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A NUMERICAL METHOD FOR CALCULATING RESONANT STATE WAVEFUNCTIONS

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A NUMERICAL METHOD FOR CALCULATING RESONANT STATE WAVEFUNCTIONS

Ризеа М.

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Численный метод вычисления волновых функций резонансных состояний

Метод начальных значений для численного решения задач типа Штурма-Лиувилля применяется для решения уравнения Шредингера для резонансных состояний.

Глубина ядерного потенциала рассматривается как собственное значение, полученное методом "стрельбы".

Используемый метод очень быстрый и не теряет своей эффективности даже для крайне малых ширин резонансов (например, 10^{-16} МэВ).

Работа выполнена в Лаборатории ядерных реакций ОИЯИ.

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Rizea M.

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A Numerical Method for Calculating Resonant State Wavefunctions

An initial-value method of numerical solving of Sturm-Liouville problems is applied to find the solution to the Schrödinger equation which corresponds to a resonance situation.

The depth of the nuclear potential is regarded as an eigenvalue, which is obtained by iteration. Having established the nuclear potential, the resonant wavefunction is generated by integrating numerically the Schrödinger differectial equation inwards from large radii using the initial conditions of $G(r)$, where G is the irregular Coulomb function.

The method of integration is Numerov's one, which has some advantages compared with other methods. For example, it is more accurate than the finite-difference methods and simpler than the Runge-Kutta method. In addition, the accuracy is increased by using the Richardson extrapolation technique.

The eigenvalue is found by the Newton method, which ensures second order convergence, and therefore it is faster than other procedures, e.g., repeated bisection.

Because the solution is exactly on resonance, no searching for the phase shift is required. Consequently, the suggested procedure may be employed even if the resonance widths are extremely narrow (e.g., 10^{-16} MeV).

The final result was used to determine resonance widths for very narrow states.

The investigation has been performed at the Laboratory of Nuclear Research, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1978

1. Introduction

The term of "resonance" or "quasi-bound state" often appears in nuclear physics.

It is related to the excited states, which may be considered to consist of a core nucleus plus a single nucleon or cluster (an alpha particle, for example).

If the radial potentials involved have the form indicated in Fig. 1, discrete states may exist at various energies E.

The states are classified as

- bound, if $E<0$
- quasi-bound, if $0<E<E_b$
- unbound, if $E>E_b$.

The case of quasi-bound states is of particular interest and many methods have been developed for solving the Schrödinger equation which describes these states.

The quasi-bound state wavefunctions are usually obtained as solutions (eigenfunctions) of a Sturm-Liouville problem associated with the Schrödinger equation.

In formulating the Sturm-Liouville problem, it is possible to consider either the energy or the depth of the nuclear potential as eigenvalue.

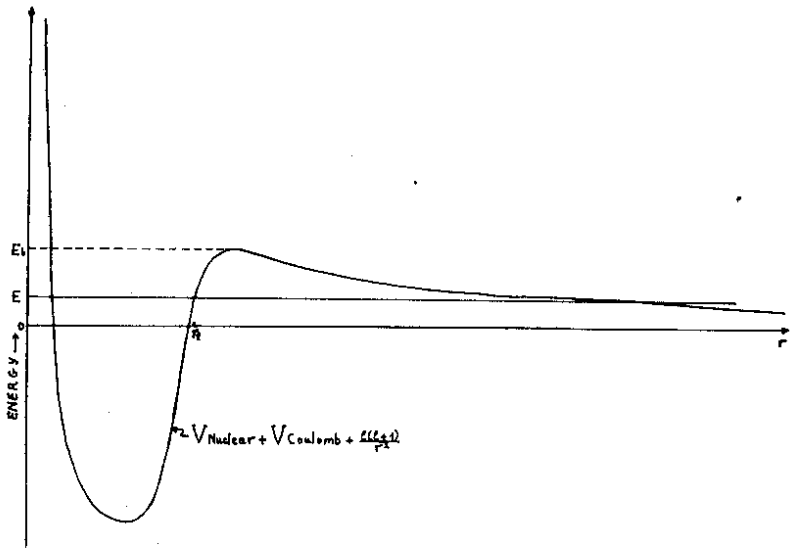

Fig. 1 A graph of the effective potential with a binding condition which corresponds to a quasi-bound resonant state.

