Modified two-potential approach to tunneling problems

S.A. Gurvitz,1, 2 P.B. Semmes,3 W. Nazarewicz,4, 5, 6 and T. Vertse7, 2

1Department of Particle Physics, Weizmann Institute of Science, Rehovot 76100, Israel
2Joint Institute for Heavy Ion Research, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831
3Physics Department, Tennessee Technological University, Cookeville, Tennessee 38505
4Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996
5Physics Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831
6Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, PL-00681, Warsaw, Poland
7Institute of Nuclear Research of the Hungarian Academy of Sciences
8H-4001, Debrecen, Hungary

One-body quantum tunneling to continuum is treated via the two-potential approach, dividing the tunneling potential into external and internal parts. We show that corrections to this approach can be minimized by taking the separation radius inside the interval determined by simple expressions. The resulting modified two-potential approach reproduces the resonance’s energy and the width, both for narrow and wide resonances. We also demonstrate that, without losing its accuracy, the two-potential approach can be modified to a form resembling the R-matrix theory, yet without any uncertainties related to the choice of the matching radius.

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I. INTRODUCTION

The quantum mechanical tunneling through a classically forbidden region is an ubiquitous phenomenon in physics, which has been extensively studied since the early days of quantum mechanics. In 1927, Hund was the first to point out the possibility of “barrier penetration” between two discrete states. In the same year, Nordheim considered the case of tunneling between continuum states. Subsequently, Oppenheimer performed a calculation of the rate of ionization of the hydrogen atom, and Gamow, Gurney and Condon explained alpha decay rates of radioactive nuclei in terms of the tunneling effect.

While the semi-classical treatment of tunneling turned out to be very successful in many applications, the numerical calculation offers very little insight into the physical process. In addition, the validity of the standard WKB formula is rather restricted. Other methods, although more accurate, contain various uncertainties. For example, the results of the commonly used R-matrix theory are often sensitive to the choice of the matching radius, and the theoretical error is difficult to estimate.

The treatment of the tunneling problem can be essentially simplified by reducing it to two separate problems: a bound state problem and a non-resonant (scattering) state problem. This can be done consistently in the two-potential approach (TPA) (see also Refs. 12, 13), representing the barrier potential as a sum of the “inner” and the “outer” terms, containing only bound and only scattering states, respectively. This approach not only provides better physical insights than many other approximations but it is also simple and accurate.

In this paper we propose further developments and a modification of the TPA, and present a detailed comparison of this approach with the results of numerical calculations based on the Gamow-state (resonant-state) formalism. The resulting analytical expressions are easy to interpret and they can be straightforwardly extended to the non-spherical case.

The paper is organized as follows. In Sect. II, the TPA is briefly described. Section III deals with the quantal correction terms to the TPA. The minimization of these terms prescribes unambiguously the “window” for the separation radius that divides the original barrier potential into inner and outer terms. In this case, by considering examples of wide and narrow nuclear resonances, we demonstrate that the TPA yields results which are practically the same as those of the resonant-state calculation. In Sec. IV, we present a modification of the TPA. The resulting expressions resemble those of the R-matrix theory, yet without any uncertainties related to the matching radius, see Sec. V. Finally, the summary of our work is contained in Sec. VI.

II. TWO-POTENTIAL APPROACH

Consider a quantum well $V(r)$ with a barrier, which contains a quasi-stationary state at the $E_{res}$. The coordinate space can be divided into two regions, the “inner” region, $0 < r < R$, and the “outer” region, $r > R$, where $R$ is taken inside the barrier (see Fig. 1). Accordingly, one can introduce the two auxiliary potentials: the inner
FIG. 1: The “inner” \((U; \text{top})\) and the “outer” \((\tilde{W}; \text{bottom})\) parts of the potential \(V(r)\) defined as in Eqs. (1) and (2), respectively. The separation radius \(R\) is chosen well inside the barrier. The energy of the metastable state is \(E_0\) and \(V_0=V(R)\). The barrier radius is denoted by \(\bar{R}\) and \(r_1,2\) are the classical turning points.

