Resonance expansions in quantum mechanics

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Received 29 July 2005

The goal of this contribution is to discuss various resonance expansions that have been proposed in the literature.

PACS: 3.65-w
Key words: Resonance expansions; Gamow states

1 Introduction

The Gamow (or resonance) states are the wave functions of resonances. These states are eigensolutions of the Schrödinger equation subject to a "purely outgoing boundary condition." The Gamow states were introduced by Gamow [1] in 1928 to describe α decay (see also [2]). Some years later, in 1939, Siegert made use of the Gamow states to obtain a resonance expansion of the scattering function for potentials of finite range [3] which was further developed by Humblet and Rosenfeld [4]. In 1955, Peierls pointed out the relationship between the residues of the propagator at the resonance poles and the Gamow states [5]. The properties of the Gamow states and its applications have been considered by many authors, see for example [6–20]. A pedestrian introduction to these states can be found in [21].

The Gamow states can be used to obtain resonance expansions of wave functions and propagators. The purpose of this paper is to discuss the main features of several of such expansions and to point out some of their differences. For the sake of simplicity, we shall restrict our discussion to potentials of finite range. The potentials will be three dimensional and spherically symmetric except in Section 4, where they will be assumed to be one dimensional.

2 Berggren's and Berggren-like resonance expansions

In order to derive Berggren's expansion [8], we start out with a completeness relation in terms of the bound and scattering states,

$$1=\sum_{n=1}^{N_{\rm b}}|K_n\rangle\langle K_n|+\int_0^\infty {\rm d}k\,|k^+\rangle\langle^+k|\,, \tag{1}$$

where 1 is the identity operator, $|K_n\rangle$ are the bound states and $|k^+\rangle$ are the scattering states. We are assuming that the potential holds $N_{\rm b}$ bound states. By deforming the integral of Eq. (1) into the contour $\Gamma_{\rm B}$ of Fig. 1, and by using Cauchy's theorem, we extract the contributions from the resonance states that are hidden in the continuum integral and write them in the same form as the bound state contributions:

$$1=\sum_{n=1}^{N_{\rm b}}|K_n\rangle\langle K_n|+\sum_{n=1}^{N_{\rm B}}|k_n^+\rangle\langle^+k_n|+\int_{\Gamma_{\rm B}} {\rm d}k\,|k^+\rangle\langle^+k|\,, \tag{2}$$

where $|k_n^+\rangle$ is the Gamow state corresponding to the nth resonance, and $N_{\rm B}$ is the number of resonances that lie in between the real axis and the contour $\Gamma_{\rm B}$. The integral in Eq. (2) is called the background.

Berggren's expansion includes only those few resonances that are supposed to be the most important in the energy range of interest. The background integral is usually assumed to give a negligible contribution in such energy range. However, the background need not always be negligible. For example, virtual poles influence low energy scattering, and the background integral in Eq. (2) cannot be neglected at low energies. (Of course, one can easily deform the contour $\Gamma_{\rm B}$ to include explicitly the effect of the virtual poles.) As well, even when the background integral is negligible, it is never zero. This is due to the fact that the bound and resonance states do not form a complete basis, and one has to include an additional sets of kets to obtain a complete basis. When the background integral is not negligible, which is the usual case encountered in applications, one needs to estimate it. For Berggren's expansion, a discretization of the background integral yields such estimation [16].

One can construct Berggren expansions of the Hamiltonian H, the resolvent $1/(z-H)$ and the evolution operator ${\rm e}^{-{\rm i}Ht}$ by simply letting those operators act on Eq. (2).

Berggren's expansion (2), sometimes with slight modifications, is the one most oftenly used in nuclear physics [12, 13, 16, 19].

