Title: THEORY OF PROTON EMITTERS

Author(s): Patrick Talou, Theoretical Division
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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Theory of proton emitters

P. Talou

*Theoretical Division, MS B283, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

**Abstract:**

Modern theoretical methods used to interpret recent experimental data on ground-state proton emission near the proton drip line are reviewed. Most of them are stationary and are aimed to compute proton decay widths $\Gamma_p$ only. Comparison is made between these approaches before being compared to experimental data. Our time-dependent approach based on the numerical solution of the time-dependent Schrödinger equation (TDSE) for initial quasi-stationary single-proton states is then introduced. It is shown that much deeper insights into the physics of this clean multidimensional quantum tunneling effect can be accessed, and that in addition to $\Gamma_p$, other physical quantities could be tested experimentally, offering new stringent tests on nuclear physics models away from the valley of $\beta$-stability. Finally, the necessity of using the TDSE approach in more complex, dynamical, problems is demonstrated.

1 Introduction

The advent of new radioactive ion beams facilities associated with powerful ancillary $4\pi \gamma$-rays detectors contributed to the recent explosion of discoveries of ground-state proton emitters along the proton drip line \[1\]. Far from the valley of $\beta$-stability, these proton resonances exhibit a strong single-particle character, providing invaluable nuclear structure informations which are otherwise difficult to access.

From a theoretical point of view, these extremely narrow resonances ($\Gamma \approx 10^{-22} - 10^{-15}$ MeV) can be conveniently interpreted as single-particle quasi-stationary states, decaying by quantum tunneling through the potential barrier created by the interaction proton-daughter nucleus. Several stationary schemes have been devoted to the computation of the proton decay width $\Gamma_p$, which is itself simply related to the partial proton half-life $T_{1/2}^p = h\ln 2/\Gamma_p$. Avoiding the treatment of the full dynamics of the tunneling problem, these approaches consider instead "Gamow" states associated to complex eigenvalues.

Sections 2 and 3 provide a brief overview of these stationary methods; theoretical results are then compared to each other and to experimental data. In Section 4, the TDSE is solved numerically for initial quasi-stationary single-proton states. General conclusions on quantum tunneling in one and two dimensions are then drawn.

In D. Rudolph et al. pioneering experiments [3], a proton is emitted from a well deformed rotational band in the parent nucleus, leaving the daughter nucleus in a spherical excited state. Such a complex situation in which the shape of the nucleus changes during the emission of the proton, is obviously intractable with traditional stationary tools. A first very crude model of this phenomenon is introduced in the last Section, and studied within the TDSE scheme. Final remarks and prospects conclude this proceeding.
2 Stationary approaches

Although the decaying of a quasi-stationary state by quantum tunneling is intrinsically a time-dependent problem, most theoretical approaches treat it as a stationary problem. Indeed, a quasi-stationary state can be defined as an eigenstate of the hamiltonian with outgoing boundary conditions. The resulting eigenvalues lie in the complex plane, and can be written as $E_0 - i\Gamma/2$, where $E_0$ represents the location of the resonance, while $\Gamma$ corresponds to its width.

Below is a brief description of the stationary theoretical methods used so far to infer $\Gamma_p$.

2.1 Semi-classical method

If the decaying parent nucleus is spherical, the proton tunnels through an isotropic potential barrier, and the problem is one-dimensional only. In such a case, the semi-classical approximation WKB gives, for deep subbarrier states, a very simple estimate of the width $\Gamma_p$:

$$\Gamma_p^{WKB} = N\frac{\hbar^2}{4\mu} \exp \left\{ -2 \int_{r_1}^{r_2} k_p(r) dr \right\},$$

where

$$\hbar k_p(r) = \sqrt{2\mu (V(r) - Q_p)},$$

is the classical momentum, and $\{r_0, r_1, r_2\}$ are the classical turning points (defined by $V(r) = E$). $\mu$ is the reduced mass and $Q_p$ the kinetic energy of the emitted proton. The normalization factor $N$ is

$$N^{-1} = \int_{r_1}^{r_2} \frac{dr}{k_p(r)} \cos^2 \left( \int_{r_0}^r k_p(r') dr' - \frac{\pi}{4} \right).$$

The $\cos^2$ term can often be approximated by its average value of $1/2$. This approximation, the results of which being closer to experimental data, is used in the present calculations.