Problems of the first type are solved in refs. 1 and 2 by the continuous analog of Newton's method (see ref. 3).

Other methods for solving such problems are suggested in refs. 4 and 5.

In ref. 6, DeVries solves a problem of the second type, using a method related to the bound states.

A solution to both types of problems may also be found by searching for the phase shift and requiring that it goes through $\pi/2$ (see, e.g. , ref. 7).

In order to compute the phase shift, one can use, for example, the procedure suggested in ref. 8, which is based on the numerical quadrature of the integral form of the Schrödinger equation.

An initial-value method for eigenvalue problems is applied here to solve a second type problem.

The method converges rapidly and is useful even if the state involved is very narrow, because no searching for the phase shift is required.

2. The Sturm-Liouville Problem for Quasi-Bound States.

The solution to the radial Schrödinger equation with typical boundary conditions is required.

In this study, the following form of the equation is considered

$$\frac{d^2u_\ell(r)}{dr^2} + \left[k^2 + \frac{2\mu}{\hbar^2}V(r) - \frac{\ell(\ell+1)}{r^2}\right]u_\ell(r) = 0, \quad (1a)$$

where $\mu = \frac{A_P A_T}{A_P+A_T}$ is the reduced mass, $k^2 = \frac{2\mu E}{\hbar^2}$, and ℓ is the angular momentum.

The potential $V(r)$ is the sum of Coulomb, spherical nuclear and spin-orbit potentials

$$V(r) = V_C(r) + V_N(r) + V_{SO}(r).$$

The Coulomb potential is chosen to be that due to a homogeneously charged sphere of radius R_o

$$V_C(r) = \begin{cases} \frac{Z_P Z_T e^2}{2R_o}\left(-3 + \frac{r^2}{R_o^2}\right) & \text{if } r < R_o \\ -\frac{Z_P Z_T e^2}{r} & \text{if } r \geq R_o \end{cases} \quad (2)$$

where $R_o = r_o A_T^{1/3}$.

The nuclear potential has a Woods-Saxon form

$$V_N(r) = V_o \, V_{WS}(r), \tag{3}$$

where $V_{WS}(r) = 1/(1 + \exp \frac{r - R_o}{a_o})$, (4)

and a_o is the diffuseness.

The spin-orbit potential is given by

$$V_{SO}(r) = \langle \ell \cdot s \rangle \; V_{SO} \frac{2}{r} \frac{dV_{WS}(r)}{dr}, \tag{5}$$

where $\langle \ell \cdot s \rangle = \frac{1}{2}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right]$ and $\vec{j} = \vec{\ell} + \vec{s}$.

A first boundary condition is

$$u_\ell(r) \xrightarrow[r \to 0]{} 0 . \tag{1b}$$

The solution of the Schrödinger equation for large r is a linear combination of the regular and irregular Coulomb functions which look like, respectively,

$$F \sim \sin \theta_r \quad \text{and} \quad G \sim \cos \theta_r , \tag{6}$$

where $\theta_r = \rho - \eta \ln(2\rho) - \ell \frac{\pi}{2} + \sigma$, $\rho = kr$ and $\eta = \frac{Z_p Z_T e^2 \mu}{\hbar^2 k}$.

(The Coulomb functions are solutions to the following differential equation $\frac{d^2u}{d\rho^2} + \left[1 - \frac{2\eta}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right]u = 0$).

The solution which corresponds to a quasi-bound resonant state must behave like G(r) at large radii (boundary condition (1c)).

This condition may be obtained as follows.

By introducing the phase shift δ_ℓ, one knows that the solution for large r is $u_\ell \sim \sin(\theta_r + \delta_\ell)$. For resonance, $\delta_\ell = \frac{\pi}{2}$ and hence $u_\ell \sim \cos \theta_r$. (There are several definitions of resonant states in quantum mechanics. If the width of the state is narrow, the above definition holds with good accuracy).

It is not possible to satisfy the conditions (1b) and (1c) with any arbitrary $\mathcal{V}_N(r)$.

Then, for fixed radius R_0 and diffuseness a_0, it will be necessary to vary V_0 until the boundary conditions are satisfied.

