Complex density of continuum states in resonant quantum tunneling

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We introduce a complex-extended continuum level density and apply it to one-dimensional scattering problems involving tunneling through finite-range potentials. We show that the real part of the density is proportional to a real “time shift” of the transmitted particle, while the imaginary part reflects the imaginary time of an instanton-like tunneling trajectory. We confirm these assumptions for several potentials using the complex scaling method. In particular, we show that stationary points of the potentials give rise to specific singularities of both real and imaginary densities which represent close analogues of excited-state quantum phase transitions in bound systems.

The density of discrete energy spectra of bound quantum systems forms a bridge between classical and quantum mechanics. The derivation of so-called trace formulas in the 1970’s [1–3] showed that detailed information on quantum spectra is deducible from purely classical properties of the system. While the oscillatory component of the level density is related to classical periodic orbits, the smooth component is determined by the size of the accessible phase space at given energy $E$. Non-analyticities of the phase-space volume function lead to singularities of quantal spectra known as the excited-state quantum phase transitions (ESQPTs) [4–8]. In particular, for one-dimensional (1D) systems, these singularities express anomalous time relations caused by discontinuous or divergent periods of classical orbits.

The question addressed in this work is whether the densities of continuum energy eigenstates in unbound systems [9, 10] allow for similar semiclassical interpretations. Such systems participate in fundamental processes including molecules, atoms, nuclei and elementary particles [11, 12]. Quantum tunneling, besides being considered to play an essential role in the evolution of early universe [13], represents an important tool of modern technologies (see e.g. Ref. [14]). Time relations in scattering and tunneling processes and their semiclassical foundations are vividly discussed topics [15, 16], which with recent advent of the attosecond metrology become available to experimental study (see e.g. Ref. [17]).

We focus on 1D scattering problems involving resonant tunneling in multibarrier potentials $V(x)$. These processes have no direct classical counterparts, but their analogues have been searched in terms of a complex generalization of classical mechanics [18–22]. Our present work brings new arguments supporting these efforts. We find that a suitable complexly defined continuum level density reflects complex times deduced from generalized semiclassical dynamics involving instanton-like solutions. Moreover, we demonstrate that real and imaginary components of the continuum level density show ESQPT-like singularities associated with classical stationary points of potentials $V(x)$ and $-V(x)$ applied, respectively, in the allowed and forbidden regions.

Let $\hat{H}$ and $\hat{H}^{(0)}$ be Hamiltonians with continuous energy spectra describing an unbound quantum system with and without interaction, respectively. The continuum level density used in the corresponding scattering problems has been defined [9, 10] as

$$\delta \rho(E) = \lim_{\epsilon \to 0} \frac{1}{\pi} \text{Im} \text{Tr} \left[ \hat{G}(E+i\epsilon) - \hat{G}^{(0)}(E+i\epsilon) \right],$$

(1)

where $\hat{G}(E) = 1/(E-\hat{H})$ and $\hat{G}^{(0)}(E) = 1/(E-\hat{H}^{(0)})$ are Green operators associated with $\hat{H}$ and $\hat{H}^{(0)}$. Our present approach differs from this in two points: (a) we assume that both interacting and free Hamiltonians have discrete sets of complex eigenvalues and (b) we introduce the continuum level density $\Delta \rho(\mathcal{E})$ as a complex function in the complex energy domain $\mathcal{E} = E - \frac{i}{2} \Gamma$. Point (a) is realized by application of the so-called complex scaling method in combination with a finite-box approximation [23–26]. The method makes use of a similarity transformation with a non-unitary operator $\tilde{S}$, which maps the original Hamiltonians to equivalent non-Hermitian images $\tilde{H}_{\text{NH}} = \tilde{S} \hat{H} \tilde{S}^{-1}$ and $\tilde{H}_{\text{NH}}^{(0)} = \tilde{S} \hat{H}^{(0)} \tilde{S}^{-1}$. For a finite box size, these images have discrete sets of complex eigenvalues $\xi_k = E_k - \frac{1}{2} \Gamma_k$ and $\xi_k^{(0)} = E_k^{(0)} - \frac{1}{2} \Gamma_k^{(0)}$ with integer index $k$. As discussed below, some of these states can be interpreted as resonance states with real energies $E_k$ and widths $\Gamma_k \geq 0$. Generalization (b) is achieved by defining the continuum level density as

$$\Delta \rho(\mathcal{E}) = \frac{i}{\pi} \text{Re} \left( \frac{1}{\mathcal{E} - \tilde{H}_{\text{NH}}} - \frac{1}{\mathcal{E} - \tilde{H}_{\text{NH}}^{(0)}} \right),$$