Due to its great simplicity, the WKB formalism has been used extensively over the years in the study of nuclear decays by particle emission. Nevertheless, this approach suffers several important drawbacks. First, it is valid for deep subbarrier states only. Second, only the order of magnitude of $\Gamma$ can be inferred. Finally, its extension to deformed nuclei is a very difficult and cumbersome task. For this purpose, the more general path integral approaches, like instantons/bounces, should be used. To my knowledge, such an approach has not been implemented yet for proton emitters.

2.2 “Matching” method

While the accurate determination of complex solutions of the Schrödinger equation with outgoing boundary conditions appears to be a difficult task, proton widths $\Gamma_p$ can be inferred by simply looking at the asymptotic wave functions of the problem [5]. At large distances, the nuclear potential vanishes, and only the spherical Coulomb potential remains.
For a spherically symmetric potential, the single-particle wave function of the proton in the state \((lj)\) behaves asymptotically as

\[ r\psi_{lj}^{out}(r) = N_{lj} \left[ G_l(k_pr) + i F_l(k_pr) \right], \]

where \(N_{lj}\) is a normalization constant, and \(F_l\) and \(G_l\) are the regular and irregular Coulomb functions, respectively. The determination of \(N_{lj}\) provides the required information

\[ \Gamma_{lj}(R) = \frac{\hbar^2 k}{\mu} |N_{lj}|^2 = \frac{\hbar^2 k}{\mu} \frac{R^2 |\psi_{lj}(R)|^2}{G_l^2(R) + F_l^2(R)}. \]   

(3)

This quantity becomes independent of \(R\) for large distances, i.e., outside the range of the nuclear potential.

The extension of this approach to axially deformed nuclei is straightforward. Following the same “matching” idea, and looking at a specific exit channel \((l_p j_p)\), the partial decay width reads

\[ \Gamma_{l_p j_p}(R) = \frac{\hbar^2 k}{\mu} \frac{R^2 |\psi_{l_p j_p}(R)|^2}{G_{l_p}^2(R) + F_{l_p}^2(R)}, \]

(4)

which again becomes independent of \(R\) for sufficiently large distances. Here, the wavefunction \(\psi_{lj}(r)\) is the spherical component \((lj)\) of the total quasi-stationary wavefunction \(\phi_K(r)\):

\[ \phi_K(r) = \sum_{j \geq K} \psi_{lj}(r) [Y_l(\hat{r}) \chi_{1/2}]_{j_K}. \] 

(5)

where \(K\) is the projection of the total angular momentum on the nuclear axis of symmetry. Finally, a more general expression can easily be derived to encompass the decay to excited states in the daughter nucleus (see [5] for details).

### 2.3 Distorted wave method

Within standard reaction theory formalism, the proton emission can be interpreted as one particular reaction channel characterized by a transition amplitude \(T(A + 1, Z + 1; A, Z)\). The resonance width associated with such an amplitude is given by

\[ \Gamma = 2\pi |T(A + 1, Z + 1; A, Z)|^2, \]

(6)

where the amplitude \(T\) can be derived within the distorted wave approach

\[ T(A + 1, Z + 1; A, Z) = \langle \psi_{Ap} \Psi_{Ap} | V_{Ap} | \Psi_{A+1} \rangle. \]

\(\psi_{Ap}\) represents the relative motion of the proton with respect to the daughter nucleus, \(\Psi_{Ap}\) is the product of the intrinsic wave functions of the proton and the daughter nucleus, \(\Psi_{A+1}\) is the quasi-stationary state of the parent nucleus, and \(V_{Ap}\) represents the interaction between the proton and the daughter nucleus (approximated by a simple one-body potential).
For spherically symmetric nuclei, the width $\Gamma$ of Eq. (6) becomes

$$\Gamma^{DW} = \frac{4\mu}{\hbar^2 k} \left| \int_0^\infty F_t(r) \left[ V - V_C^0 \right] \phi_{ij}(r) dr \right|^2,$$

