Comparison of *S*-matrix and WKB methods for half-width calculations

S. Mahadevan,[1] P. Prema,[1] C. S. Shastry,[1] and Y. K. Gambhir[2]
[1]*Department of Physics, Amrita Vishwa Vidyapeetham, Ettimadai Coimbatore 641105, India*
[2]*Department of Physics, I.I.T. Powai, Mumbai 400076, India*
(Received 25 April 2006; revised manuscript received 29 July 2006; published 8 November 2006)

The calculated Q values and half widths of α-decay of superheavy elements using both the S-matrix and the WKB methods are analyzed. The calculations are carried out using the microscopically derived α-daughter potentials for the parents appearing in the α-decay chain of super heavy element ($A = 277$, $Z = 112$). Both the S-matrix and the WKB methods though yield comparable results for smaller, in fact negative log $\tau_{1/2}$ values, the former is superior. However, for the case of positive log $\tau_{1/2}$ it is found that the S-matrix method though exact, runs into some numerical difficulties.

DOI: 10.1103/PhysRevC.74.057601 PACS number(s): 24.10.−i, 11.55.−m, 21.10.Tg, 23.60.+e

With the discovery of many superheavy elements beyond $Z = 100$ and their decay processes involving, among others, α-decay chains have revived interest in the careful analysis of Q value of α-decay and the corresponding decay constant. The α-decay of super heavy nuclei has been intensively investigated in recent years [1–11]. If α-decay is understood as a two body phenomena involving the daughter and parent nucleus, a proper approach requires a reliable input of α-daughter nucleus potential. These potentials are introduced either phenomenological [e.g., Woods-Saxon (WS) shape with adjustable parameters] or are generated microscopically in the $t\rho\rho$ approximation (double folding model) using explicitly the calculated nuclear (both proton and neutron) densities. Once such a potential is given the usual procedure of calculating Q value and decay constant is to use WKB type approximations to obtain the energies of long-lived states of the effective potential. In the α-decay problem, the effective potential is the sum of the nuclear potential, electrostatic potential and the centrifugal term. This potential generates a huge pocket in between the Coulomb barrier and the centrifugal barrier and in principle can generate bound states with $E < 0$ and resonant states with $E > 0$ with finite lifetime. For a typical α-decay system of our interest, the Coulomb barrier height is about 25 MeV, whereas Q values are in the range 5–10 MeV. Because of the long Coulomb tail, at energies near Q value, the barrier width is quite large of the order of 7–8 fm. As a result the resonance which pertains to α-decay will have in most cases, extremely narrow width. Hence resonance energies can be calculated using WKB method applicable for bound states. Thus in such cases, the positive energy resonant states and bound state energies can be expected to satisfy the equation

$$\int_{r_1}^{r_2} [k^2 - V_{\text{eff}}(r)]^{\frac{1}{2}} dr = \left(n + \frac{1}{2}\right)\pi, \tag{1}$$

where k^2 and $V_{\text{eff}}(r)$ are energy and effective potential respectively in $\hbar^2 = 2m = 1$ units; they have dimension L^{-2}. The effective potential V_{eff} includes the centrifugal term $(l + 1/2)^2/r^2$, as required in the WKB formula. Here r_1 and r_2 denote the two inner turning points.

When this formula is used, in general, one gets a number of positive eigenvalues; however, for the study of α-decay, the eigenvalue which corresponds to the Q value of the α-decay is to be identified. Once this eigenvalue is identified, the decay constant can be calculated using the WKB formula involving exponential Gamow factor and the assault frequency factor $A_f(k_R)$ adopting the procedure used by Elton [12]. The WKB approximation yields the following expression for half width corresponding to $k^2 = k_R^2$

$$\frac{\Gamma_R}{2} = A_f(k_R) \exp\left[-2\int_{r_2}^{r_3} \left(V_{\text{eff}}(r) - k_R^2\right)^{1/2} dr\right], \tag{2}$$

where

$$A_f(k_R) = \frac{2\left\{k_R^2 + \int_{r_1}^{r_2} dr\, V_{\text{eff}}(r)/(r_2 - r_1)\right\}}{r_B\left[V_B - \left(k_R^2\right)\right]^1/_2}. \tag{2a}$$

In Eq. (2a) V_B is the barrier height located at $r = r_B$.