The inner potential contains a bound state, \(\Phi_0(r)\) \((E=E_0)\), representing an eigenstate of the “inner” Hamiltonian \(H_0 = K + U(r)\), where \(K = -\nabla^2/2m\) is the kinetic energy term \((\hbar=1)\). One can demonstrate \(\ref{footnote:1}\) that the energy and the width of the quasi-stationary state, associated with the complex-energy poles of the total Green’s function \(G(E) = (E-K-V)^{-1}\), are obtained from the following equation

\[
E = E_0 + \langle \Phi_0 | W | \Phi_0 \rangle + \langle \Phi_0 | W \tilde{G}(E) W | \Phi_0 \rangle. \tag{3}
\]

Here \(W(r) = W(r) - V_0\), and the Green’s function \(\tilde{G}\) is given by

\[
\tilde{G}(E) = G_0(E) \left[ 1 + \tilde{W} \tilde{G}(E) \right], \tag{4}
\]

where

\[
G_0(E) = \frac{1 - \Lambda}{E + U_0 - K - U}, \quad \Lambda = |\Phi_0 \rangle \langle \Phi_0|. \tag{5}
\]

The resonance energy \(E_{\text{res}} = \Re(E)\) and the width \(\Gamma = -2\Im(E)\) of a quasi-stationary state obtained from Eq. (4) are independent of the choice of the separation radius \(R\).

Equation (4) can be solved iteratively by using the standard Born series for the Green’s function \(G\), i.e. by expanding \(G\) in powers of \(G_0\). Yet, the corresponding expansion for the quasi-stationary state energy converges very slowly. For that reason, we proposed \(\ref{note:1}\) a more efficient expansion scheme in which \(G\) is expanded in powers of the Green’s function \(G_\tilde{W}(E) = (E - K - \tilde{W})^{-1}\), corresponding to the outer potential \(\tilde{W}\). From Eq. (4) it immediately follows that

\[
\tilde{G} = G_\tilde{W} + G_\tilde{W} (U - U_0) \tilde{G} - \tilde{G} G_\tilde{W} \Lambda \left( 1 + \tilde{W} \tilde{G} \right), \tag{6}
\]

Iterating Eq. (6) in powers of \(G_\tilde{W}\) and then substituting the result into (5), one finds the desirable perturbative expansion for the energy and the width of the resonance. By truncating this series, one obtains the following first-order relation valid for the isolated metastable state:

\[
E = E_0 + \langle \Phi_0 | W | \Phi_0 \rangle + \langle \Phi_0 | W G_\tilde{W}(E) W | \Phi_0 \rangle. \tag{7}
\]

The above equation can be solved iteratively for \(E = E_r - i\Gamma/2\) by assuming that the energy shift \(\Delta = E_r - E_0\) and the width \(\Gamma\) are small compared to \(E_0\) and \(V_0-E_0\). In such a case, one can put \(G_\tilde{W}(E) \approx G_\tilde{W}(E_0)\), thus reducing Eq. (7) to

\[
E = E_0 + \langle \Phi_0 | W | \Phi_0 \rangle + \langle \Phi_0 | W G_\tilde{W}(E_0) W | \Phi_0 \rangle. \tag{8}
\]

By using the Schrödinger equation for \(G_\tilde{W}\) one finally obtains the TPA expressions \(\ref{footnote:1}\) for the width \(\Gamma\) and for the energy shift \(\Delta = E_{\text{res}} - E_0\) of the quasi-stationary state:

\[
\Gamma = \frac{1}{mk} |\Phi_0(R)\chi_k'(R) - \Phi_0'(R)\chi_k(R)|^2, \tag{9}
\]

\[
\Delta = -\frac{\Phi_0^2(R)}{2mk} [\alpha \chi_k'(R) + \chi_k(R)] [\alpha \chi_k'(R) + \chi_k(R)], \tag{10}
\]

where \(k = \sqrt{2mE_0}, \alpha = \sqrt{2m(V(R) - E_0)}, \chi_k(r) = \Re(\chi_k^{(+)}(r))\), and \(\chi_k^{(+)}(r)\) stands for the irregular (outgoing) solution of the Schrödinger equation for the outer potential.

It follows from Eqs. (9) and (10) that both \(\Gamma\) and \(\Delta\) are given in terms of bound and scattering state wave functions. Thus TPA essentially simplifies the treatment of tunneling, because the standard approximation schemes can be used for evaluation of \(\Phi_0\) and \(\chi_k\). For instance, by applying the semi-classical approximation, one obtains the improved Gamow formula for \(\Gamma\) \(\ref{footnote:1}\), \(\ref{footnote:1}\), which is useful for different applications \(\ref{footnote:1}, \ref{footnote:1}\). In particular, an extension of Eqs. (9) and (10) to the multi-dimensional case can be found in Ref. \(\ref{footnote:1}\).
III. CORRECTIONS TO TPA AND THE CHOICE OF THE SEPARATION RADIUS