(2)

where the traces are evaluated as sums over the discrete eigenvectors, whose energies $\xi_k$ and $\xi_k^{(0)}$ represent poles of $\Delta \rho(\mathcal{E})$. In the infinite-box limit, the real part of Eq. (2) on the real energy axis, Re$\Delta \rho(E - 0) \equiv \text{Re} \Delta \rho(E) = \text{Re} \rho(E) - \text{Re} \rho^{(0)}(E)$, has to coincide with density (1). The meaning of Im$\Delta \rho(E)$ is discussed below.
Let us briefly overview properties of the density (2). From the residue theorem we see that a contour integral of $\Delta \rho(\mathcal{E})$ along a closed loop in the complex plane $\mathcal{E}$ gives twice the difference between the number of eigenvalues of $\tilde{H}_{\text{NH}}$ and $\tilde{H}_{\text{NH}}(0)$ inside the loop. We expect that $\mathcal{E}_k$ and $\mathcal{E}_k^{(0)}$ for $E$ much larger than the energy range of interaction $\tilde{V} = \tilde{H} - \tilde{H}(0)$ are very close to each other, so contributions of these eigenstates to Eq. (2) approximately cancel. The essential part of $\Delta \rho(\mathcal{E})$ therefore comes from a finite number (in the finite-box approximation) of eigenstates at smaller energies $E$. The $\rho(\mathcal{E})$ term in Eq. (2) reads

$$\begin{align*}
\text{Re} \rho(\mathcal{E}) &= \frac{1}{\pi} \sum_k \frac{-\frac{1}{2} (\Gamma_k - \Gamma_k)}{(E-E_k)^2 + \frac{1}{4} (\Gamma_k - \Gamma_k)^2}, \\
\text{Im} \rho(\mathcal{E}) &= \frac{1}{\pi} \sum_k \frac{E-E_k}{(E-E_k)^2 + \frac{1}{4} (\Gamma_k - \Gamma_k)^2},
\end{align*}$$

and the $\rho^{(0)}(\mathcal{E})$ term is expressed analogously. Below we will analyze $\Delta \rho(\mathcal{E})$ on the real energy axis, i.e., for $\Gamma = 0$. The real part of $\rho(\mathcal{E})$ represents a generalization of the level density $g(E) = \sum_k \delta(E - E_k)$ of a bound system with discrete energies $E_k$ to the smooth form $\text{Re} \rho(\mathcal{E}) = \sum_k \delta_{\Gamma_k}(E - E_k)$, where $\delta_{\Gamma_k}(\Delta E) = \frac{1}{2\pi} \frac{1}{\sqrt{\Gamma_k}} \delta(E - E_k)$ is a normalized Breit-Wigner peak (Cauchy distribution) with the maximum at $\Delta E = 0$ and the full width at half-maximum $\Gamma$. An analogous expression applies to $\text{Re} \rho^{(0)}(\mathcal{E})$, so $\text{Re} \Delta \rho(\mathcal{E})$ consists of positive and negative peaks centered at energies $E_k$ and $E_k^{(0)}$, respectively. If the widths $\Gamma_k$ are close to zero, an additional smoothing may be needed to get rid of sharp local structures and reveal a robust energy dependence of the level density. This can be achieved by adding a small positive imaginary component $i\epsilon$ to energy $E$, i.e., by setting $\Gamma = -i\epsilon$ in Eqs. (3), (4) and their $\rho^{(0)}(\mathcal{E})$ analogues. Hence we introduce smoothed level densities $\rho(\mathcal{E}) = \rho(\mathcal{E}) + i\epsilon \rho(E)$. We find that $\rho^{(0)}(\mathcal{E}) = \rho^{(0)}(\mathcal{E})$ and $\rho^{(0)}(\mathcal{E}) = \rho^{(0)}(\mathcal{E}) - \rho^{(0)}(\mathcal{E})$.