However one should note that in the above approach the decaying state should be understood as the resonance state of the α-daughter nucleus two-body system. In scattering theory [13–15] a sharp resonance state is understood as a positive energy state with finite and relatively long lifetime or equivalently a narrow width. The most rigorous definition of resonance state and its width can be obtained from the analytic S-matrix theory of potential scattering [13–15]. In this approach the bound states and resonances are integrated in a unified manner and are represented as poles of S-matrix in the complex momentum (k) or equivalently in the complex energy plane. Accordingly the poles of S-matrix along the positive imaginary k axis represent the bound states and the poles representing the resonances are distributed symmetrically with respect to the imaginary axis in the lower half of the k-plane just below the real k axis. One can equivalently obtain the poles in the complex energy (k^2) plane.

In the S-matrix approach one starts with time independent Schrödinger wave equation. Since the α-decay is likely to occur when the daughter nucleus and α-system are in s ($l = 0$) state we confine our discussion to s state. Its generalization to higher partial waves, if needed, is fairly straight forward. For $s(l = 0)$ state the equation reads

$$\frac{d^2u}{dr^2} + (k^2 - V(r))u = 0; \tag{3}$$

k^2 and $V(r)$ denote energy and well behaved short range potential, respectively.

Then one writes u as a linear combination of Jost solutions $F(k, r)$ and $F(-k, r)$ such that

$$u \underset{r\to\infty}{\longrightarrow} \frac{1}{2ik}\,[f(-k)\,e^{-ikr} - f(k)\,e^{ikr}]. \tag{4}$$

The coefficients $f(\pm k)$ are known as Jost functions and are given by Wronskions

$$f(\pm k) = W[u, F(\pm k, r)]. \tag{5}$$

The S-matrix is given by

$$S(k) = \frac{f(k)}{f(-k)}. \tag{6}$$

It is well known that poles generated by zeros of $f(-k)$in the lower half of complex k-plane denote resonances provided the poles are close to the real k-axis.

Let $k_p = k_r - ik_i$, with $k_r > k_i > 0$, denotes a resonant position. Then

$$k_p^2 = k_r^2 - k_i^2 - i2k_rk_i = E_R - i(\Gamma_R/2). \tag{7}$$

Here E_R and Γ_R, denote the resonance energy and width, respectively. The width $\Gamma_R = |4k_rk_i|$ is related to decay constant λ, mean life τ and half-life $\tau_{1/2}$ through the relations $\Gamma_R = \hbar/\tau = 0.693\hbar/\tau_{1/2} = \hbar\lambda$.

In short, one needs to calculate the zeroes of $f(-k)$ in the appropriate region of the complex k plane by adopting a numerical technique. In applying this method to alpha decay problem, we have to use the appropriate Coulomb distorted Jost functions which can be obtained as linear combinations of regular and irregular Coulomb wave functions. The S-matrix in this case is a product of s-wave Coulomb S-matrix $S_c\,(k)$ and the "nuclear" S-matrix $S_n\,(k)$. The method of calculating these are well known in optical model [16–19]. However, care is needed to retain numerical accuracy when complex k is used. The resonances are represented by the poles of $S_n\,(k)$ as stated earlier. In order to obtain the pole position of S-matrix in k-planes we adopted Newton–Raphson iterative method starting with reasonable trial values [20–22]. This iterative procedure converges to the pole position, i.e., the zero position of $f(-k)$, fairly fast.