The accuracy of Eqs. (9) and (10) can be determined by evaluating the leading correction terms. There are two types of corrections to TPA: (a) those due to the replacement of $\tilde{G}$ by $G_W$ in Eq. (3) leading to Eq. (7), and (b) those due to the replacement of $G_W(E)$ by $G_W(E_0)$ in Eq. (7) leading to Eqs. (9), (10). The correction terms of the first type, $(\Delta \Gamma)_{1}$, can be obtained by iterating (8). One finds from the first iteration (10):

$$\frac{(\Delta \Gamma)_{1}}{\Gamma} \simeq \frac{mV''(R)}{16[2m(V_0 - E_0)]^{3/2}}.
$$

Equation (11) might suggest that an optimal choice of the separation radius corresponds to $V'(R) = 0$, i.e., the maximum of $V(r)$. However, it has been demonstrated numerically [16, 17] that if the top of the barrier is close of the first type, $(\Delta \Gamma)_{1}$ becomes appreciable so that Eqs. (9) and (10) become less accurate. The reason is that the energy shift $\Delta$ becomes appreciable so that $(\Delta \Gamma)_{1}$ cannot be replaced by (10).

This can be illustrated by considering a square-well potential discussed in Ref. [15]: $V(r) = l(l+1)/2m^2 - U_0$ for $r < R_1$, and $V(r) = l(l+1)/2m^2$ for $r \geq R_1$, where the top of the barrier coincides with the closing potential (see Fig. 2). For a P-wave resonance, the numerical calculation gives $E_{\text{res}} = 1$ keV and $\Gamma = 55.9$ eV. The separation radius in the potential $U(r)$ lies at $E_0=275$ keV. The top of the centrifugal barrier is at $V(R_1)=1.16$ MeV.

![FIG. 2: Metastable state in the square-well potential of Ref. [15]. The potential parameters ($U_0=51.6$ MeV and $R_1=6$ fm) correspond to a P-wave resonance at $E_{\text{res}} = 1$ keV and $\Gamma = 55.9$ eV. The bound state in the potential $U(r)$ lies at $E_0=275$ keV. The top of the centrifugal barrier is at $V(R_1)=1.16$ MeV.](image)

$U(\bar{r})$ has a bound state at $E_0=275$ keV. However, the corresponding energy shift, $\Delta = -300$ keV, is of the same order of magnitude as the energy $E_0$ of the bound state. Consequently, the replacement of $G_W(E)$ by $G_W(E_0)$ in (10) leads to large corrections to the resonance energy and the width so that Eqs. (9) and (10) cannot be used.

Let us estimate the correction term $(\Delta \Gamma)_{2} = \Gamma(E_0 + \Delta) - \Gamma(E_0)$ due to such a replacement. One can use the semi-classical Gamow formula, $\Gamma \propto \exp(-2\int_{r_1}^{r_2} |p(r)| dr)$, with $r_1$ and $r_2$ being the inner and outer classical turning points, respectively, and $|p(r)| = \sqrt{2m[V(r) - E_0]}$. Approximating $V(r)$ for $r_1 < r < r_2$ by the inverted harmonic oscillator, one obtains

$$\frac{(\Delta \Gamma)_{2}}{\Gamma} \simeq \Delta \int_{r_1}^{r_2} \frac{\sqrt{2m}}{\sqrt{V(r) - E_0}} dr \approx \pi \frac{\sqrt{2m(r_2 - r_1)}}{2\sqrt{V - E_0}} \Delta,$$

where $V = \text{max } V(r)$ and $\Delta$ is given by Eq. (11).

Thus, in order to reduce the correction term $(\Delta \Gamma)_{2}$, one needs to minimize the energy shift $\Delta$. It follows from (10) that $\Delta$ can be strongly suppressed by taking the separation radius $R$ deeply inside the barrier. Indeed, Eq. (10) contains a product of regular and irregular wave functions, which do not vary considerably under the barrier. However, the factor $|\Phi_0(R)|^2$ decays exponentially with $R$. Therefore, by taking the separation radius $R$ far away from the boundary, $R \gg r_1$, one finds that $\Delta \rightarrow 0$, and $E_0 \rightarrow E_{\text{res}}$. As a result, (10) can be replaced by (8), leading to Eqs. (9) and (10).

To illustrate this point, let us again consider the example of a P-wave resonance discussed above. By taking the separation radius $R > R_1$, we readily find that $\Delta \rightarrow 0$ as $R - R_1$ increases, and $E_0 \rightarrow E_{\text{res}} = 1$ keV. The resulting value of $\Gamma = 55.3$ eV is very close to the Gamow-state value of the resonance width. The separation radius $R$ cannot be chosen too close to the outer classical turning point since in such a case $V(R) \rightarrow E_0$ and the correction term (11) becomes important. In fact, Eqs. (11) and (12) define the lower and upper limits of $R$.