If we now introduce the notations

$$q(r) = -\frac{2\mu}{\hbar^2}\left[\mathcal{V}_C(r) + \mathcal{V}_{SO}(r)\right] + \frac{\ell(\ell+1)}{r^2} - k^2$$

$$p(r) = \frac{2\mu}{\hbar^2}V_{WS}(r)$$

$$\lambda = V_0 \qquad (7)$$

$$y(r) = u_\ell(r)$$

$$x = r,$$

Eq. (1) assumes the standard form of a Sturm-Liouville problem, i.e.,

$$y''(x) - q(x)y(x) + \lambda p(x)y(x) = 0, \qquad (8a)$$

$$y(0) = 0, \qquad (8b)$$

$$y(x) \underset{x\to\infty}{\sim} G. \qquad (8c)$$

We shall reduce this problem, which is defined on the interval $0 \leq x < \infty$, to a problem defined on a finite interval $[a,b]$.

It is known that for such problems there exists an infinite sequence of eigenvalues

$$\lambda_1 < \lambda_2 < \lambda_3 < \ldots \qquad (9)$$

In addition, there exist corresponding eigenfunctions $y_n(x)$, which are twice continuously differentiable.

It is also known that the n-th eigenfunction has n-1 distinct zeros in (a,b). (Some restrictions are necessary: $p(x)$ and $q(x)$ are continuous on $[a,b]$, $p(x) > 0$, $\forall x \in [a,b]$).

In our particular problem only one eigenvalue, respectively, only one eigenfunction may be required.

It is possible to indicate this value by the number of nodes of the corresponding eigenfunction.

The eigenvalue will be found by iteration and an initial guess is required to start the iteration process.

Such an estimate may be obtained by using information concerning the number of nodes (see Section 5).

After calculating the eigenvalue (V_0), the eigenfunction (u_ℓ) is found by the numerical integration of Eq. (1a) inwards from large radii using the initial values of G(r).

This is our quasi-bound state wavefunction.

A normalization condition will make the wavefunction unique. We use the following condition

$$\int_0^\infty \left| u_\ell (r) \right|^2 dr = 1 . \qquad (10)$$

3. Initial-Value Method for Eigenvalue Problems.

Using a general form for the boundary conditions, we consider the following Sturm-Liouville problem on the interval $[a,b]$

$$y''(x) - q(x)y(x) + \lambda p(x)y(x) = 0 , \qquad (11a)$$

$$a_1 y(a) + a_2 y'(a) = 0, \; a_1^2 + a_2^2 \neq 0 , \qquad (11b)$$

$$b_1 y(b) + b_2 y'(b) = 0, \; b_1^2 + b_2^2 \neq 0 . \qquad (11c)$$

We may relate the solution of (11) to an initial-value problem as follows.

For any fixed λ we consider

$$v''(x) - q(x)v(x) + \lambda p(x)v(x) = 0 , \qquad (12a)$$

$$a_1 v(a) + a_2 v'(a) = 0 , \qquad (12b)$$

$$c_1 v(a) + c_2 v'(a) = 1 . \qquad (12c)$$

Here c_1 and c_2 are any constants such as $a_1c_2 - a_2c_1 \neq 0$.

Then the two initial conditions are linearly independent and a unique nontrivial solution of the initial-value problem (12) exists. We denote this solution by $v(\lambda, x)$ and consider the transcedental equation

$$\varphi(\lambda) \equiv b_1 v(\lambda, b) + b_2 v'(\lambda, b) = 0 . \qquad (13)$$

Clearly each eigenvalue λ_n must satisfy this equation. Also, every root λ^* of this equation is an eigenvalue of (11) and the corresponding solution $v(\lambda^*, x)$ of (12) is a corresponding eigenfunction of (11).

Thus, the Sturm-Liouville problem (11) has been reduced to finding the roots of Eq. (13) and corresponding solutions of the initial-value problem (12).

Of course, it would be preferable to use a high-order iteration scheme, for example, Newton's method, in order to determine the roots of Eq. (13).

