# Asymptotic Behavior of the Wave Packet Propagation through a Barrier: the Green's Function Approach Revisited

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**Abstract.** To model the decay of a quasibound state we use the modified two-potential approach introduced by Gurvitz and Kalbermann [1,2]. This method was used in the past for calculating the decay width and the energy shift of an isolated quasistationary state [5]. We follow the same approach in order to propagate the wave-packet in time with the ultimate goal of extracting the momentum-distribution of emitted particles. The advantage of the method is that it provides the time-dependent wave function in a simple semi-analytic form. We intend to apply this method to the modeling of metastable states for which no direct integration of the time-dependent Schrödinger equation is available today.

The Two Potential Approximation (TPA), introduced in Refs. [1,2], turned out to be an extremely successful tool for the description of a metastable state. Simple expressions based on the TPA made it possible to obtain a very precise estimate of the lifetime of a very narrow resonance without the need of introducing an explicit time dependence. In this work, we use the TPA in order to derive the equations describing the time evolution of the wave function of a particle tunneling through a spherically symmetric barrier.

Let us consider a particle moving in a central potential $V(r)$ with a barrier. Asymptotically, i.e., at large values of $r$, we assume that $V(r)\to 0$. In the TPA, $V(r)$ can be decomposed as

$$V(r) \;=\; U(r) \;+\; W(r)\,, \tag{1}$$

where

$$U(r) = \begin{cases} V(r) & \text{if } r < R \\ V(R) & \text{if } r > R \end{cases} \tag{2}$$

is an auxiliary potential that produces a bound state at energy $E_0$ close to the energy of the metastable state, and $W(r)$ is a "closing" potential which is treated perturbatively. The separation radius $R$ should be chosen far from the classical turning points [3].

At $t$=0 the initial state is taken to be the bound eigenstate $\Phi_0(\vec{r})$ of the auxiliary Hamiltonian

$$H_0 = T + U(r) \tag{3}$$

(we take $\hbar$=1). In the following, we assume that $\Phi_0(\vec{r})$ is well isolated, i.e., it is well separated from the remaining bound states of $U(r)$ having the same quantum numbers. In such a case, at $t$>0, the wave packet represented by the wave function $\Psi(\vec{r},t)$ can be expanded in the basis $\{\Phi_0(\vec{r}), \Phi_k(\vec{r})\}$:

$$\Psi(\vec{r},t) = b_0(t)\Phi_0(\vec{r})e^{-iE_0t} \;+\; \int \frac{d^3k}{(2\pi)^3}\, b_k(t)\Phi_k(\vec{r})e^{-iE_kt}\,, \tag{4}$$

with the initial conditions $b_0(t=0)$=1 and $b_k(t=0)$=0. In Eq. (4) the wave functions $\Phi_k(\vec{r})$ represent the continuum and $E_k = V(R) + k^2/2m$. We shall refer to the first and second terms above as $\Psi_I(\vec{r},t)$ and $\Psi_{II}(\vec{r},t)$, respectively.

To evaluate the two components, $\Psi_I(\vec{r},t)$ and $\Psi_{II}(\vec{r},t)$, we apply the Laplace transform. In terms of the Laplace-transformed expansion coefficients $b(t)$,

$$\tilde{b}(\varepsilon) \;=\; \int_0^\infty b(t)e^{i\varepsilon t}\, dt, \tag{5}$$

the Laplace transform of (4) can be written as

$$\Psi_I(\vec{r},\varepsilon + E_0) = \tilde{b}_0(\varepsilon)\,\Phi_0(\vec{r})\,, \tag{6}$$

$$\Psi_{II}(\vec{r},\varepsilon + E_0) = \int \frac{d^3k}{(2\pi)^3}\, \tilde{\bar{b}}_k(\varepsilon_k)\,\Phi_k(\vec{r})\,, \tag{7}$$

where $\bar{b}_k(t) = e^{-iV(R)t}b_k(t)$ and $\varepsilon_k = \varepsilon + E_0 + V(R) - E_k$.