In the following, we discuss the TPA results for proton and neutron resonances in the realistic average nuclear potential. The approximate TPA expressions are compared to the resonant states results obtained using the GAMOW code [18].

A. Comparison with Gamow-state calculations

Consider single-nucleon resonances in the Woods-Saxon (WS) potential $V_{WS}(r)$ represented by a sum of central, spin-orbit, centrifugal, and Coulomb terms. Here, we apply the parametrization of Ref. [16], namely: $R_0=1.17A^{1/3}$ fm, $a = 0.75$ fm for the central term, and $U_0^o = 0.2U_0$ and $R_0^o = 1.01A^{1/3}$ for the spin-orbit potential. We calculate $\Delta$ and $\Gamma$ according to Eqs. (9) and (10) by varying the separation radius $R$ inside the barrier, starting with the barrier radius, $R_1$, corresponding to the maximum of $V(r)$. 
TABLE I: TPA calculations for the $0h_{11/2}$ and $2s_{1/2}$ proton resonances with energy $E_{\text{res}}=1.5\text{ MeV}$ in a WS potential. The calculated widths $\Gamma_{\text{TPA}}$ and the corresponding corrections $\Delta \Gamma$ are shown relative to $\Gamma_{\text{TPA}}$ for several values of the separation radius $R$. The actual accuracy of the TPA, $\Delta\Gamma/\Gamma$, is given in the last column. If the correction is marked zero, it means that it is below 0.1%.

| $R - \bar{R}$ (fm) | $\Delta$ (keV) | $\Gamma_{\text{TPA}}$ (MeV) | $(\Delta \Gamma)_1/\Gamma_{\text{TPA}}$ | $(\Delta \Gamma)_2/\Gamma_{\text{TPA}}$ | $(\Delta \Gamma)/\Gamma$ |
|---------------------|---------------|-----------------------------|---------------------------------|---------------------------------|-----------------|
| $0h_{11/2}$ Gamow state: $E_{\text{res}}=1.5\text{ MeV}$, $\Gamma=4.918\text{ E-18 MeV}$ | 0             | -1.9                        | 4.931 E-18                      | 0                               | -1%             |
| 1.59                | -0.27         | 4.919 E-18                  | 0                               | -0.15%                          | 0               |
| 4.28                | -5.0 E-3      | 4.919 E-18                  | 0                               | 0                               | 0               |
| $2s_{1/2}$ Gamow state: $E_{\text{res}}=1.5\text{ MeV}$, $\Gamma=6.709\text{ E-14 MeV}$ | 0             | -3.3                        | 6.727 E-14                      | 0                               | -2.3%           |
| 3.45                | -0.11         | 6.709 E-14                  | 0                               | -0.1%                           | 0               |
| 8.05                | -1.2 E-3      | 6.746 E-14                  | 0                               | -0.7%                           | 0               |

TABLE II: Same as in Table I except for the neutron $0i_{13/2}$ and $1f_{5/2}$ resonances.

| $R - \bar{R}$ (fm) | $\Delta$ (keV) | $\Gamma_{\text{TPA}}$ (MeV) | $(\Delta \Gamma)_1/\Gamma_{\text{TPA}}$ | $(\Delta \Gamma)_2/\Gamma_{\text{TPA}}$ | $(\Delta \Gamma)/\Gamma$ |
|---------------------|---------------|-----------------------------|---------------------------------|---------------------------------|-----------------|
| $0i_{13/2}$ Gamow state: $E_{\text{res}}=1\text{ MeV}$, $\Gamma=1.834\text{ E-6 MeV}$ | 0             | -11.9                       | 1.869 E-6                       | 0                               | -3%             |
| 3.45                | -0.47         | 1.844 E-6                   | -1.2%                           | -0.1%                           | -0.5%           |
| 5.96                | -6.1 E-2      | 1.847 E-6                   | -1.5%                           | 0                               | -0.7%           |
| $1f_{5/2}$ Gamow state: $E_{\text{res}}=1\text{ MeV}$, $\Gamma=9.271\text{ E-2 MeV}$ | 0             | -109                         | 1.227 E-1                       | 0                               | -25%            |
| 2.05                | -51.4         | 1.089 E-1                   | -10.1%                          | -12%                            | -17%            |
| 4.05                | -7.2          | 9.876 E-2                   | -12%                            | -1.7%                           | -6.5%           |
| 4.57                | +2.7          | 9.408 E-2                   | -17%                            | +0.6%                           | -1.5%           |