Needless to say, the completeness relation (2) is a formal expression that must be understood within the rigged Hilbert space as part of a "sandwich" with well-behaved wave functions f and g:

$$(f,g)=\sum_{n=1}^{N_{\rm b}}\langle f|K_n\rangle\langle K_n|g\rangle+\sum_{n=1}^{N_B}\langle f|k_n^+\rangle\langle^+k_n|g\rangle+\int_{\Gamma_B} {\rm d}k\,\langle f|k^+\rangle\langle^+k|g\rangle\,. \tag{3}$$

Expression (3) is valid only when the wave functions $f(r)$ and $g(r)$ fall off at infinity faster than any exponential.

As we mentioned above, Berggren's expansion includes only the resonances that carry the most influence in the energy range under consideration. One can incorporate the contribution of other resonances by enclosing other poles of the fourth quadrant of the k-plane. For example, by using the contour $\Gamma_{\rm M}$ of Fig. 1, one obtains [17]

$$1=\sum_{n=1}^{N_{\rm b}}|K_n\rangle\langle K_n|+\sum_{n=1}^{N_{\rm M}}|k_n^+\rangle\langle^+k_n|+\int_{\Gamma_{\rm M}}{\rm d}k\,|k^+\rangle\langle^+k|\,, \tag{4}$$

where $N_{\rm M}$ is the number of (proper) resonances in between the contour Γ_M and the real axis. By substituting $|k^+\rangle = S(k)|k^-\rangle$ into Eq. (1), where $S(k)$ is the S matrix and $|k^-\rangle$ is the "out" Lippmann-Schwinger ket, and by using the contour $\Gamma_{\rm BG}$ of Fig. 1, one obtains another expansion [11]:

$$1=\sum_{n=1}^{N_{\rm b}}|K_n\rangle\langle K_n|+\sum_{n=1}^{N_{\rm BG}}|k_n^-\rangle\langle^+k_n|+\int_{\Gamma_{\rm BG}}{\rm d}k\,|k^-\rangle S(k)\langle^+k|\,, \tag{5}$$

where $N_{\rm BG}$ is the number of resonances in the fourth quadrant of the complex plane. One can also include virtual states in an obvious way.

Likewise the completeness relation (2), the completeness relations (4) and (5) are to be understood as part of a "sandwich" with well-behaved functions f and g. However, unlike the completeness relation (2), the completeness relations (4) and (5) do not make sense as they stand. The reason is that, in order to properly derive those expansions, it is necessary that the analytic continuation of the integrands $\langle g|k^+\rangle\langle^+k|f\rangle$ and $\langle g|k^-\rangle S(k)\langle^+k|f\rangle$ tends to zero as k tends to infinity in the fourth quadrant of the complex plane. However, those integrands diverge exponentially in that limit. For example, if $f(r)$ is an infinitely differentiable function with compact support, then its wave number representation $f(k)=\langle^+k|f\rangle$ diverges exponentially on the infinite arc. Therefore, one has to use either a regulator or a time-dependent approach:

$${\rm e}^{-{\rm i}Ht}=\sum_{n=1}^{N_{\rm b}}{\rm e}^{-{\rm i}K_n^2t}|K_n\rangle\langle K_n|+\sum_{n=1}^{N_{\rm BG}}{\rm e}^{-{\rm i}k_n^2t}|k_n^+\rangle\langle^+k_n|+\int_{\Gamma_{\rm M}}{\rm d}k\,{\rm e}^{-{\rm i}k^2t}|k^+\rangle\langle^+k|\,,\quad t>0\,. \tag{6}$$

The expansions (4) and (5) are now understood as the (singular!) limit when $t\to 0$ of the expansion (6). Note that the expansion (6) is valid for $t>0$ only, yet another reminder that resonances ought to be understood in a time-asymmetric, time-dependent manner. We shall further discuss time-dependent expansions in the next section.

A side effect of the divergence of the integrand $\langle g|k^-\rangle S(k)\langle^+k|f\rangle$ at the infinite arc is that the so-called "Hardy axiom" [11, 22] is flawed. The reason is that the "Hardy axiom" assumes that $\langle f|k^-\rangle$ and $\langle^+k|g\rangle$ are Hardy functions, and therefore $\langle f|k^-\rangle$ and $\langle^+k|g\rangle$ should tend to zero in the infinite arc of the fourth quadrant of the complex k-plane. On the contrary, the quantum mechanical wave functions $\langle f|k^-\rangle$ and $\langle^+k|g\rangle$ diverge (exponentially!) in that limit, and therefore they cannot be Hardy functions.