If the eigenvalue λ_n is required, then, for given initial guess $\lambda_n^{(0)}$, the successive approximations to λ_n are obtained by the formula

$$\lambda_n^{(\nu+1)} = \lambda_n^{(\nu)} - \frac{\varphi(\lambda_n^{(\nu)})}{\varphi'(\lambda_n^{(\nu)})} , \quad \nu = 0,1,2,\ldots \qquad (14)$$

In order to estimate the derivative $\varphi'(\lambda) = \frac{d\varphi(\lambda)}{d\lambda}$, we use the so-called variational equation for Eq. (12). Thus,

$$\varphi'(\lambda) \equiv b_1 w(\lambda, b) + b_2 w'(\lambda, b) , \qquad (15)$$

where $w(\lambda, x) = \frac{\partial v(\lambda, x)}{\partial \lambda}$ is the solution of the variational problem

$$w'' - q(x)w + \lambda p(x)w + p(x)v(\lambda,x) = 0, \qquad (16a)$$

$$w(\lambda,a) = 0, \qquad (16b)$$

$$w'(\lambda,a) = 0. \qquad (16c)$$

This problem is obtained by the formal differentiation of the initial-value problem (12).

A complete theoretical justification of the exposed procedure is contained in ref. 9.

In practice, we proceed as follows.

We consider a uniform network $x_i = a + ih$, $i = 0,1,\ldots,N$, $h = \frac{b-a}{N}$ and determine an approximate solution of (12) by a numerical method.

We denote this numerical solution for any fixed λ by $\bar{v}_i(\lambda)$, $\bar{v}'_i(\lambda)$, $i = 0,1,\ldots,N$.

The function $\varphi(\lambda)$ will be approximated by

$$\Phi(\lambda) \equiv b_1\bar{v}_N(\lambda) + b_2v'_N(\lambda). \qquad (17)$$

Using the values $\bar{v}_i(\lambda)$ instead of $v(\lambda,x_i)$ in Eq. (16a), we also solve (16) numerically to determine an approximation to $\varphi'(\lambda)$

$$\Phi'(\lambda) \equiv b_1\bar{w}_N(\lambda) + b_2\bar{w}'_N(\lambda), \qquad (18)$$

where $\bar{w}_i(\lambda)$, $\bar{w}'_i(\lambda)$ is the numerical solution of problem (16).

The approximations to the root λ_n will be really given by

$$\lambda_n^{(\nu+1)} = \lambda_n^{(\nu)} - \frac{\Phi(\lambda_n^{(\nu)})}{\Phi'(\lambda_n^{(\nu)})}, \quad \nu = 0,1,\ldots \qquad (19)$$

Of course, it would be desirable to obtain more accurate values for $\bar{v}_i(\lambda)$ before introducing them in Eq. (16a).

This is possible by using the Richardson extrapolation technique (see, e.g. , ref. 10, p. 186) for the solution of (12).

4. Application of the Method.

The suggested algorithm may be realized only on a finite interval $[a,b]$, while the initial physical problem is defined on the semiaxis $[0, \infty)$.

In practice, the problem (8) may be reduced to a Sturm-Liouville problem on the finite interval $[0,r_{max}]$, by taking as r_{max} a sufficiently large radius at which the contribution of central Woods-Saxon and spin-orbit potentials to the total potential is negligible (from the point of view of the available precision).

To start the numerical integration of Eqs. (12) and (16), which are of the form $y'' = f(x,y)$, the following Runge-Kutta method is used (see ref. 10, p. 268)

$$\begin{aligned} y_{i+1} &= y_i + h\left[y'_i + \tfrac{1}{6}(k_1 + 2k_2)\right] \\ y'_{i+1} &= y'_i + \tfrac{1}{6}(k_1 + 4k_2 + k_3) \\ k_1 &= hf(x_i, y_i) \\ k_2 &= hf(x_i + \tfrac{h}{2}, y_i + \tfrac{h}{2}y'_i + \tfrac{h}{8}k_1) \\ k_3 &= hf(x_i + h, y_i + hy'_i + \tfrac{h}{2}k_2)\,. \end{aligned} \qquad (20)$$

In order to avoid an infinite value at the origin (the term $\frac{\ell(\ell+1)}{r^2}$ is involved), a very small radius $\varepsilon > 0$ is taken as a first node of the network.

