Liouville transformations and quantum reflection

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Abstract

Liouville transformations of Schrödinger equations preserve the scattering amplitudes while changing the effective potential. We discuss the properties of these gauge transformations and introduce a special Liouville gauge which allows one to map the problem of quantum reflection of an atom on an attractive Casimir–Polder well into that of reflection on a repulsive wall. We deduce a quantitative evaluation of quantum reflection probabilities in terms of the universal probability which corresponds to the solution of the \( V_{\text{CP}} = -C_4/z^4 \) far-end Casimir–Polder potential.

Keywords: Schrödinger equation, quantum reflection, Casimir-Polder

1. Introduction

Quantum reflection is a phenomenon that has been known since the early days of quantum mechanics. The reflection of atoms close to a surface from the attractive van der Waals potential has already been studied in the 1930s by Lennard-Jones [1, 2]. While the atom’s classical motion would be increasingly accelerated towards the surface, the quantum matter waves are reflected back because of the rapid variation of the potential close to the surface. In fact, the reflection probability approaches unity for atoms at low energies.

The attractive Casimir–Polder (CP) force arises from the coupling of the atom and surface by the fluctuations of the electromagnetic field. It generalizes the van der Waals force by taking into account retardation effects due to the finite speed of light. Quantum reflection from the Casimir–Polder potential was first studied experimentally for He and H atoms on liquid helium films [3–5] and more recently for ultracold atoms or molecules on solid surfaces [6–12]. Meanwhile, many theoretical papers have studied various fundamental aspects and applications of quantum reflection [13–21]. More recently, it has been noticed that quantum reflection could be useful for storing and guiding cold antihydrogen atoms [22–25] and that it should play a role in any experiment where antihydrogen atoms interact with a matter plate (see [26–28] and references therein).

Paradoxical results appear in the study of quantum reflection (QR) from the Casimir–Polder interaction. The probability of quantum reflection not only increases when the velocity of the incident atom is decreased, but also when the magnitude of the interaction is decreased. For example, the probability of quantum reflection is larger for atoms falling onto silica bulk than onto metallic mirrors [26] and is even larger for nanoporous silica [27]. This paradox is qualitatively explained by the fact that atoms get closer to the surface for a weaker potential, so that the CP potential becomes steeper and quantum reflection probability larger.

In this paper, we propose a quantitative treatment of these paradoxical behaviors based on Liouville transformations. Such transformations are gauge transformations of the Schrödinger equation, which map problems corresponding to different potentials into one another, while leaving scattering amplitudes invariant. In the case of QR on a CP potential studied in this paper, a special Liouville gauge can be introduced to transform the potential from an attractive CP well into a repulsive wall. The paradoxical features of the initial QR problem become intuitive predictions of the transformed problem. Furthermore, QR probabilities can then be described in terms of the universal solution associated with the \( V_{\text{CP}} = -C_4/z^4 \) far-end (CP) potential.

In section 2, we recall the usual treatment of the QR problem, based on deviations from the semiclassical WKB
approximation [13]. We present in section 3 the Liouville transformations which transform Schrödinger equations into equivalent ones corresponding to different potentials. We then introduce in section 4 a special choice which maps the original problem of QR on a CP well into a more intuitively understood problem of reflection on a repulsive wall. In section 5 we study the $V_\Omega = -C_\Omega/z^4$ potential which shows non trivial symmetry properties while being representative of the CP interaction in the far-end. We finally use these results (section 6) to give a simple evaluation of QR probabilities, in terms of the universal function associated with this problem and of one scattering length parameter depending on the full CP potential.

2. Quantum reflection

We consider a cold atom of mass $m$ incident with a velocity $v < 0$ parallel to the $z$-axis upon the CP potential $V(z)$ in the half-space $z > 0$ above the material surface located at $z = 0$, as represented in figure 1. We consider a plane material surface, so that the vertical motion is decoupled from the horizontal one.

The vertical motion is then described by a 1D Schrödinger equation:

\[ \Psi''(z) + F(z) \Psi(z) = 0, \]

\[ F(z) \equiv \frac{2 m (E - V(z))}{\hbar^2}. \]

The primes represent the derivative of a function with respect to its argument. The CP potential $V(z)$ is attractive, with characteristic inverse power laws at both ends of the $z$-domain, the cliff-side close to the surface $z \to 0$ and the far-end $z \to \infty$:

\[ V(z) \simeq V_3(z), \quad V_3(z) \equiv -C_3/z^4, \]

\[ V(z) \simeq V_4(z), \quad V_4(z) \equiv -C_4/z^4. \]

In (1), $E = \frac{1}{2}mv^2$ is the energy associated with the motion orthogonal to the plane. It may be the result of a free fall from a height $h$ above the surface $E = mgh$, where $g$ is the acceleration of gravity. This semi-classical treatment of the free fall is possible when $E$ is much larger than the energy $E_1$ of the first gravitational quantum state above the surface [28, 29]:

\[ E_1 \equiv \left( \frac{\hbar^2 m g^2}{2} \right)^{\frac{1}{4}} \lambda_1 \simeq 1.407 \text{ peV}, \]

where $\lambda_1 \simeq 2.338$ is the absolute value of the first zero of the Airy function $Ai$. In the following, we use $E_1$ as the unit for $E$ so that the validity of the semi-classical treatment of the free fall above the surface is simply $E/E_1 \gg 1$. This condition also corresponds to $h/h_1 \gg 1$ where $h_1 \equiv E_1/mg$ is the associated unit for the free fall height $h$, that is the height $\simeq 13.7 \mu$m of the classical turning point for the first quantum state [29].

