_0 Z^{-1/3}$, and a_0 = Bohr radius. It is calculated within the Majorana method [29]. This last approach was used in Ref. [28] to calculate the PSFs.

In this work, we go further in accuracy and take into account the influence of the nuclear structure by deriving the potential $V(r)$ from a realistic proton density distribution in the daughter nucleus. This is done by solving the Schrödinger equation for a Woods-Saxon (WS) potential. In this case,

$$V(r) = \alpha\hbar c \int \frac{\rho_e(\vec{r'})}{|\vec{r} - \vec{r'}|} d\vec{r'}, \quad (8)$$

where the charge density is

$$\rho_e(\vec{r}) = \sum_i (2j_i + 1) v_i^2 |\Psi_i(\vec{r})|^2, \quad (9)$$

with Ψ_i being the proton (WS) wave function of the spherical single-particle state i and v_i being its occupation amplitude. The factor $(2j_i + 1)$ reflects the spin degeneracy. The screening effect is taken into account in the same manner as in Ref. [28].

To compute the PSFs, the electron phase factors $f_{jk}^{(0)}$ must be obtained from the solutions of the Dirac equation by neglecting the neutrino mass:

$$f_{11}^{(0)} = |f^{-1-1}|^2 + |f_{11}|^2 + |f_1^{-1}|^2 + |f_1^{-1}|^2, \quad (10)$$

with

$$f^{-1-1} = g_{-1}(\epsilon_1) g_{-1}(\epsilon_2), \quad f_{11} = f_1(\epsilon_1) f_1(\epsilon_2); \quad (11)$$

$$f_1^{-1} = g_{-1}(\epsilon_1) f_1(\epsilon_2), \quad f_1^{-1} = f_1(\epsilon_1) g_1(\epsilon_2). \quad (12)$$

The values of the f and g functions are approximated with the solutions on the surface (method I from Ref. [28]):

$$g_{-1}(\epsilon) = g_{-1}(\epsilon, R); f_1(\epsilon) = f_1(\epsilon, R) \quad (13)$$

For the two-neutrino DBD, the PSFs are

$$G_{2\nu} = \frac{2\tilde{A}^2}{3 \ln 2 g_A^4 (m_e c^2)^2} \int_{m_e c^2}^{T_0 - m_e c^2} \int_{m_e c^2}^{T_0 - \epsilon_1} \int_0^{T_0 - \epsilon_1 - \epsilon_2} \times d\epsilon_1 d\epsilon_2 d\omega_1 f_{11}^{(0)} w_{2\nu} (\langle K_N \rangle^2 + \langle L_N \rangle^2 + \langle K_N \rangle \langle L_N \rangle), \quad (14)$$

where $T_0 = Q_{\beta\beta} + 2m_e c$ is the total energy released in the decay and $\langle K_N \rangle$ and $\langle L_N \rangle$ are expressions (known in the theory of DBD) that depend on the electron and neutrino ($\omega_{1,2}$) energies and on the g.s. energies of the initial nucleus and of the excited states of the intermediate nucleus [22–28]. $\tilde{A} = 1.12 A^{1/2}$ (in MeV) gives the energy of the giant Gamow-Teller resonance in the intermediate nucleus, and

$$w_{2\nu} = \frac{g_A^4 (G \cos\theta_C)^4}{64\pi^7 \hbar} w_1^2 w_2^2 (p_1 c)(p_2 c) \epsilon_1 \epsilon_2. \quad (15)$$

The PSFs are finally renormalized to the electron rest energy and are reported in yr^{-1}.

For the $0\nu\beta\beta$ decay, the PSFs are

$$G_{0\nu} = \frac{2}{4 g_A^4 R^2 \ln 2} \int_{m_e c^2}^{T_0 - m_e c^2} f_{11}^{(0)} w_{0\nu} d\epsilon_1, \quad (16)$$

where

$$w_{0\nu} = \frac{g_A^4 (G \cos\theta_C)^4}{16\pi^5} (m_e c^2)^2 (\hbar c^2)(p_1 c)(p_2 c) \epsilon_1 \epsilon_2, \quad (17)$$

where $G = 1.16637 \times 10^{-5}\ \text{GeV}^{-2}$ is the Fermi constant and $\cos\theta_C = 0.9737$ [26]. In Eq. (16) it is convenient to redefine the PSFs by a renormalization that eliminates the constant g_A and correlates (by dividing by $4R_A^2$) the dimension of $G_{0\nu}$ with the NMEs, which are dimensionless. Thus, our PSFs are reported in yr^{-1}.