(7)

where $V_C^0$ is the point-like Coulomb interaction. For axially deformed nuclei,

$$\Gamma_{l,p,j_p}^{DW} \propto \left| M_{l_p,j_p} \right|^2,$$

(8)

where

$$M_{l_p,j_p} = \sum_{l_m} \left\langle l_p m_{l_p} \right\rangle \left\langle 1_m 1_j \right\rangle \left\langle j_p \right| \left\langle j \right| \left. V(r) - V_C^0(r) \right\rangle \left\langle l_m r \right| \left. Y_l^m(r) \right\rangle,$$

in which the last matrix element is evaluated in the intrinsic (body-fixed) system of reference. From this expression, it can be seen that an exchange of angular momentum at the nuclear surface is allowed thanks to the non-spherical part of the potential $V(r)$.

In fact, it can be shown [6] that the distorted wave method and the “matching” method give exactly identical results.

## 2.4 Coupled-channels formalism

The single-particle wave function $\psi_K(r)$ is expanded in partial spherical waves

$$\phi_K(r) = \sum_{l_j} \psi_{l_j K}(r) \left[ \bar{Y}_l(r) \chi_{1/2} \right]_{j_K}.$$  

(9)

Projecting this wave function on the state $\left[ \bar{Y}_{l'}(\vec{r}) \chi_{1/2} \right]_{j'K}$, one gets a set of coupled-channels equations

$$\left[ \frac{d^2}{dr^2} - \frac{k^2 - l(l + 1)}{r^2} \right] \psi_{\alpha K}(r) = \sum_{\alpha'} \left( V_{1\alpha\alpha'} + V_{2\alpha\alpha'} \frac{d}{dr} \right) \psi_{\alpha' K}(r),$$

(10)

where $V_{1\alpha\alpha'}$ and $V_{2\alpha\alpha'}$ are the matrix elements of the interaction taken between the angular and spin parts of the partial waves ($\alpha = l_j$).

In practice, the infinite $l$-decomposition of Eq. (9) is truncated. Equations (10) are then solved with imposing outgoing boundary conditions at large distances. A couple of methods have been developed to solve accurately this set of equations (see [7, 8] for details).
3 Numerical results and comparison with experiment

The single-particle potential used to describe the interaction between the proton and the axially deformed daughter nucleus is given by a sum of nuclear, Coulomb, and spin-orbit terms. Details of the potential can be found in Ref. [9]. For one-dimensional calculations, the potential has been taken from Ref. [4] with the parameters set WS1.

Table 1 gathers results of one-dimensional calculations for a few observed proton emitters. As mentioned earlier, DW and "Matching" approaches are identical. Our numerical calculations confirm this result (difference less than 0.05%). On the other hand, WKB values can deviate as much as 50% from the "exact" result.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Qp (keV)</th>
<th>Orbit</th>
<th>$t_{1/2}^{WKB}$</th>
<th>$t_{1/2}^{DW}$</th>
<th>$t_{1/2}^{Mat.}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{109}I$</td>
<td>829(4)</td>
<td>1$d_{5/2}$</td>
<td>10.9$\mu$s</td>
<td>10.01$\mu$s</td>
<td>10.01$\mu$s</td>
</tr>
<tr>
<td>$^{113}Cs$</td>
<td>977(4)</td>
<td>1$d_{5/2}$</td>
<td>592$ns$</td>
<td>543.45$ns$</td>
<td>543.63$ns$</td>
</tr>
<tr>
<td>$^{147m}Tm$</td>
<td>1132(5)</td>
<td>1$d_{3/2}$</td>
<td>207$\mu$s</td>
<td>208.84$\mu$s</td>
<td>208.90$\mu$s</td>
</tr>
<tr>
<td>$^{151}Lu$</td>
<td>1255(3)</td>
<td>0$h_{11/2}$</td>
<td>84.7$ms$</td>
<td>57.79$ms$</td>
<td>57.81$ms$</td>
</tr>
<tr>
<td>$^{157}Ta$</td>
<td>947(7)</td>
<td>2$s_{1/2}$</td>
<td>218$ms$</td>
<td>222.48$ms$</td>
<td>222.57$ms$</td>
</tr>
<tr>
<td>$^{161}Re$</td>
<td>1214(6)</td>
<td>2$s_{1/2}$</td>
<td>84.7$\mu$s</td>
<td>187.40$\mu$s</td>
<td>187.46$\mu$s</td>
</tr>
<tr>
<td>$^{185m}Bi$</td>
<td>1611(9)</td>
<td>2$s_{1/2}$</td>
<td>3.16$\mu$s</td>
<td>3.16$\mu$s</td>
<td>3.16$\mu$s</td>
</tr>
</tbody>
</table>

Table 1: One-dimensional computations (WKB, DW, and "Matching") of proton widths $\Gamma_p$ for several known proton emitters.