If we were treating also the interaction with the CP potential in a semiclassical approach, the function $F(z)$ would be seen as the square of the de Broglie wave-vector $k_{db}$ associated with the classical momentum $\hbar k_{db}$:

\[ k_{db}(z) \equiv \sqrt{F(z)}. \]

As the CP potential is attractive and the incident energy positive, $F$ is everywhere positive, so that a classical particle undergoes an increasing acceleration towards the surface. This behavior is mimicked by the semiclassical WKB wave-functions which propagate in the rightward and leftward directions ($\eta =+1$ and $-1$ respectively) [30]:

\[ \Psi_{WKB}^{\eta}(z) = \alpha_{db}(z) e^{i \phi_{db}(z)}, \]

\[ \alpha_{db}(z) = \frac{1}{\sqrt{k_{db}(z)}}, \quad \phi_{db}(z) = \int_{z_0}^{z} k_{db}(z') \, dz'. \]

Here, $\alpha_{db}$ is the WKB amplitude and $\phi_{db}$ the WKB phase associated with the classical action integral $\hbar \phi_{db}$. The arbitrariness of the choice of the reference point $z_0$ is fixed in the following by the far-end convention:

\[ \lim_{z \to \infty} (\phi_{db}(z) - k z) = 0, \]

\[ k = \lim_{z \to \infty} k_{db}(z) = \frac{\sqrt{2mE}}{\hbar}. \]

In a quantum treatment of the interaction with the surface [26], QR appears as a consequence of non-adiabatic transitions between the counter-propagating WKB waves (7). It can be obtained by solving the exact Schrödinger equation (1) for a wave-function written, in full generality, as a linear combination of $\Psi_{WKB}^{\eta}(z)$ with $z$-dependent coefficients $\beta_{\eta}^{z}$:

\[ \Psi(z) = \beta_{\eta}(z) \Psi_{WKB}^{\eta}(z), \]

where we use an implicit sum rule for repeated indices. These coefficients obey coupled first-order differential equations [13]:

\[ \beta_{\eta}'(z) = \beta_{\eta}(z) \frac{k_{db}(z)}{2k_{db}(z)} e^{-2i\phi_{db}(z)}. \]

This system of equations can be solved numerically and matched to the WKB solutions at both ends of the domain [18, 31, 32]. Special care has to be taken on the cliff-side where the potential diverges. The matching has to use the mathematical solutions of (1) known for the $V_3$ potential [22, 26], at the price of losing physical understanding of the problem.
The Schwarzian derivative is defined as the second derivative of the logarithmic derivative of a function, which can also be expressed in terms of the Schwarzian derivative. The difference between (1) and (13) is often described in terms of the so-called parameter \( \kappa \) defined in (10). A qualitative criterion for occurrence of QR is that the coupling term in (12) takes significant values, which may be stated as a large enough variation of the de Broglie wavelength on the length scale fixed by the de Broglie wavelength.

A less approximate discussion of this point can be based on the remark that WKB wave-functions obey an equation differing from the original (1):

\[
\Psi_{\text{WKB}}' (z) + F(z) \Psi_{\text{WKB}}(z) = \frac{\alpha_{\text{AB}}^*(z)}{\alpha_{\text{AB}}(z)} \Phi_{\text{WKB}}(z). \tag{13}
\]

The difference between (1) and (13) is often described in terms of the so-called badlands function [26]:

\[
Q(z) = -\frac{\alpha_{\text{AB}}(z)}{\alpha_{\text{AB}}(z)} = -\alpha_{\text{AB}}^*(z), \tag{14}
\]

which can also be expressed in terms of the Schwarzian derivative \( \{ \phi_{\text{AB}}, z \} \) of the WKB phase \( \phi_{\text{AB}}(z) \):

\[
Q(z) = \frac{\{ \phi_{\text{AB}}, z \}^2}{2F(z)} = \frac{\{ \phi_{\text{AB}}, z \}}{2k_{\text{AB}}^2(z)}. \tag{15}
\]

The Schwarzian derivative is defined as:

\[
[f, z] = \frac{f''(z)}{f'(z)} - \frac{3}{2} \left( \frac{f'(z)}{f(z)} \right)^2. \tag{16}
\]

In regions where the badlands function vanishes, equations (1) and (13) are identical so exact solutions of the Schrödinger equation can be written as a sum of WKB waves. The WKB waves have well defined directions of propagation, therefore no quantum reflection can occur in these areas. It follows that the regions where QR takes place are those where the WKB approximation fails and they are indicated by significant values of the badlands function.

In the case of the CP potential, the function \( Q(z) \) is peaked and vanishes not only in the far-end where \( k_{\text{AB}} \) goes to a constant, but also at the cliff-side as a consequence of the power-law variation (3). These properties have been proven by several examples in [26, 27] and are also illustrated in figure 2.

The three curves show the functions \( Q(z) \) for a hydrogen atom above a silica bulk with energies \( E \) respectively equal to \( 10^3, 10^4 \) and \( 10^5E_1 \), and \( V(z) \) calculated for a hydrogen atom and a silica bulk.