The complex level density (2) will be investigated in 1D scattering problems. Hamiltonians of these problems have the standard forms, $\tilde{H}(0) = \hat{p}^2/2m + \tilde{H}$ and $\tilde{H} = \tilde{H}(0) + \tilde{V}(x)$, where $\hat{p} = -i\hbar \frac{\partial}{\partial x}$ stands for the momentum operator, $m$ for the particle mass, and $\tilde{V}(x)$ is a potential. We assume that $\tilde{V}(x) \equiv 0$ outside a certain finite interval $(x_L, x_R)$. The usual asymptotics of wave functions is required, namely

$$\psi(x) = \begin{cases} e^{+\frac{i}{\hbar}p_+x + R(E)e^{-\frac{i}{\hbar}p_+x}} & \text{for } x < x_L, \\
T(E)e^{+\frac{i}{\hbar}p_+x} & \text{for } x > x_R, \end{cases}$$

where $p = \sqrt{2m|E-V(x)|}$, and $R(E)$ and $T(E)$ stand for reflection and transition amplitudes, respectively. The transmission amplitude is written as

$$T(E) = |T(E)| e^{i\phi(E)} = e^{i[t \ln |T(E)|]} = e^{\Phi(E)},$$

where $\phi(E)$ is a real phase shift of the transmitted wave and $\Phi(E)$ is a complex phase including $-i\ln |T(E)|$.

It is known that the real continuum level density (1) expresses the change of the real phase shift $\phi(E)$ with energy [9]. In analogy, we write

$$\begin{align*}
\Delta \rho(E) &= \frac{1}{\pi} \frac{d}{dE} \Phi(E) = \frac{1}{\pi} \frac{d}{dE} \phi(E) - \frac{i}{\pi} \frac{d}{dE} \ln |T(E)|. \quad (7)
\end{align*}$$

This implies that real and imaginary parts of $\Phi(E)$ can be obtained by an integration of the respective part of $\Delta \rho(E)$, which, for expressions of the form (3) and (4), can be done explicitly. So the complex continuum level density contains complete information on both functions $\phi(E)$ and $|T(E)|$. Using the smoothed density $\Delta \rho(\mathcal{E}) = \Delta \rho(E + i\epsilon)$ instead of $\Delta \rho(E)$, one obtains a smoothed complex phase $\tilde{\Phi}(E) \equiv \Phi(E) - i \ln |T(E)|$.

Phase shifts of wave functions in scattering problems are related to some suitably defined “time delays” [15, 16, 27–29]. For example, the so-called Eisenbud-Wigner time [27] is given as $\Delta t = \hbar \frac{\partial}{\partial E} \phi$, which near the center of a single resonance yields a delay $\Delta t \propto \hbar/\Gamma_k$ proportional to the average lifetime, whereas far from the resonances $\Delta t \approx 0$ [16]. To avoid sharp changes of the time delay, we calculate it from the smoothed phases. The smoothed complex phase $\tilde{\Phi}(E)$ results in the complex time shift

$$\Delta T(E) \equiv \hbar \frac{d}{dE} \tilde{\Phi}(E). \quad (8)$$

The meaning of real and imaginary components of $\Delta T(E)$ follows from semiclassical considerations. Indeed, the transmitted wave at $x = x_R$ is approximated by

$$T(E)e^{\frac{i}{\hbar}p_Rx_R} = e^{\frac{i}{\hbar}p_Lx_L} e^{\frac{i}{\hbar} \left[ \int_{x_L}^{x_R} \sqrt{2m|E-V(x)|} + C \right]} ,$$

where constant $C$ includes phase shifts between allowed and forbidden regions [30]. From Eq. (8) we obtain

$$\begin{align*}
\text{Re} \Delta T(E) &= \int_{E \geq V(x)} dx' \sqrt{m \frac{m}{2(E-V(x))} - \frac{m}{2(E-V(x))} } , \\
\text{Im} \Delta T(E) &= \int_{E < V(x)} dx' \sqrt{m \frac{m}{2(E-V(x))} } .\quad (10)
\end{align*}$$