Results. The single-particle densities inside the daughter nucleus, needed to derive the potential $V(r)$, are obtained by solving the Schrödinger equation for a spherical WS potential, including spin-orbit and Coulomb terms. The universal parametrization was employed as in Ref. [30]. The occupation amplitudes are obtained within the BCS approach [31]. Further, the Dirac equation is solved for the electron moving in the potential $V(r)$, created by the proton distribution, by using the power series method from Ref. [32]. We built up a numerical code that uses an algorithm similar to that used in Ref. [33]. The asymptotic normalization to unity is done as in Ref. [34]. The solutions of the electron wave functions are computed numerically by approximating them with infinite polynomials whose coefficients at different distances r are connected analytically by the particular forms of the Dirac equations and by the values of the Coulomb potential. Therefore, the numerical values of the wave functions can be calculated step by step, by increasing the distance r. At very large distances, the behavior of the wave functions must resemble that of the Coulomb function. This last condition provides a way to renormalize the amplitude to unity and to determine the phase shift. To solve the integrals (14) and (16), we compute the values of the electron wave functions and these values are interpolated. Because the wave function values at the nuclear surface vary rapidly for energies close

TABLE I. Values of the PSFs for transitions to the g.s. (first line) and to the excited 0_1^+ state (second line). The relative differences in percentage ε (%) between other previous calculations (indicated by references) and our results are displayed in the last rows of each section. $Q_{\beta\beta}$ and $Q^1_{\beta\beta}$ are the kinetic energies available in the corresponding decays.

	Nucleus											
	^{48}Ca	^{76}Ge	^{82}Se	^{96}Zr	^{100}Mo	^{110}Pd	^{116}Cd	^{128}Te	^{130}Te	^{136}Xe	^{150}Nd	^{238}U
						$G_{2\nu}$ (10^{-21} yr^{-1})						
$Q_{\beta\beta}$ (MeV)	4.272	2.039	2.995	3.350	3.034	2.018	2.814	0.866	2.527	2.458	3.371	1.145
$Q^1_{\beta\beta}$ (MeV)	1.275	0.917	1.507	2.202	1.904	0.548	1.057		0.733	0.879	2.630	0.204
[24,25]	16200	53.8	1830		3860			0.35	1970	2030	48700	
[27]	16200	52.6	1740	7280	3600		2990	0.344	1940	1980	48500	
	0.376	0.0769	4.80	190	101		0.89		18.6	0.485	4850	
[28]	15600	48.2	1600	6820	3310	138	2760	0.269	1530	1430	36400	14.6
	0.363	0.0698		175	60.6	0.00484	0.873		0.0757	0.362	4330	0.000464
Present	15500	43.9	1480	5940	2910	120	2580	0.253	1460	1370	34200	115
work	0.37	0.0595	3.71	131	45.8	0.00332	0.695		0.0771	0.356	3990	0.00326
ε [24,25]	4.3	18.4	−2.2		4.1			27.7	25.9	32.5	29.8	
ε [27]	4.3	16.5	−7.5	−4.4	−2.8		13.7	26.5	24.7	30.8	29.5	
	1.6	22.6	22.7	31.1	54.7		21.9		99.6	26.6	17.7	
ε [28]	0.6	8.9	7.5	12.9	12.1	13.0	6.5	5.9	4.6	4.2	6.0	>100
	−1.9	14.8		25.1	24.4	31.4	20.4		−1.8	1.7	7.9	>100
						$G_{0\nu}$ (10^{-15}yr^{-1})						
[24,25]	26.1	2.62	11.4		18.7			0.748	19.4	19.4	85.9	
[27]	26.0	2.55	11.1	23.1	45.6		18.9	0.671	16.7	17.7	78.4	
[28]	24.8	2.36	10.2	20.6	15.9	4.82	16.7	0.588	14.2	14.9	63.0	33.6
	0.299	0.178		4.57	3.16	0.0884	0.716		0.309	0.613	27.3	0.753
Present	24.9	2.34	10.1	20.3	15.7	4.79	16.6	0.555	14.1	14.6	62.0	31.1
work	0.305	0.187	0.917	3.30	3.07	0.108	0.719		0.357	0.659	27.0	1.18
ε [24,25]	4.6	10.7	11.4		16.0			25.8	27.3	24.7	27.8	
ε [27]	4.2	8.2	9.0	12.1	65.6		12.2	17.3	18.4	17.5	20.9	
ε [28]	−0.4	0.9	1.0	1.5	1.3	0.6	0.6	5.6	0.7	2.0	1.6	7.4
	−2.0	−5.1		27.8	2.9	−22.2	−0.4		−15.5	−7.5	1.1	−57