Table 1. Quantum reflection probabilities \( R \) for hydrogen atoms falling on a silica bulk plate, with different incident energies \( E \), given in units of \( E_1 \) (see (5)). The three last columns correspond to the plots on figure 2, while the first one is given only as an indication of the trend of QR probability for the lowest gravitational quantum state.

| \( E \) \( \times 10^3E_1 \) | 1 | 10 | \( 10^2 \) | \( 10^3 \) | \( 10^4 \) | \( 10^5 \) |
|---|---|---|---|---|---|---|
| \( R \) [%] | 98.5 | 95.4 | 86.1 | 63.2 | 28.0 | 5.6 |

In spite of its effectiveness, the method described in this section suffers several drawbacks. First QR is a scattering process with incident matter waves reflected or transmitted when crossing the badlands, but this scattering process is poorly defined as the potential diverges at the cliff. Second the correlation of the peak value of \( Q \) with the QR probability is observed, but a quantitative interpretation of this correlation is missing. In fact, the role of the badlands function is discussed by comparing the two different problems associated with (1) and (13), and not by studying the equation of physical interest (1). All these drawbacks are cured in the sequel of this paper, thanks to the introduction of Liouville transformations of the Schrödinger equation [33].

### 3. Liouville transformations

The Schrödinger equation (1) is an example of a Sturm-Liouville equation under Liouville normal form [34]. What is called the WKB approximation by physicists was in fact introduced by Liouville [35] and Green [36] for studying properties of such equations, long before Wentzel [37], Kramers [38] and Brillouin [39] used it in the context of quantum mechanics. The transformations used in the present paper increase when the peak values increases, that is also when the energy decreases.
were introduced by Liouville in 1837 [35] and we follow here the convention of Olver [40–42] for naming them after Liouville (see the notes at the end of ch 6 in [40]).

Liouville transformations have been used to obtain approximate solutions [43–45]. They have been also used to study second-order differential equations applied to solvable Schrödinger equations [46–50]. We want to emphasize at this point that we use here the Liouville transformations to describe equivalent scattering problems corresponding to different potentials, with no approximation, for potentials not belonging to a class of solvable problems.

After these historical remarks, we define the Liouville transformations [41] which correspond to coordinate changes with correlated rescalings of the wave-function. The coordinate change maps the physical $z$-domain into a $\tilde{z}$-domain with $\tilde{z}(z)$ a smooth monotonous function ($\tilde{z}'(z) > 0$). Equation (1) for $\Psi(z)$ keeps the same form for the rescaled wave-function $\Psi(\tilde{z})$:

$$\Psi(\tilde{z}) = \sqrt{\tilde{z}'(z)} \Psi(z),$$

$$\tilde{\Psi}'(\tilde{z}) + F(z) \tilde{\Psi}(z) = 0,$$  

with a transformed function $\tilde{F}(\tilde{z})$:

$$\tilde{F}(\tilde{z}) = \frac{F(z) - \frac{1}{2} \{z, \tilde{z}\}}{\tilde{z}'(z)^2}.$$  

The curly braces denote the Schwarzian derivative (16) of the coordinate transformation $\tilde{z}(z)$.

The composition of two Liouville transformations $z \to \tilde{z}$ and $\tilde{z} \to \hat{\tilde{z}}$ is a Liouville transformation $z \to \hat{\tilde{z}}$, and the group properties of this composition law is ensured by Cayley's identity for Schwarzian derivatives [41]:

$$\{ \tilde{z}, z \} = (\tilde{z}'(z))^2 \{ \tilde{z}, \tilde{z} \} + \{ z, \tilde{z} \}.$$  

When this identity is applied to inverse transformations ($\tilde{z} = z$), the following relation is obtained:

$$0 = (\tilde{z}'(z))^2 \{ \tilde{z}, \tilde{z} \} + \{ \tilde{z}, \tilde{z} \},$$

so that the transformation (19) can also be written:

$$\tilde{F}(\tilde{z}) = z'(z)^2 F(z) + \frac{1}{2} \{ z, \tilde{z} \}.$$  

The Wronskian of two solutions $\Psi_1, \Psi_2$ of the Schrödinger equation is a constant, independent of $z$ and antisymmetric in the exchange of the two solutions:

$$\mathcal{W}(\Psi_1, \Psi_2) = \mathcal{W}(\Psi_2(z) - \Psi_1(z)) \mathcal{W}(\Psi_2(z)).$$  

The Liouville transformations preserve this Wronskian:

$$\mathcal{W}(\Psi_1, \Psi_2) = \tilde{\mathcal{W}}(\tilde{\Psi}_1, \tilde{\Psi}_2),$$

and this property has important physical consequences, as shown in the following section.