The integral in Eq. (10) is taken across all classically allowed (for given $E$) regions between $x_L$ and $x_R$ and represents the time that a classical particle needs to pass these regions. The subtracted term is the transmission time of a free particle. On the other hand, the integral in Eq. (11), taken across all classically forbidden regions, is related to complex-time solutions of the classical equations of motions inside the potential barriers.

The use of complex time in the description of tunneling processes within the framework of the path integral was initiated by McLaughlin [18] and later developed e.g. in Refs. [2, 19–22]. In particular, the well known instanton solution [19] applies the Wick rotation $t \rightarrow -it$ to
derive the semiclassical tunneling probability. This approach was generalized to tunneling through multibarrier potentials, for which a notriivial evolution of time $T$ in the complex plane was considered [22]. In these problems, the continuous path $T(s)$, characterized by a steadily increasing real parameter $s$, has a shape of a descending staircase, whose segments corresponding to motion in classically allowed regions are parallel with the real time axis $(\frac{d}{ds}T = 1)$, while the segments associated with tunneling through forbidden regions go vertically along the negative imaginary axis $(\frac{d}{ds}T = -i)$. Complex-extended Hamilton equations render the momentum switching between pure real and imaginary values at classical turning points between allowed and forbidden regions, while the coordinate evolves solely in the real domain. The evolution in forbidden regions is equivalent to the motion with energy $-E$ in an inverted potential $-V(x)$.

These considerations lead to a semiclassical expression of the continuum level density in 1D scattering. Combining Eqs. (7) and (8), we get the formula

$$\Delta \rho(E) = \frac{1}{\pi \hbar} \Delta T(E), \quad (12)$$

which together with Eqs. (10) and (11) represents a semiclassical estimate of both real and imaginary parts of the smoothed density. The real and imaginary parts of the time shift $\Delta T(E)$ correspond to real and imaginary times accumulated in the above-described staircase evolution of $T(s)$, the real part being reduced by subtracting the passage time of a free particle. We note an apparent similarity of Eq. (12) with the relation $\bar{\rho}(E) = t_0(E)/2\pi \hbar$ between the smoothed level density of a bound system and the period $t_0$ of classical orbits at energy $E$. The denominators in these formulas differ by a factor 2 because the time shift $\Delta T(E)$ includes only a half of the full return trajectory. Therefore, the scattering and bound systems rely upon rather similar semiclassical descriptions, in which the scattering systems with continuous energy require the use of complex instead of real quantities.

We test Eq. (12) in 1D scattering systems with several sample potentials (see Fig. 1) using the complex scaling method [31, 32] (for reviews see Refs. [23–25]). The method is based on a similarity transformation $\hat{S} = e^{\theta/2}e^{-\theta \hat{p}\hat{x}/\hbar} \equiv S(\theta)$, where $\theta$ is a real scaling parameter. The coordinate and momentum operators transform as $\hat{S}\hat{x}\hat{S}^{-1} = e^{i\theta}\hat{x}$ and $\hat{S}\hat{p}\hat{S}^{-1} = e^{-i\theta}\hat{p}$, which makes it possible to turn discrete resonant solutions $\psi_k(x)$ of the stationary Schrödinger equation with Hamiltonian $\hat{H}$ into normalized eigenstates of the transformed non-Hermitian Hamiltonian $\hat{H}_{NH}(\theta) = \hat{S}\hat{H}\hat{S}^{-1} \equiv H_{NH}$. Indeed, the resonant solution associated with a pole of the scattering matrix at the complex momentum $p_k = |p_k|e^{-i\alpha_k}$ with $\alpha_k \in (0, \pi)$ has the form of an outgoing (transmitted) wave $\psi_k(x) = e^{ip_kx/\hbar}$ for $x < x_l$, and $x > x_R$, which after the complex scaling transformation becomes a square-integrable function if $\theta - \alpha_k \in (0, \pi)$.