The initial conditions (12b) and (12c), which for $x_0 = 0$ would have the form $v(\lambda,0) = 0$, $v'(\lambda,0) = \text{constant}$, become

$$v(\lambda,\varepsilon) = \frac{(k\varepsilon)^{\ell+1}}{(2\ell+1)!!}\,, \qquad (12b')$$

$$v'(\lambda,\varepsilon) = \frac{v(\lambda,\varepsilon)}{\varepsilon}\,. \qquad (12c')$$

(The behaviour of the solution $u_\ell(r)$ to the Schrödinger equation (1a) in the vicinity of the origin was taken into account, i.e.

$$u_\ell(r) \xrightarrow[r\to 0]{} \hat{j}_\ell(kr) \xrightarrow[r\to 0]{} \frac{(kr)^{\ell+1}}{(2\ell+1)!!} ,$$

where $\hat{j}_\ell$ is the Riccati-Bessel function; see, e.g. , ref. 7).

The initial conditions of the variational problem (16) will be

$$w(\lambda, \varepsilon) = 0, \qquad (16b')$$

$$w'(\lambda, \varepsilon) = 0. \qquad (16c')$$

After obtaining the values of $v(\lambda, \varepsilon+h)$ and $w(\lambda, \varepsilon+h)$ by the Runge-Kutta method, the integration is continued on the network $x_i = \varepsilon + ih$ $(i = 0,1,2,\ldots,m;\ x_m = r_{max})$ by Numerov's method

$$y_i - 2y_{i-1} + y_{i-2} = \frac{h^2}{12}(f_i + 10f_{i-1} + f_{i-2}), \qquad (21)$$

where $f_j = f(x_j, y_j)$.

(The order of the method is $O(h^4)$; see ref. 10, p. 280).

The boundary condition (1c) is expressed by

$$\left.\frac{u'_\ell}{u_\ell}\right|_{r_{max}} = \left.\frac{G'}{G}\right|_{r_{max}} , \qquad (1c')$$

which leads to the following form of the function $\phi(\lambda)$

$$\phi(\lambda) \equiv \bar{v}'_m(\lambda) G_m - \bar{v}_m(\lambda) G'_m , \qquad (17')$$

where $\bar{v}_m(\lambda)$ is the value in x_m of the numerical solution of the problem (12a), (12b'), (12c'), $G_m = G(x_m)$, and

$$\bar{v}'_m(\lambda) \approx \frac{\bar{v}_{m+1}(\lambda) - \bar{v}_{m-1}(\lambda)}{2h}$$

$$G'_m \approx \frac{G(x_m+h) - G(x_m-h)}{2h} . \qquad (22)$$

The Coulomb function G was computed by the subroutine RCWFN (see ref. 11).

The convergence of the process defined by Eq. (19) is seen from the decrease of the quantity

$$\Delta_{\nu+1} = \frac{\left|\lambda_n^{(\nu+1)} - \lambda_n^{(\nu)}\right|}{\left|\lambda_n^{(\nu+1)}\right|} = \frac{\left|\frac{\Phi(\lambda_n^{(\nu)})}{\Phi'(\lambda_n^{(\nu)})}\right|}{\left|\lambda_n^{(\nu+1)}\right|} \qquad (23)$$

(the relative error).

The process finishes, if $\Delta_\nu < \delta$, where δ is small enough.

By computing $q(x_i)$ and $p(x_i)$ and storing them before starting the integration and by taking into account the common terms of equations (12a) and (16a), the pair $(\bar{v}_i(\lambda), \bar{w}_i(\lambda))$ may be obtained at each step by very simple computations.

After obtaining the required eigenvalue, the resonant state wavefunction u_ℓ is generated from starting values of G(r) at r_{max} and r_{max}-h by the Numerov method.

The normalization condition (10) is approximated by

$$\int_0^{r_c} |u_\ell(r)|^2 \, dr = 1 \, . \qquad (10')$$

The r_c cutoff radius is taken to lie in the neighbourhood of the first exterior node of u_ℓ and it was proved numerically that any radius in this region yields the same normalization, if E is sufficiently below E_b.