When $\Psi$ is a solution of (1), its complex conjugate $\Psi^*$ is also a solution, and the probability density current $j(z)$ is proportional to the Wronskian of $\Psi^*$ and $\Psi$:

$$j(z) \equiv \frac{\hbar}{2im} \mathcal{W}(\Psi^*, \Psi).$$

As the probability density $\rho = \Psi^* \Psi$ is time-independent in the problem studied in this paper, $j(z)$ is a constant $j$ independent of $z$. It follows from (24) that this constant is invariant under Liouville transformations $j = \hat{j}$. We emphasize that the probability density $\rho$ is neither constant nor preserved by the transformation, as one deduces from (17) that $\rho(z) = \tilde{\rho}(\tilde{z})\rho(\tilde{z})$. We also note that the WKB functions, which are exact solutions of (13) and approximate solutions of (1) at both ends of the $z$-domain, obey the following relations (which will be used below):

$$\mathcal{W}\left(\Psi_{\ell\text{WKB}}^*, \Psi_{\bar{WKB}}^\ell\right) = 2\mathcal{W}_{\ell\bar{\ell}}^\text{WKB}.$$  

We recall now that the scattering amplitudes can be written in terms of Wronskians of solutions of the Schrödinger equation [51]. To this aim, we note that $Q(z)$ goes to 0 at the left and right ends of the $z$-domain, so that we can define exact solutions $\Psi_{\ell}^\ell$ and $\Psi_{\bar{\ell}\ell}^\text{WKB}$ of (1) which match the asymptotic WKB waves there:

$$\Psi_{\ell}^\ell(z) \to \Psi_{\ell\text{WKB}}^\ell(z), \quad \Psi_{\bar{\ell}\ell}^\text{WKB}(z) \to \Psi_{\bar{\ell}\text{WKB}}^\ell(z).$$

These four solutions are schematized in figure 3.

As the WKB waves $\Psi_{\ell\text{WKB}}^\ell$ and $\Psi_{\bar{\ell}\text{WKB}}^\ell$ are complex conjugates of each other, this is also the case for the exact solutions matching them at left or right ends:

$$\left(\Psi_{\ell}^\ell\right)^\ast = \Psi_{\bar{\ell}}^\ell, \quad \left(\Psi_{\bar{\ell}\ell}^\text{WKB}\right)^\ast = \Psi_{\ell\text{WKB}}^\bar{\ell}.$$  

A generic solution $\Psi(z)$ of (1) can then be decomposed over the left or right basis:

$$\Psi(z) = a_{\ell}^L \Psi_{\ell}^\ell(z) = a_{\bar{\ell}}^R \Psi_{\bar{\ell}}^\ell(z).$$

For each decomposition, the amplitudes can be collected in column matrices related by a transfer matrix:

$$a_{\ell}^L = T_{\ell\bar{\ell}} a_{\bar{\ell}}^R \quad \Rightarrow \quad \Psi_{\ell}^\ell = T_{\ell\bar{\ell}}^\ast \Psi_{\bar{\ell}}^\ell.$$  

These solutions and associated amplitudes can alternatively be defined in terms of outgoing and incoming waves with the usual identification:

$$\left(\begin{array}{c} \Psi_{\text{out}}^+ \\ \Psi_{\text{out}}^- \end{array}\right) = \left(\begin{array}{c} \Psi_{\ell}^+ \\ \Psi_{\bar{\ell}}^- \end{array}\right), \quad \left(\begin{array}{c} \Psi_{\text{in}}^+ \\ \Psi_{\text{in}}^- \end{array}\right) = \left(\begin{array}{c} \Psi_{\ell}^\ell \\ \Psi_{\bar{\ell}}^\text{WKB} \end{array}\right).$$
The out and in amplitudes are related by the unitary scattering matrix (SS† = I):

\[ a_{out}^* = S^\dagger a_{in}^\dagger, \]

which can be obtained from the transfer matrix (see [52]):

\[ S = \begin{pmatrix} S_+^+ & S_+^- \\ S_-^+ & S_-^- \end{pmatrix} = \frac{1}{T_+^\dagger} \begin{pmatrix} 1 & -T_+^- \\ T_+^+ & 1 \end{pmatrix}. \]

\[ T = \begin{pmatrix} T_+^+ & T_+^- \\ T_-^+ & T_-^- \end{pmatrix}, \quad \text{det} T = 1. \]

As the Wronskian of solutions \( \Psi_L^\dagger \) or \( \Psi_R^\dagger \) is a constant, it can be evaluated in particular in the asymptotic regions where these exact solutions reduce to WKB waves. They therefore obey the same relations as in (26):

\[ \mathcal{W} \left( (\Psi_L^\dagger)^\dagger, \Psi_R^\dagger \right) = \mathcal{W} \left( (\Psi_R^\dagger)^\dagger, \Psi_L^\dagger \right) = 2I_0 \nu. \]

The information on the scattering is then contained in the Wronskians involving solutions at the left and right ends:

\[ \mathcal{W} \left( (\Psi_L^\dagger)^\dagger, \Psi_R^\dagger \right) = 2(I^\dagger T)^\dagger_0. \]

Since the matrices \( T \) and \( S \) are expressed in terms of Wronskians by using (36) and (33), it follows from (24) that they are invariant under Liouville transformations (\( T = T \) and \( S = S \)). In particular, the reflection and transmission amplitudes \( r = S_+^+ \) and \( t = S_-^- \) defined for waves incoming from the far-end are preserved (\( r = \tilde{r} \) and \( t = \tilde{t} \)) and can be calculated equivalently after any Liouville transformations.

It is worth stressing again that these gauge transformations relate equivalent scattering problems to one another, while not necessarily making the resolution simpler. In specific cases, for example the model studied in section 5, they may lead to non trivial symmetry properties. In the general case, we show in the next section that a special gauge choice brings satisfactory answers to all questions raised at the end of section 2.