The results of the complex scaling method for the Hamiltonian $\hat{H} = \hat{H}^{(0)} + \hat{V}(x)$ with potentials from Fig. 1 are shown in Fig. 2. For a fixed $\theta$, only the resonances with complex energies $E_k = |E_k|e^{-i\beta_k}$ satisfying $\beta_k = 2\alpha_k < 2\theta$ emerge (red dots below the diagonal), while those with $\beta_k \geq 2\theta$ form background states (in the infinite-size limit forming so-called “rotated continuum”) that approximately satisfy the condition $\frac{1}{2}E = \tan \theta$ (red dots along the diagonal). More resonances (with larger $\beta_k$) may pop out if $\theta$ is increased, but this is usually limited by some numerical constraints. The effect of these hidden resonances on the level density must be included in the contribution of the background states for...
a given $\theta$. Moreover, the complex scaling transformation with the same $\theta$ performed on the free Hamiltonian $\hat{H}^{(0)}$ yields only the background states (blue dots along the diagonal), and for large enough $E$ the background contributions in $\text{Re} \rho(E)$ and $\text{Re} \rho^{(0)}(E)$ approximately cancel each other [26]. So $\text{Re} \Delta \rho(E)$ is formed mostly by contributions of resonances not too far from the real axis, and the same holds also for $\text{Im} \Delta \rho(E)$. Close to $E=0$, however, both background contributions combine in a nontrivial way and need to be evaluated carefully.

The potentials employed here have a general form

$$ V(x) = (a + bx + cx^2) \ e^{-\eta x^2}, \quad (13) $$

where $a, b, c$ and $\eta$ are adjustable parameters (see the caption of Fig.1). For each potential, the calculation is done with some optimized values of the classicality parameter $\hbar/\sqrt{m}$ and angle $\theta$ (see the caption of Fig.2). For the sake of simplicity all quantities are considered to be dimensionless. In the finite-box approximation we assume that $V(x) = \infty$ for $|x| > \frac{1}{2}L$. The finite length $L$ makes the set of background states discrete, but its value is chosen large enough to keep this set dense and to yield the resonances at $\beta_k < 2\theta$ stabilized (invariant under an increase of $L$). Though the potentials in Eq. (13) are not restricted to any finite support interval, they decrease exponentially with increasing $|x|$. This means that $x_L$ and $x_R$ in Eqs. (9) and (10) can be chosen almost arbitrarily.

In the following calculations we set $-x_L = \frac{1}{2}L = +x_R$.

Figure 3 shows the main result of this work. It compares the real and imaginary parts of the smoothed continuum level density $\Delta \rho(E)$ with the real and imaginary parts of the time shift $\Delta T(E)$ from Eqs. (10) and (11). Note that the described method for the evaluation of $\Delta \rho(E)$ fails close to $E = 0$, so the low-energy region is excluded. Results in panels (a), (b) and (c) of Fig.3 refer to the potentials in the corresponding panels of Fig.1.

In accord with formula (12), we observe a satisfactory match of the $\Delta \rho(E)$ and $\Delta T(E)$ curves in Fig.3. The agreement is expected to further improve with decreasing parameters $\hbar/\sqrt{m}$ (more resonances) and $\epsilon$ (less smoothening). The match is very good in panels (a) and (b), and less good in panel (c), where the density curves are more smoothed as the corresponding potential gives a larger oscillatory component of $\Delta \rho(E)$. In any case, the density and time curves in all panels of Fig.3 show the same qualitative features, particularly the step-, peak- and dip-like singularities at the energies associated with stationary points of the respective potentials. These singularities reflect the fact that classical stationary points inside the interaction region induce anomalous changes of the complex time shifts. As follows from the previous discussion, the singularities in $\text{Re} \Delta T(E)$ are connected with stationary points of $V(x)$, while those in $\text{Im} \Delta T(E)$ refer to stationary points in $-V(x)$.