In table 2, theoretical and experimental half-lives are compared. The experimental spectroscopic factors $S_p^{exp}$ are defined as the ratio between theoretical and experimental half-lives. Strong deviations from unity can reveal important deformation or/and configuration mixing. Theoretical predictions give reliable results for most nuclei. $^{185m}Bi$ is an exception which cannot be described within such a simple single-particle approach (see [4] for a discussion). Other exceptions are $^{109}I$ and $^{113}Cs$. These nuclei are however expected to be deformed [13] and drive the need for deformed calculations.

Using the deformed formalisms described above, a fit to experimental data can be achieved allow-
ing the quadrupole deformation $\beta_2^{\text{exp}}$ to be a free parameter. A check comparison between $\beta_2^{\text{exp}}$ and theoretical predictions $\beta_2^{\text{th}}$ from Möller for instance [13] provides good consistency to this approach.

In summary, reliable calculations of the proton widths $\Gamma_p$ for spherical and deformed ground-state proton emitters can be achieved within these stationary schemes.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Qp (keV)</th>
<th>Nilsson orbit</th>
<th>$\beta_2^{\text{exp}}$</th>
<th>$\beta_2^{\text{th}}$ [13]</th>
<th>$t_{1/2}^{\text{exp}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{109}I$</td>
<td>829(4)</td>
<td>$1/2 + [420]$</td>
<td>0.05 – 0.1 [10]</td>
<td>0.16</td>
<td>103(5)μs</td>
</tr>
<tr>
<td>$^{113}Cs$</td>
<td>977(4)</td>
<td>$3/2 + [421]$</td>
<td>0.1 – 0.15 [10]</td>
<td>0.21</td>
<td>17(2)μs</td>
</tr>
<tr>
<td>$^{131}Eu$</td>
<td>950(8)</td>
<td>$3/2 + [411]$</td>
<td>0.3 [12]</td>
<td>0.33</td>
<td>17.8(19)ms</td>
</tr>
<tr>
<td>$^{131}Eu$</td>
<td>811(7)</td>
<td>$3/2 + [411]$</td>
<td>0.3 [12]</td>
<td>0.33</td>
<td>$23_{-6}^{+10}$ ms</td>
</tr>
<tr>
<td>$^{141}Ho$</td>
<td>1169(8)</td>
<td>$7/2 - [523]$</td>
<td>0.25 – 0.35 [11]</td>
<td>0.29</td>
<td>4.2(4)ms</td>
</tr>
</tbody>
</table>

Table 3: Nuclear deformations $\beta_2^{\text{exp}}$ predicted from experimental proton half-lives of deformed nuclei.

4 Beyond the stationary picture

Ground-state proton emission is a clean quantum tunneling problem. To get more insights into this physics and to encompass its important dynamical features, the full TDSE describing the evolution of the system proton-daughter nucleus should be solved.

The TDSE for the proton quasi-stationary state $\psi_{qs}$ is

$$i\hbar \frac{\partial}{\partial t} \psi_{qs}(r, t) = \mathcal{H}(r, t) \psi_{qs}(r, t).$$

We will assume for now that the hamiltonian $\mathcal{H}$ is independent of time. If the parent nucleus is axially deformed, the total angular momentum $I_p$ is not a good quantum number anymore, but $K$, its projection on the z-axis of symmetry is. Hence, the quasi-stationary state becomes $\psi_{qs}(\rho, z, \varphi, t) = f_{qs}(\rho, z, t)e^{iK\varphi}$ and the hamiltonian in the cylindrical $(\rho, z)$ plane reads

$$\mathcal{H}(\rho, z) = -\frac{\hbar^2}{2\mu} \left\{ \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial \rho^2} + \frac{\partial^2}{\partial z^2} - \frac{K^2}{\rho^2} \right\} + V(\rho, z),$$

where $V(\rho, z)$ is the single-particle potential described in Ref. [9].