### 4. Special gauge choice

In this section, we choose a special Liouville gauge which shows interesting properties. Precisely, we choose a coordinate \( z \) proportional to the WKB phase \( \phi \) which maps the initial problem of QR on an attractive well into a different problem of reflection on a repulsive wall. This special gauge choice brings satisfactory answers to all questions raised above. In particular, it leads to a perfectly well-defined scattering problem with no interaction in the asymptotic states, and it also allows to understand the variation of the QR probability in a rigorous as well as intuitive manner.

The special gauge choice is fixed by the following definition of the coordinate \( z \) and associated quantities identified by boldfacing:

\[ z \equiv \frac{\phi_{db}(z)}{x}, \quad \Psi(z) = \sqrt{z(z)} \Psi(z), \]

\[ F(z) = \frac{F(z) - \frac{1}{2}[z, z]}{z(z)^{1/2}} = x^2(1 - Q(z)), \]

where we have noticed that \([z, z] = [\phi_{db}, z]\) and then used the definition (15) of \( Q(z) \). The scale constant \( x \) is arbitrary at this point, but will be fixed soon. Equation (38) can be rewritten in terms of energy and potential:

\[ F(z) \equiv E - V(z), \quad E = x^2, \quad V(z) = x^2Q(z). \]

As \( Q(z) \) goes to zero at both ends of the physical domain \( z \in ]0, \infty[ \), the interaction potential \( V \) tends to 0 at both ends of the transformed domain \( z \in ]-\infty, \infty[ \). It thus corresponds to a well-defined scattering problem with no interaction in the asymptotic input and output states.

Using the expression (14) of \( Q(z) \), a positivity property can be demonstrated for the integral of \( V \):

\[ I \equiv \int_{-\infty}^{\infty} V(z)dz = -\kappa \int_0^{\infty} \alpha_{db}(z)\alpha'_{db}(z)dz = \kappa \int_0^{\infty} (\alpha_{db}(z))' dz > 0, \]

where the integrated term, which should appear in the integration by parts between the first and second lines, vanishes at left and right ends (\( \alpha_{db}a_{db}' \to 0 \) for \( z \to 0 \) and \( z \to \infty \)). Whereas the initial potential \( V \) was everywhere negative, the shape of the transformed potential \( V \) is mostly a repulsive wall, even though \( V \) may be negative in some parts of the \( z \) -domain. We will see now that the transformed equation has classical turning points where \( F = 0 \) or \( E = V \), for not too large values of the original energy \( E \).
potential:

\[ \lambda = \sqrt{k\ell}, \quad \kappa = \sqrt{2mE\ell}, \quad \ell = \frac{\sqrt{2mC_4}}{E}. \]  

This choice will lead to functions \( V(z) \) having nearly identical peak shapes for different energies \( E \), at least for not too large values of \( E \). In fact, these functions reproduce a universal function \( V_d(z) \) when the initial potential \( V(z) \) matches the form of the far-end tail \( V(z) \) of the CP potential. This model is studied in section 5 and it is shown there that the universal function \( V_d(z) \) has a peak value at \( z = \zeta \) where:

\[ \zeta = \frac{\ell}{\kappa} = \frac{C_4}{E}. \]  

The plots in figure 4 show \( E \) and \( V \) for CP potentials \( V \) calculated between a hydrogen atom and a silica bulk [26] and 3 incident energies \( E \) respectively equal to \( 10E_i, 10^2E_i \) and \( 10^3E_i \). The transformed energies \( E \) are represented as the 3 horizontal lines and the transformed potentials \( V(z) \) as the 3 curves. With \( E \) always positive and \( V(z) \) mostly positive, a logarithmic scale is used along the vertical axis, in order to make some details more apparent.

We see in figure 4 that the peaks for the functions \( V \) are nearly the same for the different initial energies. This is due to the fact that, for the parameters chosen here, these peaks correspond to distances \( z \sim \zeta \) such that the exact CP potential \( V(z) \) is close to its far-end tail \( V_d(z) \). The deviations appearing on the plots correspond to values of \( z \) closer to the cliff-side, where \( V_d(z) \) is indeed a poor representation of \( V(z) \). As \( V \) is nearly the same for the different problems whereas \( E = x^2 = k\ell \), it follows that classical turning points appear in the transformed problem for not too large energies \( E \propto \kappa^2 \). For the plots drawn in figure 4 the turning points appear for \( E = 10, 10^2E_i \), but not for \( E = 10^3E_i \).

The existence of classical turning points in the transformed problem is in striking contrast with the initial problem of QR on an attractive well, which did not show turning points. This initial QR problem has been transformed into the more intuitive problem of ordinary reflection on a repulsive wall, with exactly identical scattering amplitudes. The fact that the QR probability goes to unity when \( \kappa \to 0 \) is now understood as an immediate consequence of the increasing reflection expected for a particle with a lower and lower energy \( E \) coming onto a repulsive wall with a more or less fixed peak value.

In a similar manner, we can understand the dependence of QR probabilities on the absolute magnitude of the CP potential. To do so we consider hydrogen atoms falling onto a perfect mirror, a silicon bulk or a silica bulk, which give rise respectively to weaker and weaker CP interaction [26]. Figure 5 shows the constants \( E \) and the functions \( V(z) \) for a fixed energy \( E = 10^2E_i \approx 1.4 \text{ neV} \). The potentials correspond to values for the far-end tails, \( C_4 \) and \( \ell \), which decrease from perfect mirror to silicon to silica. As in figure 4, the transformed potentials \( V \) have similar peak shapes, which tend to align on the universal curve calculated for a pure \( V_d \) potential and shown as the dashed curve. In contrast, the transformed energies \( E \propto k\ell \) decrease with \( \ell \), which immediately explains why the QR probability increases [26].