Effects of the stationary points on the time shifts in Fig.3 can be classified as follows:

(i) A quadratic maximum of the potential at an energy $E_0$ leads to a logarithmic divergence $\propto -\ln |E - E_0|$ of the time shift [6]. This concerns the maximum of $V(x)$ in panel (a) of Fig.1, and the two maxima of $V(x)$ and one maximum of $-V(x)$ in panel (c). So in panel (a) of Fig.3 we observe one divergence in $\text{Re} \Delta T(E)$, while in panel (c) we get two divergences in $\text{Re} \Delta T(E)$ and one in $-\text{Im} \Delta T(E)$. Note that if the singularity appears in imaginary time, it is inverted in both time and energy directions since in the forbidden regions we do transformation $E \to -E$ and let time pass in the $-i$ direction.

(ii) A quadratic minimum of the potential at $E = E_0$ produces a step-like dependence $\propto \theta(E-E_0)$ of the time shift (where $\theta$ is a step function equal to 0 for negative arguments and to 1 otherwise) [6]. This is the case of all structures in Fig.1 mentioned in item (i), but in the inverse sense. So in panel (a) of Fig.3 we have one step singularity of $-\text{Im} \Delta T(E)$, and in panel (c) two step singularities of $-\text{Im} \Delta T(E)$ and one of $\text{Re} \Delta T(E)$.

(iii) A degenerate (higher than quadratic) extreme of
the potential causes divergent time shifts in both minimum and maximum cases [6]. This concerns the flat potential in Fig. 1(b). A quartic maximum of \( V(x) \) at \( E_0 \) leads to a power-law divergence \( \text{Re}\Delta T(E) \propto |E - E_0|^{-1/4} \). The corresponding quartic minimum of \(-V(x)\) gives rise to the dependence \(-\text{Im}\Delta T(E) \propto \Theta(E_0 - E)|E - E_0|^{-1/4}\).

All the above singularities are reproduced in Fig. 3 by the curves \( \text{Re}\Delta T(E) \) and \( \text{Im}\Delta T(E) \), and their correlates are seen in the associated curves \( \text{Re}\Delta\rho(E) \) and \( \text{Im}\Delta\rho(E) \). We know that singular energy dependencies of the level density in bound quantum systems are connected with the ESQPTs, which for systems with a single degree of freedom \( f \) originate in non-analytic variations of classical periods of closed orbits [4–6]. The present analysis therefore generalizes the concept of the \( f = 1 \) ESQPT from bound to scattering systems. It turns out that in the latter case the known classification of ESQPTs needs to be applied separately to both normal and inverted potentials. We point out that semiclassical calculations of tunneling resonances—already revealing an anomaly connected with the barrier maximum—were reported earlier in Refs. [33, 34]. The present work transcends the older results by disclosing the role of the complex tunneling time in the semiclassical solutions, and by classifying the singularities of the continuum level density through the known typology of ESQPTs.

In summary, we have investigated the description of 1D scattering processes in terms of the continuum level density. We have extended the existing definition of \( \Delta\rho(E) \) to the complex domain and related its real and imaginary parts on the real energy axis to the real and imaginary time shifts associated with complex tunneling trajectories. Fundamental relations (7) and (12) have been proposed. As a confirmation of our surmise, we have clearly identified singularities of \( \Delta\rho(E) \) caused by classical stationary points for several test potentials \( V(x) \). The forms of these singularities are consistent with the types of ESQPTs in bound systems with \( f = 1 \). In particular, the singularities in \( \text{Re}\Delta\rho(E) \) reflect stationary points of \( V(x) \) in the classically allowed regions, while the singularities in \( \text{Im}\Delta\rho(E) \) reflect stationary points of \(-V(x)\) in classically forbidden regions. The latter singularities highlight the relevance of complex-time (instanton-like) classical solutions of the tunneling problem.

We anticipate that our results extend to \( f > 1 \) systems in which the ESQPTs affect higher derivatives of the level density [6, 35]. Such an extension is directly deducible from the present analysis for systems which effectively reduce to 1D problems due to an underlying symmetry.

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