Assuming a spherically symmetric potential $V(r)$, the coefficient $\tilde{b}_0(\varepsilon)$ is given by [2]

$$\tilde{b}_0(\varepsilon) \;=\; \frac{i}{\varepsilon - \varepsilon_0}\,, \tag{8}$$

with

$$\varepsilon_0 = \Delta - i\,\frac{\Gamma}{2} \;=\; -\sqrt{\frac{\pi}{2}}\,\frac{|\phi_0(R)|^2}{2mk_0}\,[\alpha\chi_{lk_0}(R) + \chi'_{lk_0}(R)]\,[\alpha\chi^{(+)}_{lk_0}(R) + \chi^{(+)\prime}_{lk_0}(R)]\,, \tag{9}$$

where $\alpha = \sqrt{2m(V_0 - E_0)}$ and $k_0 = \sqrt{2m(E_0 + \varepsilon_0)}$. In this work, $\phi_0(r)$ is the radial wave function of $\Psi_0$, and $\chi_{lk}(r)$ and $\chi_{lk}^{(+)}(r)$ are, respectively, the regular and outgoing waves of the Hamiltonian with the potential $\tilde{W}(r) = W(r) + V(R)$. Note that our radial continuum functions satisfy the orthogonality and completeness relationships

$$\int_0^\infty \chi_{lk}^*(r)\, \chi_{lk'}(r)\; dr \;=\; \delta(k - k')\,, \tag{10}$$

$$\int_0^\infty \chi_{lk}^*(r)\, \chi_{lk}(r')\; dk \;=\; \delta(r - r')\,. \tag{11}$$

Compared with expressions in Refs. [1,2], this results in an additional factor of $\sqrt{\pi/2}$ in the front of every $\chi$ [4].

With the above definitions, the radial part of the first component in Eq. (4) is

$$\psi_I(r,t) \;=\; \frac{\phi_0(r)}{r}\; e^{-i(E_0+\varepsilon_0)t}\,. \tag{12}$$

The coefficients $\tilde{\tilde{b}}_k(\varepsilon_k)$ are determined by solving the system of integral equations

$$\varepsilon\tilde{b}_0(\varepsilon) = i + W_{00}\tilde{b}_0(\varepsilon) + \int \frac{d^3k}{(2\pi)^3}\; \tilde{W}_{0k}\tilde{\tilde{b}}_k(\varepsilon_k)\,, \tag{13}$$

$$\varepsilon_k\tilde{\tilde{b}}_k(\varepsilon_k) = W_{k0}\tilde{b}_0(\varepsilon) + \int \frac{d^3k'}{(2\pi)^3}\; \tilde{W}_{kk'}\tilde{\tilde{b}}_{k'}(\varepsilon_{k'})\,,$$

with $\tilde{W}_{kk'} \equiv \langle\Phi_k|\tilde{W}|\Phi_{k'}\rangle$. The solution of (13) can be formally written as

$$\tilde{\tilde{b}}_k(\varepsilon_k) = \frac{1}{\varepsilon_k}\,\langle\Phi_k\,|\Big(1 \;+\; \tilde{W}\tilde{G}_0 \;+\; \tilde{W}\tilde{G}_0\tilde{W}\tilde{G}_0 \;+\; \cdots\Big)\,W\,|\,\Phi_0\rangle\;\tilde{b}_0(\varepsilon)\,,$$

where

$$\tilde{G}_0 \;=\; \int \frac{d^3k}{(2\pi)^3}\;\frac{|\Phi_k\rangle\,\langle\Phi_k|}{\varepsilon_k}\,. \tag{14}$$

The outgoing part of the wave function, $\Psi_{II}(\vec{r},\varepsilon)$, can now be expressed in terms of $\Psi_I(\vec{r},\varepsilon)$ as

$$\tilde{\Psi}_{II}(\vec{r},\varepsilon + E_0) = \int d^3r'\; \tilde{G}(\varepsilon + E_0; \vec{r}\,', \vec{r}\,')\; W(r')\; \tilde{\Psi}_I(\vec{r},\varepsilon + E_0)\,, \tag{15}$$

where we now introduce the Green's function

$$\tilde{G}(E) = \tilde{G}_0(E) + \tilde{G}_0(E)\,\tilde{W}\,\tilde{G}(E) \;=\; (1 - \Lambda)(E - H + \Lambda\tilde{W})^{-1}, \tag{16}$$

with $\Lambda = |\Phi_0\rangle\langle\Phi_0|$ being the projection operator on $\Phi_0$. The Green's function $\tilde{G}(E)$ is approximated in the spirit of Ref. [2] by neglecting the contribution from

$\Lambda$, and then by replacing the potential $V(r)$ by $\tilde{W}(r)$. This gives $\tilde{G}(E) \approx G_{\tilde{W}}(E)$, where

$$G_{\tilde{W}}(E) = (E - H_{\tilde{W}})^{-1} \tag{17}$$

is the Green's function of $H_{\tilde{W}} = T + \tilde{W}$.