We note that a similar discussion has been given in [33] to explain the results obtained in [27] for hydrogen atoms above nanoporous silica with different porosities.

### 5. Symmetry of the \( V_4 \) model

In this section, we discuss the model potential \( V_4(z) = -C_4/z^4 \) which is representative of the CP interaction in the far-end. Furthermore, this model is interesting in itself because it obeys a symmetry which enforces non trivial properties.

For the \( V_4 \) model, the WKB wave-vector has the simple form:

\[ k_{\text{ab}}(z) = \sqrt{\kappa^2 + \frac{\ell^2}{z^4}}. \]  

This leads to a non trivial symmetry property for the Liouville transformation corresponding to inversion:

\[ \hat{z} = -\frac{z^2}{z}, \]  

which maps the physical domain \( z \in [0, \infty] \) into an inverted domain \( \hat{z} \in [-\infty, 0] \), while exchanging the roles of the cliff-side and far-end.

The inversion (44) is a homographic function, so that its Schwarzian derivative \( \{z, \hat{z}\} \) vanishes. If \( \hat{z} \) is another map, chosen arbitrarily, Cayley’s identity (20) leads to \( \{\hat{z}, \hat{z}\} = \{\hat{z}(z)\} \{\hat{z}, \hat{z}\} \). When \( \hat{z} = \phi_{\text{ab}} \), one deduces that the sadlands function defined as in (15) for the original and
inverted coordinates are identical:

\[
Q(z) = \frac{\phi_{\text{db}, z}}{2k_{\text{db}}^2(z)} = \frac{\phi_{\text{db}, \tilde{z}}}{2k_{\text{db}}^2(\tilde{z})} = \tilde{Q}(\tilde{z}), \quad (45)
\]

with \(\tilde{\phi}_{\text{db}}(\tilde{z}) \equiv \phi_{\text{db}}(z), k_{\text{db}} \equiv k_{\text{db}}(z), \tilde{k}_{\text{db}} \equiv \tilde{k}_{\text{db}}(\tilde{z}).\)

The badlands function may be written explicitly:

\[
Q(z) = \frac{5\kappa^2\ell^2}{\left(k^2\ell^2 + \frac{\ell^2}{z^2}\right)^2} = \frac{5\kappa^2\ell^2}{8 \cosh^2(2u)} \quad u \equiv \ln \frac{z}{\zeta}, \quad (46)
\]

and it reaches its peak value at \(z = \zeta\), that is also \(\tilde{z} = \tilde{\zeta} = -\zeta\). This peak value scales as the inverse of \(\kappa^2\ell^2\), when multiplied by the latter value (see (41)), it leads to the universal function:

\[
V_4(z) = \frac{5}{\left(\frac{\ell^2}{z^2} + \frac{\ell^2}{\zeta^2}\right)^2} = \frac{5}{8 \cosh^2(2u)} u \equiv \ln \frac{z}{\zeta}, \quad (47)
\]

with a peak value \(\frac{5}{8}\) and a relation between \(z\) and \(u\) still to be discussed.

The WKB phase and the coordinate \(z\) also obey symmetry properties under the inversion:

\[
z = \phi_{\text{db}} \equiv \int_{u_0}^u \frac{\ell^2}{2} \cosh(2u') \, du',
\]

\[
= z_0 + \int_0^u \frac{\ell^2}{2} \cosh(2u') \, du', \quad (48)
\]

with \(z_0\) the value corresponding to the inversion center:

\[
z_0 \equiv z(\zeta) = \frac{1}{\sqrt{2}} f'\left(\frac{1}{2}\right)^{\frac{1}{2}}. \quad (49)
\]

Equations (47) and (48) constitute an explicit parametric representation of the universal function \(V_4(z)\) proving that it is symmetrical with respect to the inversion \(u \rightarrow -u\), that is also \(z - z_0 \rightarrow -(z - z_0)\). Another representation in terms of hypergeometric functions is given in appendix B, where other homogeneous forms of the potential \(V(z)\) are also considered.

The QR probability calculated for the \(V_4\) model [53, 54], denoted \(R_4\) in the following and plotted in figure 6, is a universal function of the dimensionless parameter \(\kappa \ell\). It can be calculated by numerically solving the Schrödinger equation for the potential \(V_4(z)\) or \(V_4(z)\). Alternatively, it can be obtained by the analytical method summed up in appendix A.

6. Discussion of QR probabilities

We now present the values obtained for QR probabilities, and compare the exact results for the full CP potential with those obtained for the \(V_4\) model.