We begin with the high-$\ell$ narrow proton resonance $0h_{11/2}$. The parameters of the WS potential are appropriate for $^{147}$Tm, which is a proton emitting nucleus. The potential depth, $U_0=-61.8823\text{ MeV}$, was adjusted to the energy $E_{\text{res}}=1.5\text{ MeV}$. The resulting barrier radius is $\bar{R}=8.54\text{ fm}$ ($V(\bar{R})=17.44\text{ MeV}$) and the inner and outer turning points are $r_1=6.33\text{ fm}$ and $r_2=71.15\text{ fm}$, respectively. Since $E_{\text{res}}<V(\bar{R})$, the calculated $0h_{11/2}$ resonant state has a very small width, $\Gamma=6.695\text{ E-14 MeV}$. The results of TPA calculations are shown in Table I for different values of $R \geq \bar{R}$, together with the corresponding correction terms to TPA: $(\Delta \Gamma)_1/\Gamma_{\text{TPA}}$ and $(\Delta \Gamma)_2/\Gamma_{\text{TPA}}$. Table II also displays the actual accuracy of the TPA, $(\Delta \Gamma)/\Gamma$, where $(\Delta \Gamma)=\Gamma-\Gamma_{\text{TPA}}$. Since $\bar{R}>r_1$, the energy shift $\Delta$ is small for $R=\bar{R}$. Therefore, the results of TPA are in a good agreement with the resonant-state calculations already for $R=\bar{R}$. Next we consider the low-$\ell$, broader $2s_{1/2}$ resonance at $E_{\text{res}}=1.5\text{ MeV}$, which is considerably closer to the top of the barrier $V(\bar{R})=9.43\text{ MeV}$ ($\bar{R}=9.34\text{ fm}$). As shown in Table I, also in this case $\Gamma_{\text{TPA}}$ nicely agrees with the numerical result, and the accuracy of the TPA is well estimated by Eqs. (11) and (12).

Table II displays the TPA results for the $0i_{13/2}$ and $1f_{5/2}$ neutron resonances in $^{133}$Sn at an energy $E_{\text{res}}=1\text{ MeV}$. Here $\Gamma$ is much larger due to the absence of the Coulomb barrier. As in the proton case, there is very good agreement with numerical calculations, provided that $R$ is taken far away from the turning points, inside the window determined by (11) and (12), and the results of TPA weakly depend on the separation radius $R$. This suggests that the separation radius can be eliminated altogether from the TPA expressions. As demonstrated in the following section one can indeed modify the TPA in such a way.

IV. MODIFIED TWO-POTENTIAL APPROACH

A tunneling potential can always be written as a sum of attractive and repulsive parts, $V(r) = V_{\text{att}}(r) + V_{\text{rep}}(r)$, where $V_{\text{rep}}(r)$ becomes dominant at distances beyond the barrier radius (see Fig. 3). Therefore, starting with some

radius $\bar{r}$, the total potential $V(r)$ can be well approximated by its repulsive part $V_{\text{rep}}(r)$. $R$ and $r_2$ denote the TPA separation radius and the outer turning point ($V(r_2) = E_0$), respectively.

FIG. 3: For $r > \bar{r}$ the tunneling potential $V(r)$ can be approximated by its repulsive part $V_{\text{rep}}(r)$. $R$ and $r_2$ denote the TPA separation radius and the outer turning point ($V(r_2) = E_0$), respectively.

For instance, in the case of a square-well potential of Fig. 2, Eq. (13) is satisfied for any nuclear part can disregarded with a desired accuracy $\eta \ll 1$:

$$|1 - V_{\text{rep}}(r)/V(r)| \leq \eta \quad \text{for } r \geq \bar{r}. \quad (13)$$

Usually, the repulsive part $V_{\text{rep}}(r)$ is well known, as well as the two linearly independent (regular and irregular) solutions $F_k(r)$ and $G_k(r)$ of the corresponding
Schrödinger equation. For instance, if \( V_{\text{ep}}(r) \) is a sum of Coulomb and centrifugal potentials, then \( F_k(r) \) and \( G_k(r) \) are the standard Coulomb functions. This implies that any solution of the Schrödinger equation with the potential \( V(r) \) can be written for \( r > \bar{r} \) as the linear combination of \( F_k(r) \) and \( G_k(r) \).