to $m_e c^2$, we took additional mesh points in the vicinity of this region to improve the numerical accuracy. Our results are presented in Table I for 12 nuclei of experimental interest. In the first (upper) part of the table the PSF values, $G_{2\nu}$, for the $2\nu\beta\beta$ decay mode, for the transitions to the g.s (first row in the grouping) and to excited 0_1^+ states (second row in the grouping) are displayed. For comparison, similar results are also displayed, indicating the references where they are taken from. The maximum available kinetic energies $Q_{\beta\beta}$ and $Q^1_{\beta\beta}$ for the transitions to the g.s. and excited 0_1^+ states, respectively, are given as well. In the last rows the relative differences in percentage between other results and ours $\{[\epsilon = G_{2\nu}(\text{Ref.}) - G_{2\nu}(\text{ours})]/G_{2\nu}(\text{Ref.})\}$ are shown for comparison. The PSF values, $G_{0\nu}$, for the $0\nu\beta\beta$ decay mode and the relative differences are presented in a similar way in the second (lower) part of the table. The relative differences between our $G_{2\nu}$ values and other results for the transitions to the g.s. are within 18.4% for the light nuclei. For the heavier nuclei, with $A > 128$, where the influence of the potential $V(r)$ is stronger, the relative differences are larger (between 25% and 32.5%), as compared with Refs. [24,27], while the agreement with Ref. [28] is excellent with one exception: ^{238}U. For the transitions to the excited 0_1^+ state the agreement with previous results is within 31.4%, with a few exceptions (^{100}Mo and ^{130}Te from Ref. [27] and ^{238}U from Ref. [28]), which should be revised. For $G_{0\nu}$ the agreement between our results and the previous ones is better than in the 2ν case and follows the same features discussed above. We notice the excellent agreement with the results from Ref. [28] for the transitions to the g.s., but also notice a few cases that should be revised (^{100}Mo and ^{238}U for transitions to the 0_1^+ state). The differences in PSF values could mainly come from two sources: the quality of the approach and the accuracy of the numerical methods that are used. On the one hand it is clear that an improved treatment of the electron wave functions (relativistic treatment with inclusion of the finite nuclear size and electron screening effects and using a realistic Coulomb potential) is preferable to a less rigorous one, as it is also highlighted in Ref. [28]. Related to this, because the influence of the structure of the daughter nucleus was never investigated, we performed the calculations with expressions of $V(r)$ either given by a uniform charge distribution or derived from a realistic proton density distribution. The differences we got between the two calculations are within 5% for both $G_{0\nu}$ and $G_{2\nu}$. On the other

hand, as we already mentioned, the f and g functions obtain their maximum values in the vicinity of $m_e c^2$ and, hence, a more rigorous treatment of the numerical integration in that region is necessary. An inadequate numerical treatment can change significantly the results.

Conclusions. In summary, we performed an independent calculation of the PSFs involved in $\beta^-\beta^-$ decays modes, for transitions to the g.s. and excited 0_1^+ states for 12 nuclei of experimental interest. The Coulomb distortion of the electron wave function is obtained by solving numerically the Dirac equation including the finite nuclear size and electron screening effects. In addition to other previous approaches, we used a Coulomb potential derived from a realistic proton density distribution in the daughter nucleus. The relative differences between other results and ours are within ≈32%, with a few exceptions that have to be revised. The differences between the PSF values can come, in part, from the rigor of the approach used in their calculation and, in part, from the accuracy of the numerical method used for integration. Because the PSFs are important ingredients both for the estimation of the DBD lifetimes and for the extraction of some key nuclear model parameters, a deeper investigation of these issues and a rigorous calculation of them is still needed.

Acknowledgments. This work was supported by a grant from the Romanian Ministry of National Education, CNCS UEFISCDI, Project No. PCE-2011-3-0318, and Contract No. 58/28.10/2011.