We first recall that the QR probability goes from unity at \(\kappa \rightarrow 0\) to zero at \(\kappa \rightarrow \infty\). Its departure from unity at low energies is described by a scattering length \(a\) defined by the

\[
R_4(\kappa) \equiv |r(\kappa)|^2 \approx 1 - 4ka, \quad b \equiv -3a. \quad (51)
\]

Table 2 gives \(\ell\) and \(b\) for a hydrogen atom above a perfect mirror, a silicon bulk and a silica bulk, given in atomic units \(a_0 \approx 52.9\) pm.

| mirror | perfect | silica |
|--------|---------|--------|
| \(b\) \([a_0]\) | 543.0 | 435.2 | 272.6 |
| \(\ell\) \([a_0]\) | 520.1 | 429.8 | 321.3 |

general relation:

\[
r(\kappa) \approx - (1 - 2i\kappa a). \quad (50)
\]

The scattering length is a complex number, the imaginary part of which determines the quantum reflection probability:

\[
R(\kappa) \equiv |r(\kappa)|^2 \approx 1 - 4k\beta, \quad \beta \equiv -3a. \quad (51)
\]

Table 2 gives \(\ell\) and \(b\) for a hydrogen atom above a perfect mirror, a silicon bulk and a silica bulk, as obtained from the full calculations in [26]. The table shows that the equality \(b = \ell\) typical of the \(V_4\) model [23] is no longer true for the full CP potential, with large variations in particular for the case of silica bulks.

We show in figure 7 the calculated QR probabilities \(R\) as a function of the dimensionless parameter \(k\ell\) for the scattering problems corresponding to table 2. The full curves represent the values calculated for perfect mirrors, silicon and silica bulks [26]. They are compared to the dashed curve which corresponds to the universal function \(R_4\) (with \(b = \ell\) in this case) calculated for the pure \(V_4\) model. Using the value calculated for \(b\) for different bulks of matter, it turns out that the exact QR probabilities \(R\) are close to the expression \(R_4\) evaluated for the same value of \(k\ell\). The agreement is excellent at low energies because the peaks of \(V\) on which QR occurs correspond in these cases to values of \(z\) in the far-end tail of the CP potential. Differences between the curves \(R\) and \(R_4\) appear at large enough energies, because distances \(z\) closer to the cliff-side play a significant role.
allows quantitative evaluation of QR probabilities which can be obtained from the universal function corresponding to the pure $V_4$ model.

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Appendix A. QR probability for the $V_4$ model

In this appendix, we recall the analytical method which can be used to to solve Schrödinger’s equation for the $V_4$ model [53, 54]. The derivation presented here follows the work of [55] and uses results in [41, 56].

We first perform a Liouville transformation:

$$z \rightarrow \tilde{z}(z) = \ln \frac{z}{\zeta}, \quad \Psi(\tau) \rightarrow \tilde{\Psi}(\tilde{\tau}) = \frac{\Psi(\tau)}{\sqrt{\tau}}.$$  \hfill (A.1)

With the new variables, the Schrödinger equation for the $V_4$ model becomes a modified Mathieu equation:

$$\Psi^{(\tau)}(\tilde{\tau}) + (-a + 2q \cosh(2\tau))\Psi(\tilde{\tau}) = 0,$$  \hfill (A.2)

where $a \equiv \frac{1}{4}$ while $q \equiv \kappa = \sqrt{k^2}$. The only remaining parameter. A pair of solutions to this equation can be written as series involving products of Bessel functions:

$$\tilde{\Psi}^{(\tau)}(\tilde{z}) = \sum_{n=-\infty}^{\infty} (-1)^n A_n^{(\tau)} J_{2n+1}(\sqrt{q} e^{\tau}) J_{2n}(\sqrt{q} e^{-\tau}).$$  \hfill (A.3)

Here $\tau$ is a complex parameter yet to be determined, known as the Mathieu characteristic exponent. The coefficients $A_n^{(\tau)}$ obey the following recurrence relation:

$$(\tau^2 + 2n^2 - a) A_n^{(\tau)} + q A_{n+1}^{(\tau)} + q A_{n-1}^{(\tau)} = 0.$$  \hfill (A.4)

The infinite determinant associated with this system of equations must be zero for a non trivial solution to exist. This singles out a value of $\tau$, which can be obtained by following the procedure detailed in [55] or using the Mathematica function MathieuCharacteristicExponent(a,q). With the recurrence relation we can write the ratios $A_n^{(\tau)}/A_{n-1}^{(\tau)}$ and $A_n^{(\tau)}/A_{n+1}^{(\tau)}$ as continued fractions. These ratios go to 0 when $|n|$ increases so that we can truncate the continued fractions to obtain numerical values for $A_n^{(\tau)}$ (with $A_0^{(\tau)} = 1$).

As a result of the invariance of equation (A.2) under parity $\tilde{z} \rightarrow -\tilde{z}$ (which is the symmetry discussed in section 5), $\tilde{\Psi}^{(\tau)}(-\tilde{z})$ are also solutions, and one can show that:

$$\tilde{\Psi}^{(\tau)}(\tilde{z}) = e^{2\sigma} \tilde{\Psi}^{(\tau)}(-\tilde{z}), \quad \sigma = \ln \frac{\tilde{\Psi}^{(\tau)}(0)}{\tilde{\Psi}^{(\tau)}(0)}.$$  \hfill (A.5)
Using known results for the Bessel functions:

\[ J_n(x) \approx \frac{2}{\pi x} \cos \left( x - \frac{\nu \pi}{2} - \frac{\pi}{4} \right) \quad \text{for } x \to \infty, \quad J_n(0) = \delta_{n,0}, \]

we deduce the asymptotic behaviors:

\[ \Psi^{(\pm)}_z(z) \approx \frac{2}{\pi \sqrt{q} e^{\pm z}} \cos \left( \sqrt{q} e^z \pm \frac{\pi}{2} - \frac{\pi}{4} \right), \]

\[ \Psi'(z) \approx e^{\mp \sqrt{q} e^z} \cos \left( \sqrt{q} e^z \pm \frac{\pi}{2} - \frac{\pi}{4} \right). \quad \text{(A.6)} \]