The TDSE (11) is solved numerically on a discretized space-time grid using the time propagator method called MSD2 [14]. The initial quasi-stationary state $\psi_{qs}(r, 0)$ is chosen as an eigenstate of a slightly modified potential, following the procedure described in Ref. [15].

From the knowledge of the proton wave function in time, one can infer the following quantities:

- the total tunneling probability defined by

$$P_{\text{tun}}(t) = \int_{\text{Vout}} |\psi_{qs}(r, t)|^2 d^3r,$$
which represents the probability that the proton has been emitted by the time $t$. $V_{\text{out}}$ represents the volume outside the (spherical or deformed) nuclear surface.

- the **total decay rate** obtained from the tunneling probability via

$$\lambda(t) = \frac{1}{1 - P_{\text{tun}}(t)} \frac{dP_{\text{tun}}}{dt}.$$  

This quantity is related to the decay width $\Gamma$ via the simple expression $\Gamma = \hbar \lambda$.

In the case of an axially deformed emitting nucleus, several other quantities are of great interest.

- the **tunneling angular distribution** (or differential cross section of tunneling) estimated in spherical coordinates $(r, \theta, \varphi)$ and defined as

$$P_{\text{tun}}(t, \theta) = \frac{dP_{\text{tun}}}{d\Omega} = \int_{r_{\text{out}}(\theta)}^{\infty} |f_{qs}(r, \theta, t)|^2 r^2 dr,$$

where $r_{\text{out}}(\theta)$ is the radial position of the potential ridgecrest in the $\theta$-direction.

- the **mean value of the angular momentum** inferred from the average value of the $L^2$ operator

$$\langle L^2 \rangle(t) = \langle \psi_{qs}(t) | L^2 | \psi_{qs}(t) \rangle.$$  

- the **partial decay rate** for the particular channel $(l_p, j_p)$ inferred from

$$\left\langle Y_{l_p K}(\hat{r}) \frac{F_{l_p}(k_p \hat{r})}{r} | \psi_{qs}(r, t) \right\rangle,$$

which gives the probability for the proton to be emitted with the angular momentum $(l_p, j_p)$.

The states $K = 0, 1$ and 2 originating from the spherical orbital $1d_{5/2}$ in $^{131}Eu$\(^1\) have been chosen as initial quasi-stationary wave functions, at several hypothetical quadrupole deformations $\beta_2$ up to 0.3 (see Fig. 1). From this figure, two important remarks can be made. First, as the nuclear deformation is turned on, the wave functions keep their overall shape in the $(\rho, z)$ half-plane. This means that the wave structure is very robust against the deformation of the potential. Second, low-K states are more disturbed by the deformation than their high-K partners whose angular momentum distribution appears much narrower due to the lack of high-K neighbors in the corresponding Nilsson diagram. For small deformations, some of these "pure" states would therefore behave as if they were moving in a spherical potential.

\(^1\)A very excited state has been chosen in order to reduce the computation time and to reveal more pronounced features of the tunneling phenomenon. Also, the spin-orbit interaction has been removed in our calculations.
Figure 1: Initial quasi-stationary wave functions \( K = 0, 1, \) and 2, originating from the spherical orbital \( 1d_{5/2} \) in \( ^{131}\text{Eu} \), for several quadrupole deformations \( \beta_2 \).

In Fig. 2, the decay rate \( \lambda(t) \) and the mean value of the angular momentum \( \langle l \rangle (t) \) for the state \( K=0 \) at the deformation \( \beta_2 = 0.1 \) are plotted in time. For a spherical decaying nucleus, one would expect to observe two distinct phases in the behaviour of \( \lambda(t) \) [15]. First, a phase of strong deviations from an exponential decay law, followed by a stationary “asymptotic” phase where \( \lambda(t) \)

Figure 2: Time dependence of the decay rate \( \lambda(t) \) (top) and of the average angular momentum \( \langle l \rangle (t) \) (bottom) for the state \( K=0 \) at the nuclear deformation \( \beta_2 = 0.1 \).