As a first step we carried out detailed systematic comparative analysis of the calculated Q values and half-lives using both the WKB and S-matrix methods employing simple model potentials like rectangular and also smoother potential barriers. The later potential has a pocket followed by a more or less flat barrier and was used in an earlier work [22] to make a comparison of pocket and barrier region resonances. It is to be mentioned that the half-width calculated using WKB type barrier penetration formula is independent of the nature of the potential beyond the outer most turning point. On the other hand in an exact S-matrix approach one expects that resonant energy and half width should depend on the entire potential. In order to ascertain the importance of tail region beyond the effective barrier we calculated the resonant energy and half width for a smoother potential.

We find from this combined analysis that though the WKB and S-matrix results are similar especially for smoother potential barriers however significant differences are noticed particularly for half-lives at several places. This indicates that, if one has to seek a more accurate calculation of widths, it is important to use the S-matrix method wherever feasible.

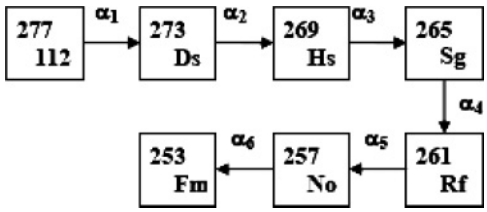

FIG. 1. α-decay chain of superheavy element $^{277}112$.

In this short communication, as an illustrative example, we present and discuss the calculated Q values and the log $\tau_{1/2}$ using the microscopically derived α-daughter potentials for the parents appearing in the α-decay chain (Fig. 1) of the super heavy element ($A = 277$, $Z = 112$) employing both the S-matrix and WKB type methods. The Q values and the half lives for this decay chain have been measured [23]. The calculations proceed in three steps: (i) The relativistic mean field (RMF) calculations [24] have been carried out for the relevant nuclei. The calculated ground state properties (binding energies, deformations, sizes) agree well with the experiment (where available) as expected [2]. (ii) The $l = 0$ (spherical) multipole part is projected out from the deformed RMF densities and then renormalized. These spherical RMF densities both for protons and neutrons along with the well known M3Y nucleon-nucleon interaction are then used in the double folding ($t\rho\rho$) approximation to generate the α-daughter nucleus potential. It is to be mentioned that the inclusion of deformation explicitly makes calculations quite complicated [25]. (iii) Next, these microscopically calculated numerical (spherical) potentials [2] have been parametrized reasonably well (see Fig. 2) in terms of attractive Woods-Saxon potential having three parameters V_0, a, R_z. The Coulomb potential is characterized by the radius parameter r_c. The Coulomb barrier height for these cases is between about 25–30 MeV and barrier location is around 10–11 fm. Finally this microscopically generated WS potential is used to calculate the Q values and the half-lives using both the WKB and the S-matrix methods.

At this stage we would like to highlight some difficulties posed in the half-life calculations when we use S-matrix method which was not so crucial in the model calculations mentioned earlier. For illustration, let us now consider the

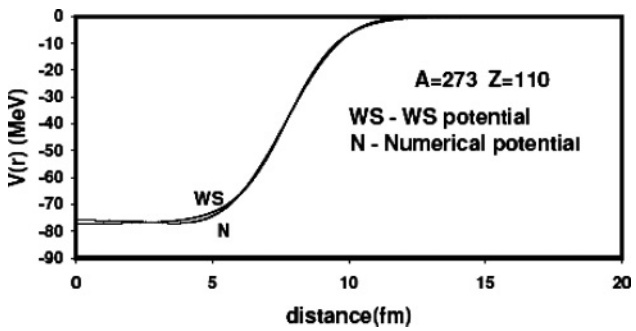

FIG. 2. The microscopic numerical potential of α-nucleus ($A = 273$, $Z = 110$) fitted with the WS shape: $V(r) = V_o/[1 + \exp((r - R_z)/a)]$ with $V_o = -77.15$ MeV, $a = 0.96$ fm, and $R_z = 7.73$ fm.