Consider the bound-state wave function \( \Phi_0(r) \) of the inner potential \( U(r) \) of Eq. (4). Since \( U(r) \approx V_{\text{ep}}(r) \) for \( \bar{r} \leq r \leq R \), \( \Phi_0(r) \) can be expanded in this region as

\[
\Phi_0(r) = c_1 G_k(r) + c_2 F_k(r),
\]

where \( k = (2mE_0)^{1/2} \). The coefficients \( c_{1,2} \) and the energy \( E_0 \) are obtained from matching of the logarithmic derivatives at \( r = \bar{r} \) and \( r = R \):

\[
\frac{c_1 G'_k(R) + c_2 F'_k(R)}{c_1 G_k(R) + c_2 F_k(R)} = -|p(R)|, \tag{15a}
\]

\[
\frac{c_1 G'_k(\bar{r}) + c_2 F'_k(\bar{r})}{c_1 G_k(\bar{r}) + c_2 F_k(\bar{r})} = \frac{\Phi'_0(\bar{r})}{\Phi_0(\bar{r})}. \tag{15b}
\]

Note that \( \Phi_0(r) \propto \exp[-|p(R)|(r-R)] \), for \( r > R \). Solving Eqs. (15) one easily finds

\[
\frac{\Phi'_0(\bar{r})}{\Phi_0(\bar{r})} = G'_k(\bar{r}) \left[ \frac{1 + \alpha \bar{r}^{-1}}{1 + \alpha \bar{r}^{-2}} \right], \tag{16}
\]

where \( \alpha = |p(\bar{r})|, \ a_k = \frac{F'_k(\bar{r})}{F_k(\bar{r})}, \ \bar{a}_k = G'_k(\bar{r})/G_k(\bar{r}) \), and

\[
f_1 = \frac{G'_k(\bar{r}) F'_k(\bar{r})}{F_k(\bar{r}) G'_k(\bar{r})}, \quad f_2 = \frac{G'_k(\bar{r}) F_k(\bar{r})}{F'_k(\bar{r}) G_k(\bar{r})}. \tag{17}
\]

The wave functions \( F_k(r) \) and \( G_k(r) \) are of the same order of magnitude in the asymptotic region, \( r \gg r_2 \). However, in the classically forbidden region the regular wave function exponentially decreases and the irregular one exponentially increases with decreasing \( r \). Using the semi-classical approximation, one can estimate \( G_k(\bar{r}) F_k(\bar{r}) \approx \exp[-f_1 R |p(r)| dr] \). Therefore, the coefficients \( f_{1,2} \) are of the order of \( \exp[-\alpha(\bar{r} - \bar{r})] \), so the corresponding terms \( f_{1,2}(1 + \bar{a}_k^{-1}) \) in Eq. (16) are exponentially suppressed and can be neglected. As a result, the matching condition (16) can be written as

\[
\frac{\Phi'_0(\bar{r})}{\Phi_0(\bar{r})} = G'_k(\bar{r})/G_k(\bar{r}). \tag{18}
\]

The above equation constitutes the MPTA condition for the resonance energy \( E_{\text{res}} = E_0 \). In contrast to Eq. (16), the relation (18) does not exhibit any explicit \( R \)-dependence. Consequently, there is no need to evaluate the bound-state wave function at large values of \( R \) well inside the barrier. Note also that for a narrow resonance the irregular wave function \( G_k(r) \) is proportional to the real part of the outgoing (Gamow) solution:

\[
\psi_{k_{\text{res}}}^\text{out}(r) \propto G_{k_{\text{res}}}(r) + i F_{k_{\text{res}}}(r) = O_{k_{\text{res}}}(r), \tag{19}
\]

with complex \( k_{\text{res}} = k - i\gamma \) and \( k_{\text{res}}^2 = 2m(E_{\text{res}} - i\Gamma/2) \). Since for small \( \Gamma \) and \( \gamma \) the imaginary parts of \( k_{\text{res}} \) and \( G_{k_{\text{res}}}(r) \) can be neglected, \( k_{\text{res}} \approx k \) and \( G_{k_{\text{res}}}(r) \approx G_k(r) \) (also for the outgoing Coulomb wave function \( O_{k_{\text{res}}}(r) = O_k(r) \)). In this case Eq. (18) represents the matching condition for the inner (bound state) wave function with the real part of the non-normalized outgoing wave. If the imaginary parts are not negligible, Eq. (18) can still be interpreted in terms of the standing-wave boundary condition at \( \bar{r} \), which means that the scattering phase shift is \( \pi/2 \). The requirement that the phase shift is equal to \( \pi/2 \) represents an alternative definition for the position of a resonance in the absence of a non-resonant phase shift.