By taking the inverse Laplace transform of (7), one obtains for the radial wave function

$$\psi_{II}(r,t) = \frac{1}{2\pi} \int_R^\infty r' dr' \; W(r')\phi_0(r') \int_{i\gamma-\infty}^{i\gamma+\infty} d\varepsilon \; e^{-i\varepsilon t} G_{\tilde{W}}(\varepsilon; r, r')\tilde{b}_0(\varepsilon - E_0) \, . \tag{18}$$

The $\varepsilon$-integral is evaluated using the residue theorem and results in the sum of the residues corresponding to the two poles of the integrand.

## Contribution due to the pole of $\tilde{b}_0(\varepsilon - E_0)$

Using the standard techniques explained in Ref. [2], we obtain

$$\psi_{II,a}(r < R, t) = \sqrt{\frac{\pi}{2}} \, \frac{\phi_0(R)}{k_0 r} \; [\alpha \chi^{(+)}_{lk_0}(R) + \chi^{(+)\prime}_{lk_0}(R)] \; \chi_{lk_0}(r) \; e^{-i(E_0+\varepsilon_0)t} \, , \tag{19}$$

and

$$\begin{aligned} \psi_{II,a}(r > R, t) = &- \frac{\phi_0(r)}{r} \; e^{-i(E_0+\varepsilon_0)t} \\ &+ \sqrt{\frac{\pi}{2}} \frac{\phi_0(R)}{k_0 r} [\alpha \chi_{lk_0}(R) + \chi'_{lk_0}(R)] \chi^{(+)}_{lk_0}(r) e^{-i(E_0+\varepsilon_0)t} \, . \end{aligned} \tag{20}$$

Note that for $r > R$ the contribution from $\psi_I$ is exactly cancelled by the first term in (20).

## Contribution due to the pole of the Green's function

The Green's function $G_{\tilde{W}}$ has a continuum of simple poles along the real $E > 0$ axis. After using the spectral representation of $G_{\bar{W}}(\varepsilon; r, r')$, one can express $\psi_{II,b}(r,t)$ as

$$\psi_{II,b}(r,t) = \frac{2m}{r} \int_R^\infty dr' \; W(r') \; \phi_0(r') \int_0^\infty dk \; \frac{e^{-i\frac{k^2}{2m}t}}{k^2 - k_0^2} \; \chi_{lk}(r) \, \chi^*_{lk}(r') \, . \tag{21}$$

The evaluation of the integral (21) represents the cornerstone of the present approach.

For now we will restrict ourselves to making some remarks regarding the asymptotic behavior of this integral at large values of $r$. We shall also assume that the potential $V(r)$ has finite range (i.e., it vanishes at large values of $r$). While this assumption cannot be used for the case of the Coulomb potential, it is still interesting to investigate the general structure of the solution for the short-range potential. In this limit, the $S$-matrix is meromorphic in the complete complex $k$-plane and [4,6]

$$[S_l(k)]^* = S_l(-k^*), \quad \text{and} \quad S_l(k) = [S_l(-k)]^{-1}. \tag{22}$$

Expressing $\chi_{lk}(r)$ in the asymptotic form:

$$\chi_{lk}(r) = \sqrt{\frac{2}{\pi}}\frac{1}{2i}\left(S_l^{1/2}(k)e^{ikr} - S_l^{-1/2}(k)e^{-ikr}\right), \tag{23}$$

one obtains for the $k$-integral in (21):

$$I(r,r',t) = \int_0^\infty dk\, \frac{e^{-i\frac{k^2}{2m}t}}{k^2-k_0^2}\, \chi_{lk}(r)\, \chi_{lk}^*(r') \tag{24}$$

$$\asymp \frac{1}{2\pi}\int_{-\infty}^\infty dk\, \frac{e^{-i\frac{k^2}{2m}t}}{k^2-k_0^2}\left[e^{ik(r-r')} - (-)^l\, S_l(k)\, e^{ik(r+r')}\right]. \tag{25}$$