case where Q value of the decay is 8 MeV and log $\tau_{1/2}$ is 3.5, say, this corresponds to $\Gamma/2 \sim 0.72 \times 10^{-25}$. This means the position of the resonance pole in the energy plane, in MeV units, is at $E = 8. - i\,0.72 \times 10^{-25}$. Hence this particular state will imply an extraordinary sharp resonance. On the other hand if log $\tau_{1/2}$ is -3.5, The S-matrix pole in complex energy plane will be at $E = 8. - i\,0.72 \times 10^{-18}$. The half width in the latter case is substantially larger. In a numerical evaluation of resonance pole it becomes quite difficult to generate reliable saturation in iteration if width is $\sim 10^{-25}$ whereas it is feasible when it is much larger and of $\sim 10^{-18}$ or more. The technical reason for this difficulty is due to the fact that if $k_p = k_r - ik_i$ is a pole of the S-matrix, $k = k_r + ik_i$ is the zero of the same. This is due to the symmetry property satisfied by the Jost functions. This may make the search of the pole when k_i is too small a very delicate task. Hence we found that width calculations using S-matrix method becomes somewhat approximate when log $\tau_{1/2}$ is significantly larger than unity. It may be pointed out that in the R-matrix and complex r-plane method [18] for calculating complex eigenvalues also, in the width calculation the accuracy for width is of the order of 10^{-4} MeV. Since the approach used by us and the method of Ref. [18] are on similar lines, the calculation of much smaller widths will face numerical complications.

In alpha decay studies such infinitesimally small widths arise because of the fact that effective height of the Coulomb barrier at resonance energy say, at 7.5 MeV is about 20 MeV or more and its barrier width is also quite large. It is due to this fact that calculation of the imaginary part pole position for resonance is going to be very difficult in several alpha decay cases. However, using sufficiently refined iterative technique we found that some of these poles can be computed when log $\tau_{1/2}$ is negative.

We developed the code to solve the Schrödinger equation for complex energy for the α-nucleus problem for the total potential which includes Coulomb potential with Coulomb parameter r_c in the usual way and the nuclear potential. As stated earlier we use WS form of nuclear potential. In the expression for the nuclear S-matrix the denominator, the zeroes of which can be identified with the poles is given by the function

$$[\phi'(R) f(\eta, -kR) - k\phi(R) f'(\eta, -kR)].$$

Here R is the matching point and η is the Coulomb parameter, $f(\eta, -kR)$ is the appropriate Coulomb Jost solution for s-wave given by $f(\eta, -kR) \propto [G_0(\eta, kR) + iF_0(\eta, kR)]$. Here F_0 and G_0 are, respectively, the regular and irregular Coulomb functions for s wave. $\phi(R)$ is the usual modified regular s-wave function of the Schrödinger equation. The symbol $'$ denotes the derivative with respect to r. The task of finding the zeros of the above function with very small imaginary part is complicated by the fact that the function $G_0(\eta, kR)$ takes exponentially large values for large η and R (see for example tables in Ref. [26]). We illustrate the origin of the complication through the following trivial example.

Suppose we are interested in finding the zero of the function $f(x) = (x - 10) \times 10^{10}$. Mathematically speaking $x = 10$ is the location of the zero. However suppose the zero is calculated with only one percent accuracy. That is instead of $x = 10$ computer gives $x = 10.1$. At this value of $x = 10.1$, $f(x) = 10^9$ which is too huge and nowhere near zero and hence does not give a feeling that we have calculated the zero of $f(x)$ to 1% accuracy. Because of these factors each case of calculation of Q and log $\tau_{1/2}$ values has to be done very diligently. As stated earlier, the cases where log $\tau_{1/2}$ values are significantly larger than unity are more difficult to handle. When log $\tau_{1/2}$ is negative, half widths are easier to compute.