Consider now Eq. (9) for the width. Since \( R > \bar{r} \), the outer wave function \( \chi_k(r) \) in the region \( r \geq R \) can be represented by the linear combination of the regular and irregular solutions of \( V_{\text{ep}}(r) \), and the corresponding coefficients in the linear combination of \( F_k(r) \) and \( G_k(r) \) are directly related to the (non-resonant) scattering phase shift for the outer potential \( \tilde{W}(r) \). One easily finds

\[
\chi_k(r) = \cos \delta_k F_k(r) + \sin \delta_k G_k(r) \quad \text{for} \quad r \geq R, \tag{20}
\]

where the phase shift \( \delta_k \) is obtained from matching of logarithmic derivatives at the separation radius \( R \):

\[
\tan \delta_k = -\frac{F_k(R)}{G_k(R)} \left( \frac{a_k - \alpha}{\bar{a}_k - \alpha} \right). \tag{21}
\]

Here we neglected the terms \( \sim \exp[-2\alpha R] \). Substituting (14) and (20) into (9) and taking into account the Wronskian relation between \( F_k(r) \) and \( G_k(r) \) one obtains:

\[
\Gamma = \cos^2 \delta_k \frac{k}{m} \left[ \frac{\Phi_0(\bar{r})}{G_k(\bar{r})} \right]^2 \left[ 1 - \frac{(\bar{a}_k + \alpha)(a_k - \alpha)}{(a_k + \alpha)(\bar{a}_k - \alpha)} \right]^2. \tag{22}
\]

Note that in the classically forbidden region \( F'_k(r)/F_k(r) \approx |p(r)| \) and \( G'_k(r)/G_k(r) \approx -|p(r)| \), so that the second term in brackets of (22) can be neglected. In addition, \( \cos \delta_k \approx 1 \), as follows from (21). As a result, one arrives at the following simple expression for the width:

\[
\Gamma = \frac{k}{m} \left[ \frac{\Phi_0(\bar{r})}{G_k(\bar{r})} \right]^2. \tag{23}
\]

Thus, similar to Eq. (18) for the resonance’s energy, the separation radius \( R \) does not appear explicitly in the expression for the width.

Equations (18) and (23) represent the final result of the modified two-potential approach (MPTA). Despite their simple appearance, these expressions are very accurate. In fact, the accuracy of the MPTA is practically the same as that of the TPA since the former was derived from the latter by neglecting only small correction terms of the order of the accuracy of the TPA itself. For instance, for the previously discussed case of the P-wave resonance in the square well potential, one finds \( E_{\text{res}} = 1 \text{keV} \) and
\( \Gamma = 55.3 \text{ eV}, \) i.e. the same result as in TPA. In general, the accuracy of the MTPA can be estimated by means of the parameter \( \eta \), which defines the lower limit for the matching radius \( \bar{r} \). However, one has to keep in mind that \( \bar{r} \) cannot be very large since the derivation of Eqs. (18) and (23) is valid only for \( \alpha (R - \bar{r}) \gg 1 \). Therefore, the value of \( \eta \) is restricted by Eq. (11) in which \( R \) is replaced by \( \bar{r} \).

It is worth noting that an expression similar to Eq. (23) was used in Refs. 19, 20 for calculating partial widths for proton emission. The corresponding formula that applies to the single channel case can be written as

\[
\Gamma (r) = \frac{k}{m} \left| \frac{\Psi_{\text{out}}^{\text{res}}(r)}{\Phi_{\text{out}}^{\text{res}}(r)} \right|^2, \tag{24}
\]

where \( r \) is large. The \( r \)-dependence of \( \Gamma (r) \) is weak but it can be reduced if one takes a more appropriate expression:

\[
\Gamma (r) = \frac{k}{m} \left| \frac{\Psi_{\text{out}}^{\text{res}}(r)}{\Phi_{\text{out}}^{\text{res}}(r)} \right|^2. \tag{25}
\]

Another expression for the width can be derived from the continuity relation for the resonant states 7, 21:

\[
\Gamma (r) = i \frac{1}{2m} \frac{\Psi_{\text{in}}^{\text{res}}(r') \Psi_{\text{out}}^{\text{res}}(r) - \Psi_{\text{in}}^{\text{res}}(r) \Psi_{\text{out}}^{\text{res}}(r')}{\int_0^1 |\Psi_{\text{in}}^{\text{res}}(r')|^2 dr'}. \tag{26}
\]

This form is completely independent of \( r \) in a wider range 21, 22 and furnishes a value which is equal to that coming from the imaginary part of the energy. However, for very narrow resonances, it is difficult to calculate the imaginary part of the energy with sufficient precision. The expression 23 derived in the MTPA replaces the Gamow wave function with the (real) bound-state wave function \( \Phi_0 \). Finally, let us emphasize that while Eq. (21) resembles the MTPA expression, it is based on different approximations and boundary conditions. On the other hand there are close connections between the MTPA and the R-matrix theory, also employing real-energy eigenstates, see Sec. V.