The integrand in Eq. (25) is a sum involving two complex functions of complex $k$,

$$\frac{1}{k^2-k_0^2}, \qquad \text{and} \qquad \frac{S_l(k)}{k^2-k_0^2}, \tag{26}$$

which have common poles at $\pm k_0$. In addition, $S_l(k)$ has an infinite number of simple poles. They are located in the lower half of the complex $k$-plane, symmetrically with respect to the imaginary axis. Following the notation of van Dijk and Nogami [7], we shall denote the poles in the fourth quadrant with $k_\nu, \nu = 1, 2, 3, \ldots$, and the poles in the third quadrant with $k_\nu, \nu = -1, -2, -3, \ldots$ It follows from Eq. (22) that

$$\mathrm{Re}(k_\nu) = -\mathrm{Re}(k_{-\nu}), \qquad \mathrm{Im}(k_\nu) = \mathrm{Im}(k_{-\nu}). \tag{27}$$

In the following, the residue of the $S_l(k)$ at the pole $k_\nu$ is denoted by $b_\nu$.

Since the complex function (26) has no essential singularity at infinity, we can apply the Mittag-Leffler theorem in order to obtain a pole expansion for (26). The pole at $k{=}-k_0$ lies in the upper half of the $k$-plane; hence it does not contribute to the integral. Consequently, Eq. (26) can be replaced by

$$\frac{1}{2k_0}\frac{1}{k-k_0}, \qquad \text{and} \tag{28}$$

$$\frac{S_l(k_0)}{2k_0}\frac{1}{k-k_0} + \sum_{\nu=-\infty}^{\infty}\frac{b_\nu}{k_\nu^2-k_0^2}\,\frac{1}{k-k_\nu}. \tag{29}$$

By substituting Eqs. (28) and (29) in (25), the integral (25) becomes

$$
I(r,r',t) = \frac{1}{4\pi\, k_0} \int_{-\infty}^{\infty} dk\ \frac{e^{-i\frac{k^2}{2m}t} e^{ik(r-r')}}{k-k_0} \tag{30}
$$
$$
- \frac{(-)^l}{2\pi} \left[ \frac{S_l(k_0)}{2k_0} \int_{-\infty}^{\infty} dk\, \frac{e^{-i\frac{k^2}{2m}t} e^{ik(r+r')}}{k-k_0} + \sum_{\nu=-\infty}^{\infty} \frac{b_\nu}{k_\nu^2 - k_0^2} \int_{-\infty}^{\infty} dk \frac{e^{-i\frac{k^2}{2m}t} e^{ik(r+r')}}{k-k_\nu} \right].
$$

The above can now be expressed in terms of the Moshinsky function

$$
\begin{aligned}
M\left(k,\mathcal{R},\tau\right) &= \frac{i}{2\pi} \int_{-\infty}^{\infty} dp\ \frac{e^{-ip^2\tau}\, e^{-ip\mathcal{R}}}{p-k} \\
&= \frac{1}{2}\, e^{-ik^2\tau}\, e^{-ik\mathcal{R}}\ \mathrm{erfc}(y)\,,
\end{aligned} \tag{31}
$$

where

$$
y \ = \ e^{-i\pi/4}\, \sqrt{\tau}\, \left( \frac{\mathcal{R}}{2\tau} - k \right)\,,
$$

where $\tau = t/2m$ and $\mathcal{R} = r \pm r'$. The integral $I(r,r',t)$ can now be calculated in the closed form:

$$
\frac{1}{2i\, k_0} \left[ M\left(k_0, r-r', \frac{t}{2m}\right) \ - \ (-)^l\, S_l(k_0)\ M\left(k_0, r+r', \frac{t}{2m}\right) \right] \tag{32}
$$
$$
+\, i\, (-)^l \sum_{\nu=-\infty}^{\infty} \frac{b_\nu}{k_\nu^2 - k_0^2}\ M\left(k_\nu, r+r', \frac{t}{2m}\right)\,.
$$

This concludes our derivation.

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