3 Time-dependent expansions

3.1 Expansion involving proper resonance poles

As is well known, the solution $\psi(t)$ to the time-dependent Schrödinger equation may be written in terms of the retarded time evolution operator $\exp(-\mathrm{i}Ht)$, where $t \geq 0$, and of the known arbitrary initial state $\psi(0)$ as

$$\psi(t) = \mathrm{e}^{-\mathrm{i}Ht}\psi(0)\,. \tag{7}$$

In coordinate representation, the retarded Green function $g(r, r'; t) = \langle r|\mathrm{e}^{-\mathrm{i}Ht}|r'\rangle$ may be written, using the Laplace transform, as [9]

$$g(r, r'; t) = \frac{\mathrm{i}}{2\pi}\int_{C_\circ} \mathrm{d}k\, G^+(r, r'; k)\, \mathrm{e}^{-\mathrm{i}k^2 t}\, 2k\,, \tag{8}$$

where $G^+(r, r'; k)$ denotes the outgoing, time-independent Green function. The contour $C_\circ$ runs parallel to the positive imaginary k-axis and bends close to the origin to run parallel to the positive real k-axis, staying always in the first quadrant of the complex k-plane, see Fig. 1. It is possible to expand the time-dependent Green function in terms of the resonance states plus a background integral by deforming appropriately the contour $C_\circ$ in the k-plane [9]. Since the variation of $G^+(r, r'; k)$ with k complex is at most exponential [23], the behavior of the integrand with k in Eq. (8) is dominated by $\exp(-\mathrm{i}k^2 t)$. A convenient choice is to deform $C_\circ$ to a contour involving two semi-circles C_s along the second and fourth quadrants of the k-plane plus a straight line C_L that passes through the origin at 45° off the real k-axis. In doing so, one passes over some poles of the outgoing Green function. In general, these include bound states and the subset of complex poles associated with the so-called proper resonance states, i.e., those poles for which $\mathrm{Re}\, k_p > \mathrm{Im}\, k_p$. By extending the integration contour up to infinity, one obtains that the semi-circles C_s yield a vanishing contribution, so one is left with a infinite sum of terms plus an integral contribution [9]:

$$\begin{aligned} g(r, r'; t) \quad &= \quad \sum_{p=1}^{\infty} u_p(r) u_p(r')\mathrm{e}^{-\mathrm{i}k_p^2 t} \\ &\quad + \frac{\mathrm{i}}{2\pi}\int_{C_L} \mathrm{d}k\, G^+(r, r'; k)\, \mathrm{e}^{-\mathrm{i}k^2 t}\, 2k\,, \end{aligned} \tag{9}$$

where, without loss of generality and for the sake of simplicity of the expressions, we have omitted the bound states. In the last equation, the sum runs through the proper resonance poles –hence the subscript p– of the outgoing Green function. In deriving expression (9), one uses that the residue of $G^+(r, r'; k)$ at the complex pole k_p is $u_p(r)u_p(r)/2k_p$, and that the resonance states are normalized according to the following condition [9]:

$$\int_0^R \mathrm{d}r\, u_p^2(r) + \mathrm{i}\frac{u_p^2(R)}{2k_p} = 1\,, \tag{10}$$

where R denotes the radial coordinate from which the potential vanishes. Note that the integral term in Eq. (9) may be written as an integral along the contour Γ_{M}.