The results are summarized in Table I. This table provides a variety of results. Under the log $\tau_{1/2}$ (WKB) column, Q-SM (Q-WKB) correspond to the WKB results obtained by using the Q values of the S-matrix (WKB) method. As stated earlier, in the alpha decay cases, it is reasonable to use Eq. (1) for obtaining Q values by WKB method. The Q values from S-matrix and WKB methods are fairly close but they differ to some extent from the corresponding experimental values. However there is difference as far as the half-life results are concerned, where WKB results seem to be better for positive log $\tau_{1/2}$. As elaborated earlier, this is because of the difficulty in finding the imaginary part of the S-matrix pole, which is too small. As expected, when half-life values are negative, the S-matrix results seem to be substantially better.

So far the calculation of Q and log $\tau_{1/2}$ values using S-matrix or WKB methods have been carried out using the potential having WS shape which gives the best least squares fits to the numerical potential. Since such a fit may not be entirely satisfactory in generating the numerical potential in all

TABLE I. Q values (in MeV) and log ($\tau_{1/2}$) obtained from S-matrix (SM) and WKB methods. r_c, R_z, a are in fm, V_0 is in MeV and $\tau_{1/2}$ is in sec. Under the log $\tau_{1/2}$(WKB) column, SM-Q (WKB-Q) correspond to the WKB results obtained by using the Q values of the S-matrix (WKB) method. Subscript $_D$ stands for the daughter and Expt. denotes the experiment.

Parameters ($V_0 = -78.0$, $r_c = 1.2$, $a = 0.95$) for all cases	Pole position in Energy plane $E = E_R - i\Gamma/2$	Q (SM)	log $\tau_{1/2}$ (SM)	log $\tau_{1/2}$ (WKB) (SM-Q)	Q (WKB)	log $\tau_{1/2}$ (WKB) (WKB-Q)	Q (Expt.)	log $\tau_{1/2}$ (Expt.)
$Z_D = 100$, $A_D = 253$, $R_z = 7.598$	$7.95 - i0.4772 \times 10^{-25}$	7.95	3.630	1.687	7.95	1.687	8.47	1.176
$Z_D = 102$, $A_D = 257$, $R_z = 7.6373$	$8.41 - i0.2302 \times 10^{-25}$	8.41	2.723	0.824	8.39	0.893	8.65	0.672
$Z_D = 104$, $A_D = 261$, $R_z = 7.7257$	$8.35 - i0.6642 \times 10^{-24}$	8.35	2.536	1.696	8.40	1.517	8.90	1.382
$Z_D = 106$, $A_D = 265$, $R_z = 7.7637$	$8.80 - i0.1306 \times 10^{-23}$	8.79	2.472	0.940	8.85	0.729	9.37	1.294
$Z_D = 108$, $A_D = 269$, $R_z = 7.6013$	$10.98 - i0.9854 \times 10^{-18}$	10.98	−3.630	−4.185	11.04	−4.340	11.25	−3.958
$Z_D = 110$, $A_D = 273$, $R_z = 7.6886$	$10.98 - i0.2976 \times 10^{-18}$	10.98	−3.110	−3.663	11.04	−3.828	11.62	−3.550

domains of r space, we have repeated some of the calculations using the exact numerical potential. The results are very similar to those obtained with the corresponding WS type potential. Even though S-matrix results for $\log \tau_{1/2}$ are better in principle, when $\log \tau_{1/2}$ is significantly larger than zero, due to extraordinary small widths involved computational difficulties arise and in such cases WKB method is preferable.

To summarize the WKB method is satisfactory for obtaining Q values and the results compare very closely with those of S-matrix. However, differences do occur for $\log \tau_{1/2}$ values.

The authors are thankful to A. Bhagwat for supplying the microscopically calculated numerical potentials and B. Sahu for his interest in the work. Partial financial support from the Department of Science and Technology (DST), Government of India under Project Nos. SR/S2/HEP-13/2004 and SR/S2/HEP-18/2004-II is gratefully acknowledged.

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