### A. MTPA: numerical examples

We present below in Table III the results of the MTPA for the widths 23 of resonances discussed in Tables I and II in the context of TPA. (Since the MTPA resonance energies are very close to the exact result, they are not displayed.) One finds that the MTPA reproduces the width almost with the same accuracy as the TPA, provided that the matching radius \( \bar{r} \) is large enough to ensure that the contribution from the nuclear attractive potential is small (\( \eta \ll 1 \)). It follows from Table III that \( \eta \) controls the accuracy of MTPA rather well, except for a broad neutron resonance \( 1f_{5/2} \) when \( \Delta \Gamma / \Gamma \) reaches 10\% at \( \bar{r} = \bar{R} + 2.96 \). In this case, the matching radius is quite far away from the barrier radius, so that the accuracy of the MTPA is given by Eq. (11) (with \( R \) replaced by \( \bar{r} \)). This is well confirmed by Table II, which shows the corresponding correction term.

### V. COMPARISON WITH THE R-MATRIX THEORY

It is interesting to compare the full expressions of the MTPA, Eqs. (18) and (23), with the results of the R-matrix theory 6. In the latter method, the space is divided into internal and external regions by a hard sphere of the radius \( a_c \), and a complete set of the internal wave functions \( u_{\lambda}(r) \) is introduced, \( \int_0^{a_c} u_{\lambda}(r) u_{\lambda}(r) dr = \delta_{\lambda \lambda'} \). The internal wave functions obey real boundary conditions for the logarithmic derivative:

\[
\frac{u'_{\lambda}(a_c)}{u_{\lambda}(a_c)} = B. \tag{27}
\]

The value of \( B \) determines the R-matrix eigenvalues \( E_{\lambda} \). It is convenient to choose \( B \) so that one of the eigenvalues would coincide with the position of the resonance where the value of the phase shift is equal to \( \pi/2 \). This defines the so-called “natural” boundary condition:

\[
\frac{u'_{\lambda}(a_c)}{u_{\lambda}(a_c)} = \Re \left[ \left( \frac{G_{\lambda \lambda}(a_c)}{G_{k \lambda}(a_c)} \right) \right]. \tag{28}
\]

In this case, one can apply the one-level approximation, i.e., approximate the resonance with a single Breit-Wigner term. The corresponding width \( \Gamma_{\lambda} \) becomes:

\[
\Gamma_{\lambda} = \frac{k}{m [1 - g_{\lambda}(a_c)] |G_{k \lambda}(a_c)|^2}, \tag{29}
\]
where \( g_\lambda \) denotes the energy derivative of the level shift \( r \).

One finds that Eqs. \( 18 \) and \( 23 \) of the MTPA formally resemble Eqs. \( 28 \) and \( 29 \) by choosing \( a_c = \bar{r} \) and taking \( g_\lambda(a_c) = 0 \). Yet, the inner wave function \( \Phi_0(r) \) of the MTPA is different from the internal wave function \( u_\lambda(r) \) of the R-matrix theory. The latter is totally confined inside the inner region, whereas \( \Phi_0(r) \) is a true “bound state” wave function of the inner potential \( U(r) \). Therefore, their normalizations are different.

The essential problem of the R-matrix theory is a proper choice of the matching radius \( a_c \), which remains a free parameter. A different choice of \( a_c \) does affect the results of R-function calculations in a one-level approximation. Moreover, there should exist an optimal matching radius, for which the results of the R-matrix calculations are close to the exact results \( 17 \). However, except for some simple cases (e.g., the square well potential), the optimal matching radius cannot be simply prescribed. In contrast, the MTPA is not sensitive to the matching radius \( \bar{r} \), provided that it is taken inside the “window” defined by Eqs. \( 11 \) and \( 13 \). This is an essential advantage of MTPA over the R-matrix method. (For critical discussion of the R-matrix expression for the resonance width, see Refs. \( 21, 22 \).)

VI. SUMMARY

This paper contains a detailed investigation of the two-potential approach to the one-body tunneling problem. It has been found that TPA becomes extremely accurate if the separation radius, dividing the entire space into the inner and the outer regions, is taken deeply inside the barrier, but not too close to the outer classical turning point. From a minimization of the leading correction terms, we obtained simple expressions for the upper and lower limits of the TPA separation radius. The high accuracy of the method was demonstrated explicitly by a detailed comparison with Gamow resonances of a realistic nuclear potential.

Furthermore, we have found that the TPA can be further simplified by taking into account the properties of regular and irregular solutions of the Schrödinger equation under the barrier. The final expressions of the modified two-potential approach formally resemble those of the R-matrix theory with the “natural” boundary conditions. However, the internal wave function of the MTPA is considerably different. In addition, contrary to the R-matrix theory, the corresponding matching radius of the MTPA is well defined. This makes MTPA particularly suitable for practical applications.

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