3.2 Expansion involving the full set of poles and resonance states

One may obtain an expansion involving the full set of bound, virtual, resonance and anti-resonance states (the latter associated with the third-quadrant poles of the S matrix) by noting that the contour in Eq. (8) may be deformed into a semi-circle C_s' along the third quadrant of the k-plane plus an integral term along the real k-axis. By extending the integration contour up to infinity, we again obtain that the contribution of the semi-circle vanishes and we are left with the expression

$$g(r,r';t) = \frac{\mathrm{i}}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k\, G^+(r,r';k)\mathrm{e}^{-\mathrm{i}k^2 t}\, 2k\,. \tag{11}$$

It turns out that under the condition $r,\, r' < R$, one may use the Cauchy expansion of the outgoing Green function

$$G^+(r,r';k) = \frac{1}{2k}\sum_{n=-\infty}^{\infty}\frac{u_n(r)u_n(r')}{(k-k_n)}\,, \qquad r,\, r' < R\,, \tag{12}$$

where the anti-resonance poles correspond to negative integer values of n. The above expression still holds when either r or r', but not both, equals R. To our knowledge, the above result was first reported, for a solvable model, by More [24]. It has been proved in the s-wave case for potentials of finite range by García-Calderón and Berrondo [25], and it has been used by several authors, see for example [26–28]. The expansion given by Eq. (12) implies that the Gamow states satisfy the relationships

$$\sum_{n=-\infty}^{\infty}\frac{u_n(r)u_n(r')}{k_n} = 0\,, \qquad r, r' < R\,, \tag{13}$$

and

$$\frac{1}{2}\sum_{n=-\infty}^{\infty} u_n(r)u_n(r') = \delta(r-r')\,, \qquad r, r' < R\,. \tag{14}$$

Substitution of Eq. (12) into Eq. (11) yields [29]

$$g(r,r';t) = \sum_{n=-\infty}^{\infty} u_n(r)u_n(r')M(k_n,t)\,, \quad r, r' < R\,, \tag{15}$$

where the M function is defined as

$$\begin{aligned} M(k_n,t) &= \frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}k\,\frac{\mathrm{e}^{-\mathrm{i}k^2 t}}{k-k_n} \\ &= \frac{1}{2}w(\mathrm{i}y_n). \end{aligned} \tag{16}$$

The function w is the complex error function [30]:

$$w(z) = \exp(-z^2)\mathrm{erfc}(-\mathrm{i}z)\,. \tag{17}$$

The argument y_n is given by

$$y_n = -\mathrm{e}^{-\mathrm{i}\pi/4} k_n t^{1/2} \,. \tag{18}$$

One may write the above solutions in a form that exhibits explicitly its exponential and non-exponential contributions by writing them in terms of an expansion involving the complex poles of the fourth quadrant of the k-plane:

$$g(r,r';t) = \sum_{p=1}^{\infty} \{u_p(r)u_p(r')\mathrm{e}^{-\mathrm{i}k_p^2 t} - [u_p(r)u_p(r')M(-k_p,t) - u_p^*(r)u_p^*(r')M(-k_p^*,t)]\} \,, \tag{19}$$

where we have used that the poles of the third quadrant satisfy, from time reversal considerations, that $k_{-p} = -k_p^*$ and that $u_{-p} = u_p^*$. Also, we have made use of the following symmetry of the w functions [30]:

$$w(\mathrm{i}y_p) = 2\mathrm{e}^{y_p^2} - w(-\mathrm{i}y_p) \,, \tag{20}$$

which holds when the argument y_p lies within the limits

$$\pi/2 < \arg y_p < 3\pi/2 \,. \tag{21}$$

This last condition is fulfilled by the proper poles of the fourth quadrant.

We note that, contrary to all previous expansions, the expansion (15) first yields an estimation of the background integral when $r, r' < R$, second it is valid when $r, r' < R$, and third it includes the contribution of the anti-resonance states explicitly.

4 Resonance expansions and the steepest descent method

Resonance expansions of the wave function in coordinate or momentum representations, and of survival amplitudes arise naturally when calculating the corresponding integrals with the steepest descent technique. The important point is that, even though the poles are the same as in other approaches (say poles of the transmission amplitude in one-dimensional scattering), their contributions may differ. In this paper, we shall illustrate the basic idea in coordinate representation and for one-dimensional scattering off a potential with support $[0,d]$, although similar manipulations can be performed in other cases. Instead of the wave number k, in this section we shall use $p/\hbar$, p being the momentum.