Figure 3: Angular momentum projection of the outgoing wave function \( \psi_{K=0} \) at \( \beta_2 = 0.1 \).
reaches a constant (the decay being exponential). In the present deformed situation, the second phase does not show a constant behaviour, but instead reveals damped oscillations in time. This oscillatory behaviour is a direct consequence of the exchange of angular momentum at the nuclear surface, illustrated by the behaviour of \( <l>(t) \). For "pure" high-\( K \) states, this second phase would instead reveal a straight line.

More precisely, one can access the \( l_p \) content of the outgoing wave function in time thanks to the projection scheme of Eq. (13). In Fig. 3 the outgoing proton wave function is projected onto the two main \( l_p =0 \) and 2 states. Finally, the tunneling angular distributions of the three deformed states \( K = 0,1,2 \) (see Fig. 4) show that the tunneling path is mainly dictated by the nuclear structure, i.e., the topology of the wave function, rather than by the deformation of the potential. Contrary to the common belief expressed for instance for \( \alpha \) decay, the main emitting direction is not necessarily along the nuclear symmetry axis.

5 Time-dependent problems

The usefulness of a dynamical approach like TDSE to study the proton decay from spherical and deformed nuclei has been largely demonstrated in the last section. Nevertheless, the dramatic advantage of TDSE in comparison to other stationary approaches is that it allows the study of problems where the interacting potential is time-dependent. Such class of problems is obviously outside the scope of traditional stationary schemes.

An example of such a complex situation is the recent discovery by D. Rudolph et al. of proton emission from a deformed second minimum in \(^{58}Cu\) to an excited state in \(^{57}Ni\) \(^3\).

As a first very crude model, let us consider the time-dependence of the nuclear deformation \( \epsilon(t)^2 \), hence of the single-particle potential \( V(\rho, z, \epsilon(t)) \), to follow a linear behaviour

\[
\epsilon(t) = \begin{cases} 
\epsilon_i \left(1 - \frac{t}{T_d}\right) & \text{for } t \leq T_d \\
0 & \text{for } t > T_d
\end{cases}
\]

(14)

where \( T_d \) is the duration of the nuclear deformation, i.e., the time it takes for the nucleus to go from its initial configuration (here, \( \epsilon_i = 0.2 \)) to its final one (here, \( \epsilon_f = 0 \)).

\(^2\)The quantity \( \epsilon \) comes from a different parametrization of the nuclear deformation than previously used. Nevertheless, for small deformations, \( \epsilon \approx \beta_2 \).
We applied this formalism to the decay of single-proton quasi-stationary $1g$ states ($K=0$ to 4) in $^{58}Cu$. The tunneling probabilities $P_{\text{tun}}(t)$ and decay rates $\lambda(t)$ for the $K=1$ state for different time-dependent scenarios are shown in Fig. 5. Obviously, the different scenarios are easily distinguishable and constitute a signature of $V(t)$ (see Ref. [16] for further explanations). In Fig. 6, tunneling angular distributions also reveal a strong influence under $\epsilon(t)$. The limiting spherical calculation ($\epsilon = 0$) simply exhibits two peaks corresponding to the spherical harmonic $Y_4^1(\theta, \phi)$, while the deformed $\epsilon = 0.2$ pattern comes from an interplay between the initial wave function structure and the anisotropic potential barrier [17].

Further and more realistic calculations should shed some light on this complex particle decay process.

6 Conclusion

Reliable theoretical calculations of proton decay width $\Gamma_p$ in spherical and deformed nuclei have been performed. Different theoretical approaches have been compared. If one is only interested in the order of magnitude of $\Gamma_p$, simple semi-classical WKB estimates are sufficient. As for getting a better accuracy, the “matching” approach of Maglione et al. should be preferred because of its intrinsic simplicity. Stepping further, the numerical solution of the TDSE describing the time evolution of the emitted proton interacting with the daughter nucleus provides a deeper understanding on this multidimensional quantum tunneling problem. In particular, the computation and experimental observation of angular distributions of p-protons emitted from oriented deformed nuclei could potentially be a powerful test of single-particle nuclear models [18]. Finally, for complex problems where the interacting potential is time-dependent, only a dynamical approach like TDSE can offer valuable physical insights.

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References


Figure 6: Tunneling angular dependencies of $\psi_{1g}$, $\Lambda=1$.