[1] F. T. Avignone, S. R. Elliott, and J. Engel, Rev. Mod. Phys. **80**, 481 (2008).
[2] H. Ejiri, Prog. Part. Nucl. Phys. **4**, 249 (2010).
[3] W. Rodejohann, Int. J. Mod. Phys. E **20**, 1833 (2011).
[4] A. Faessler, arXiv:1203.3648.
[5] J. Vergados, H. Ejiri, and F. Simkovic, Rep. Prog. Phys. **75**, 106301 (2012).
[6] V. A. Rodin, A. Faessler, F. Simkovic, and P. Vogel, Phys. Rev. C **68**, 044302 (2003).
[7] F. Simkovic, A. Faessler, V. A. Rodin, P. Vogel, and J. Engel, Phys. Rev. C **77**, 045503 (2008).
[8] F. Simkovic, A. Faessler, H. Muther, V. Rodin, and M. Stauf, Phys. Rev. C **79**, 055501 (2009).
[9] D.-L. Fang, A. Faessler, V. Rodin, and F. Simkovic, Phys. Rev. C **83**, 034320 (2011).
[10] M. Kortelainen, O. Civitarese, J. Suhonen, and J. Toivanen, Phys. Lett. B **647**, 128 (2007).
[11] M. Kortelainen and J. Suhonen, Phys. Rev. C **75**, 051303(R) (2007).
[12] S. Stoica and H. V. Klapdor-Kleingrothaus, Nucl. Phys. A **694**, 269 (2001).
[13] E. Caurier, A. P. Zuker, A. Poves, and G. Martinez-Pinedo, Phys. Rev. C **50**, 225 (1994); J. Retamosa, E. Caurier, and F. Nowacki, *ibid*. **51**, 371 (1995).
[14] E. Caurier, J. Menendez, F. Nowacki, and A. Poves, Phys. Rev. Lett. **100**, 052503 (2008).
[15] J. Menendez, A. Poves, E. Caurier, F. Nowacki, and A. Poves, Nucl. Phys. A **818**, 139 (2009).
[16] M. Horoi, S. Stoica, and B. A. Brown, Phys. Rev. C **75**, 034303 (2007).
[17] M. Horoi and S. Stoica, Phys. Rev. **81**, 024321 (2010).
[18] J. Barea and F. Iachello, Phys. Rev. C **79**, 044301 (2009); J. Barea, J. Kotila, and F. Iachello, Phys. Rev. Lett. **109**, 042501 (2012).
[19] T. R. Rodriguez and G. Martinez-Pinedo, Phys. Rev. Lett. **105**, 252503 (2010).
[20] P. K. Rath, R. Chandra, K. Chaturvedi, P. K. Raina, and J. G. Hirsch, Phys. Rev. C **82**, 064310 (2010).
[21] H. Primakov and S. P. Rosen, Rep. Prog. Phys. **22**, 121 (1959).
[22] W. C. Haxton and G. J. Stephenson, Jr., Prog. Theor. Part. Nucl. Phys. **12**, 409 (1984).
[23] M. Doi, T. Kotani, H. Nishiura, and E. Takasugi, Prog. Theor. Phys. **69**, 602 (1983).
[24] M. Doi, T. Kotani, and E. Takasugi, Prog. Theor. Phys. Suppl. **83**, 1 (1985).
[25] M. Doi and T. Kotani, Prog. Theor. Phys. **87**, 1207 (1992); **89**, 139 (1993).
[26] T. Tomoda, Rep. Prog. Phys. **54**, 53 (1991).
[27] J. Suhonen and O. Civitarese, Phys. Rep. **300**, 123 (1998).
[28] J. Kotila and F. Iachello, Phys. Rev. C **85**, 034316 (2012).
[29] S. Esposito, Am. J. Phys. **70**, 852 (2002).
[30] M. Mirea, Phys. Rev. C **78**, 044618 (2008).
[31] M. Brack, J. Damgaard, A. Jensen, H. Pauli, V. Strutinsky, and W. Wong, Rev. Mod. Phys. **44**, 320 (1972).
[32] W. Buhring, Z. Phys. **187**, 180 (1965).
[33] F. Salvat and R. Mayol, Comp. Phys. Commun. **62**, 65 (1991).
[34] F. Salvat, J. M. Fernandez-Varea, and W. Williamson, Jr., Comp. Phys. Commun. **90**, 151 (1995).