Assume that the wave packet is initially confined to the left of the potential so that it can be written, in terms of its initial momentum representation $\phi(p)$ and the scattering eigenstates of H, ψ_p, as

$$\langle x|\psi(t)\rangle = \int_C \mathrm{d}p\, \langle x|\psi_p\rangle \mathrm{e}^{-\mathrm{i}Et/\hbar}\phi(p) \tag{22}$$

where

$$\langle x|\psi_p\rangle = h^{-1/2} \begin{cases} \mathrm{e}^{\mathrm{i}px/\hbar} + R(p)\mathrm{e}^{-\mathrm{i}px/\hbar} & x \le 0 \\ T(p)\mathrm{e}^{\mathrm{i}px/\hbar} & x \ge d \,, \end{cases} \tag{23}$$

and C goes from $-\infty$ to ∞ above all singularities. The coefficients $R(p)$ and $T(p)$ are the reflection and transmission amplitudes for $p > 0$, continued analytically elsewhere. The transmitted wave packet may then be written as

$$\langle x|\psi(t)\rangle = h^{-1/2} \int_C \mathrm{d}p\, \mathrm{e}^{\mathrm{i}xp/\hbar} \mathrm{e}^{-\mathrm{i}Et/\hbar} T(p)\phi(p)\,, \tag{24}$$

and the contour C may be deformed along the steepest descent path.

These integrals may be written in the form

$$\mathcal{I} = \int_C \mathrm{d}k\, \mathrm{e}^{-\mathrm{i}(ak^2+kb)} g(k). \tag{25}$$

In simple cases, $g(k)$ is a meromorphic function. The saddle point of the exponent is at $k = -b/2a$, and the steepest descent path is the straight line $\mathrm{Im}(k) = -(\mathrm{Re}(k) + b/2a)$. By completing the square, introducing the new variable u,

$$u = (k + b/2a)/f, \quad f = (1 - \mathrm{i})(m\hbar/t)^{1/2}, \tag{26}$$

which is real on the steepest descent path and zero at the saddle point, and mapping the contour to the u-plane, the integral takes the form

$$\mathcal{I} = \mathrm{e}^{\mathrm{i}mx^2/\hbar t} f \int_{C_u} \mathrm{d}u\, \mathrm{e}^{-u^2} G(u), \tag{27}$$

where $G(u) \equiv g[k(u)]$. It is now useful to separate the pole singularities explicitly and write G as

$$G(u) = \sum_j \frac{A_j/f}{u - u_j} + H(u), \tag{28}$$

where A_j/f is the residue of $G(u)$ at $u = u_j$ and the remainder, $H(u)$, is obtained by substraction. Note that $H(u)$ is an entire function if G is meromorphic.

The integral $\mathcal{I}$ is thus separated into two integrals, $\mathcal{I} = \mathcal{I}' + \mathcal{I}''$. The first one may be reduced to known functions by deforming the contour along the steepest descent path (real-u axis) and taking proper care of the pole contribution,

$$\begin{aligned} \mathcal{I}' &\equiv \mathrm{e}^{\mathrm{i}mx^2/\hbar t} \sum_j A_j \int_{C_u} \mathrm{d}u\, \frac{\mathrm{e}^{-u^2}}{u - u_0} \\ &= -\mathrm{i}\pi \mathrm{e}^{\mathrm{i}mx^2/\hbar t} \sum_j A_j w(-u_j)\,. \end{aligned} \tag{29}$$

The second integral, which involves the remainder H, must in general be evaluated numerically,

$$\mathcal{I}'' \equiv \mathrm{e}^{\mathrm{i}mx^2/\hbar t} f \int_{C_u} \mathrm{d}u\, H(u). \tag{30}$$

However, the computational effort is greatly reduced by deforming the contour along the steepest descent path, too. When it is an entire function, it may be expressed as a series by expanding $H(u)$ around the origin and integrating term by term,

$$\begin{aligned}\mathcal{I}'' &= \mathrm{e}^{imx^2/\hbar t} f \pi^{1/2} \Bigg[H(u=0) \\ &+ \sum_{n=1}^{\infty} \frac{1 \times 3 \times ... \times (2n-1)}{2^n (2n)} H^{(2n)}(u=0) \Bigg] ,\end{aligned} \tag{31}$$

In practical applications, the first term alone gives already a very good approximation. Note the basic role of the w-functions, which may be thought of as the elementary transient mode propagators of the Schrödinger equation. Long and short time formulae are easily obtained from asymptotic expansions of $w(z)$.