5. Numerical Example.

On the basis of the suggested algorithm a FORTRAN program was written. As a test run, the wavefunction appropriate to the state $^{214}Po = {}^{210}Pb + \alpha$ was calculated. The result with

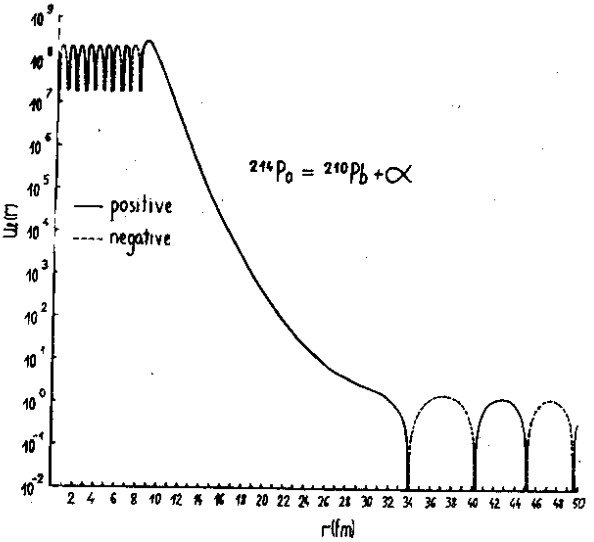

Fig. 2 Resonant state wavefunction normalized to G(r) for large r.

starting values of G(r) at large radii is shown in Fig. 2.

The additional parameters have been

$E = 7.687$, $r_o = 1.376$, $a_o = 0.625$, $\ell = 0$, $s = 0$, $n = 9$

(n is the number of internal nodes of the wavefunction).

An estimate for the initial guess $\lambda^{(o)}$ may be derived, on the basis of a classical approximation of the potential, from the condition

$$n\pi \leq \int_0^{r_t} \sqrt{\lambda p(x) - q(x)}\, dx \leq (n+1)\pi \,, \qquad (24)$$

where we used the notations (7), and r_t is the turning point (for $r > r_t$, $\lambda p(r) - q(r) < 0$).

Under the above conditions, the range $95 < \lambda < 107$ has

been obtained and we used a value of $\lambda^{(0)} = \frac{95 + 107}{2} = 101$ as an initial guess.

For $\varepsilon = 10^{-6}$, $h = 0.025$, $\delta = 10^{-8}$, $r_{max} = 28$, the sequence of successive eigenvalue approximations is shown in table 1.

Table 1

ν	$\lambda^{(\nu)}$	$\Delta\nu = \left\lvert \frac{\lambda^{(\nu)} - \lambda^{(\nu-1)}}{\lambda^{(\nu)}} \right\rvert$
0	101.00000	
1	104.51739	$3.3 \cdot 10^{-2}$
2	104.11843	$3.8 \cdot 10^{-3}$
3	104.12266	$4.1 \cdot 10^{-5}$
4	104.12266	$3.5 \cdot 10^{-9}$

The decrease of the value of $\Phi(\lambda)$ may be seen from the ratio $Q = \left\lvert \frac{\Phi(\lambda^{(k)})}{\Phi(\lambda^{(0)})} \right\rvert$.

In the present case, $Q = \left\lvert \frac{\Phi(\lambda^{(3)})}{\Phi(\lambda^{(0)})} \right\rvert = 1.18 \cdot 10^{-7}$.

The dependence of the calculation accuracy on the step h is exemplified in table 2.

Table 2

h	(3)
0.05	104.12240
0.025	104.12266
0.0125	104.12268

For h = 0.025, the computation time on the CDC-6500 of JINR, Dubna, is about 3 seconds.

The wavefunction normalized to 1 is $\psi(r) = C\, u_\ell(r)$, where $C=0.207595\cdot10^{-8}$. The constant C has been obtained from the condition $\int_0^{r_c} |\psi(r)|^2 dr = 1$, with the cutoff radius r_c = 34 fm.

The wavefunction may be used to determine the resonance width Γ. From the relation (see ref. 12)

$$\Gamma = \frac{\hbar v}{\int_0^{r_c} |u_\ell|^2 dr}, \quad v = (2E/\mu)^{\frac{1}{2}}$$

we have obtained $\Gamma = 0.55141\cdot10^{-16}$ MeV.

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