As we are looking for the reflection and transmission amplitudes \( r \) and \( t \) for a wave coming from the far-end, we search the solution \( t \Psi_L(z) \) of Schrödinger equation (A.2) which has the asymptotic behaviors:

\[ t \Psi_L(z) \approx \frac{t}{\ell} \exp \left( -i 2 \pi x_0 - \frac{\ell}{z} \right), \]

\[ t \Psi_L(z) \approx \frac{e^{-i \zeta} + re^{i \zeta}}{\sqrt{\ell}}. \quad \text{(A.7)} \]

We have used the asymptotic forms of \( \phi_{db}(z) \):

\[ \phi_{db}(z) \approx 2 \pi x_0 - \frac{\ell}{z} \quad \text{for } z \to 0, \quad \phi_{db}(z) \approx \zeta. \quad \text{(A.8)} \]

Matching the asymptotic forms (A.6–A.7), we obtain the reflection and transmission amplitudes:

\[ r = -i \frac{\sinh(\sigma)}{\sinh(\sigma + i \pi \tau)}, \quad t = \frac{\sin(\pi \tau) e^{2i \pi x_0}}{\sin(\sigma + i \pi \tau)}. \quad \text{(A.9)} \]

It has been checked that this analytical method gives the same results as a direct integration of the Schrödinger equation [26]. The resulting QR probability \( R_4 = |r|^2 \) is drawn on figure 6.

### Appendix B. Other homogeneous potentials

In this appendix, we consider the case of homogeneous potentials \( V_n(z) = -C_n/z^n \) with \( n > 2 \). This includes the already discussed case \( n = 4 \), as well as the case \( n = 3 \) which corresponds to the Van der Waals zone close to the surface and the case \( n = 5 \) which corresponds to the far-end of a slab mirror [26].

We start by introducing two relevant length scales:

\[ \zeta_n = \sqrt{\frac{C_n}{E}}, \quad \ell_n = \sqrt{\frac{2mC_n}{\hbar^2}} = \frac{1}{\sqrt{\zeta_n^2} (\zeta_n)^2}. \quad \text{(B.1)} \]

They generalize the definitions of \( \zeta \) and \( \ell \) for \( n = 4 \), \( \zeta_n \) and \( \ell_n \) measure respectively the distance at which \( E = |V_n| \) and the strength of the potential.

The WKB wavevector and phase thus read:

\[ k_{db}(z) = \kappa \sqrt{1 + \frac{x}{x_n}}, \quad x \equiv \frac{z}{\zeta_n}, \quad \text{(B.2)} \]

\[ \phi_{db}(z) = \kappa \zeta_n \int_{z_0}^{z} \sqrt{1 + \frac{1}{x_n^2}} \ dx', \quad \text{(B.3)} \]

where \( z_0 \) is chosen to enforce (9). For \( n > 2 \), we deduce:

\[ \phi_{db} = \frac{n \pi x_0}{n - \frac{2}{\sqrt{\ell}}}, \quad F \left( \frac{1}{2}, \frac{1}{n}; \frac{1}{n}; \frac{1}{x_n} \right) \right) = \frac{1}{n} \left[ \frac{1}{1 + \frac{1}{x_n^2}} \right]. \quad \text{(B.4)} \]

The badlands function:

\[ Q(z) = \frac{(n - n + 4)(1 + n) x^n}{16 (1 + x^n)^3} \quad \text{(B.5)} \]

is a peaked function reaching its maximum at:

\[ x_n = \sqrt{\frac{5 n^2 - 3 n - 8 + \sqrt{3(7 n^2 - 6 n^3 - 13 n^2 - 4 n^2 + 2)}}{4 n^2 + 2}}, \quad \text{(B.6)} \]

We define the special Liouville gauge \( z = \phi_{db}(z)/\zeta \) as in (37) and obtain \( E = x^2 \) and \( V = x^2 Q(z) \) as in (39). Up to now, we did not fix the scale factor as in (41), as \( t \equiv t_4 \) does not play any role for the potential \( V_n \) studied in this Appendix.

As the maximum value of \( Q \) scales as \( 1/\kappa_n^2 \), we choose the scale factor as:

\[ x_n = \kappa_n^2, \quad \text{(B.7)} \]

which generalizes the definition (41). This leads to universal functions \( V_n(z) \) which do not depend on any other parameter than \( n \). The functions \( V_n(z) \) are drawn on figure B1 for the cases \( n = 3, 4, 5 \), as functions of the coordinate \( z = \phi_{db}(z)/\zeta \) using the convention (B.7).

With the same convention, the integrals (40) of \( V_n \) over the real axis are real numbers depending only on \( n \) and they
can be expressed in terms of the Gamma function:

\[
I_n = \frac{n \sqrt{\pi} \Gamma \left( 2 + \frac{1}{n} \right) \sec \left( \frac{\pi}{n} \right)}{12 \Gamma \left( 1 + \frac{1}{n} \right)}. \tag{B.8}
\]

In particular, the case \( n = 4 \) corresponds to:

\[
I_4 = \frac{5 \Gamma (5/4)^2}{3 \sqrt{\pi}} \approx 0.772531. \tag{B.9}
\]

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