For applications of this technique to describe different transient phenomena, see for example [31–33].

5 Complex, effective Hamiltonians

As we shall see in this section, truncation of resonance expansions enable us to understand the origin of complex, effective Hamiltonians.

If we apply the Hamiltonian to the Berggren expansion (2), we obtain

$$H = \sum_{n=1}^{N_{\mathrm{b}}} K_n^2 \, |K_n\rangle\langle K_n| + \sum_{n=1}^{N_{\mathrm{B}}} k_n^2 \, |k_n^+\rangle\langle^+ k_n| + \int_{\Gamma_{\mathrm{B}}} \mathrm{d}k \, k^2 \, |k^+\rangle\langle^+ k| \, , \tag{32}$$

Thus, the Hamiltonian can be split into a sum of bound, resonance and background contributions:

$$H = H_{\mathrm{bound}} + H_{\mathrm{resonance}} + H_{\mathrm{background}} \, . \tag{33}$$

In matrix notation, one can write this equation as a diagonal matrix,

$$H = \begin{pmatrix} K_1^2 & & & & & & & \\ & \ddots & & & & & & \\ & & K_{N_{\mathrm{b}}}^2 & & & & & \\ & & & k_1^2 & & & & \\ & & & & k_2^2 & & & \\ & & & & & \ddots & & \\ & & & & & & k_{N_{\mathrm{B}}}^2 & \\ & & & & & & & (k^2)_{\mathrm{bg}} \end{pmatrix} . \tag{34}$$

When, for example, the first and second resonances are the most important to the problem under consideration, we can neglect everything but the contribution of those two resonances. The corresponding effective, complex Hamiltonian arises in a natural way:

$$H = \begin{pmatrix} k_1^2 & 0 \\ 0 & k_2^2 \end{pmatrix}. \qquad (35)$$

When double poles come into play, the effective Hamiltonians have non-diagonal terms [17]. Note that, contrary to PT-symmetric Hamiltonians, the eigenvalues of this effective Hamiltonian are complex.

Acknowledgement

RM acknowledges financial support from the Basque Government through reintegration fellowship No. BCI03.96.

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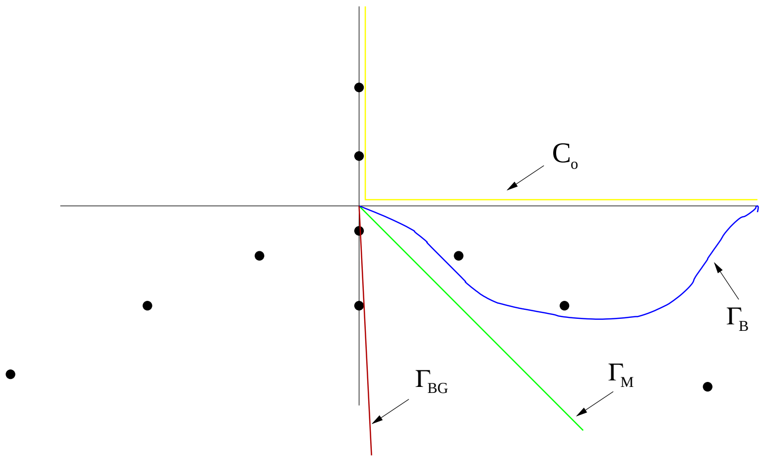

Fig. 1. Different contours yield different expansions. The bullets represent the bound, resonance, anti-resonance and virtual poles.