IOP Publishing Physica Scripta

Phys. Scr. **95** (2020) 065405 (9pp) https://doi.org/10.1088/1402-4896/ab80e6

Quantum particles in a moving potential

Miguel Ahumada-Centeno[1,5], Paolo Amore[2,5], Francisco M Fernández[3,5] and Jesus Manzanares-Martinez[4,5]

[1] Facultad de Ciencias, Universidad de Colima, Bernal Díaz del Castillo 340, Colima, Colima, Mexico
[2] Facultad de Ciencias, CUICBAS, Universidad de Colima, Bernal Díaz del Castillo 340, Colima, Colima, Mexico
[3] INIFTA, Division Quimica Teorica, Blvd. 113 S/N, Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina
[4] Departamento de Investigacion en Fisica, Universidad de Sonora, Blvd. Luis Encinas y Rosales, Hermosillo, Sonora 83000, Mexico

E-mail: mahumada0@ucol.mx, paolo@ucol.mx, fernande@quimica.unlp.edu.ar and new.jmanza@gmail.com

Received 24 October 2019, revised 15 March 2020
Accepted for publication 18 March 2020
Published 2 April 2020

Abstract

We study the behavior of a quantum particle, trapped in localized potential, when the trapping potential starts suddenly to move with constant velocity. In one dimension we have reproduced the results obtained by (Granot and Marchewka 2009 *EPL* **86** 20007), for an attractive delta function, using an approach based on a spectral decomposition, rather than on the propagator. We have also considered the cases of Pöschl-Teller and simple harmonic oscillator potentials (in one dimension) and to the hydrogen atom (in three dimensions). In this last case we have calculated explicitly the leading contribution to the ionization probability for the hydrogen atom due to a sudden movement.

Keywords: boound states, quantum wells, moving potentials

(Some figures may appear in colour only in the online journal)

1. Introduction

This paper focuses on a class of quantum mechanical problems where the Hamiltonian displays an explicit time–dependence: a typical realization of this situation, the time–dependence manifests itself through an interaction that is acting upon the system over a finite interval of time. Applications of these problems can be found in standard text of Quantum Mechanics. A different possibility, considered in this paper, is that the time-dependence can enter in the problem in a less direct way, via the boundary conditions (for instance a box whose walls start to move at a given time) or because the potential itself in the Hamiltonian starts to move. In a recent paper, [1], Granot and Marchewka have studied the interesting problem of determining the behavior of a quantum particle trapped in a localized potential, when the potential suddenly starts to move at constant speed at $t = 0$. These authors used an attractive Dirac delta potential in one dimension to model the problem, calculating exactly the probability that the particle remains confined to the moving potential or that it remains in the initial position. In addition to these two possibilities, they also observed the probability that the particle moves at twice the speed of the potential: for an observer sitting in the rest frame of the potential at $t > 0^+$ this phenomenon can be interpreted as a quantum reflection of a particle moving to the left with speed $-v$ from the well.

The problem considered in [1] is a special case of the more general problem of a quantum system with a time–dependent Hamiltonian, where the potential may change continuously with time or may be subject to a sudden perturbation. A well–known example, with exact solution, is the case of a particle in one–dimensional infinite square–well with one wall moving at constant velocity, originally discussed by Doescher and Rice [2] long time ago (exact solutions for infinite square-wells with a wall moving with different laws were later found by Makowski and Dembinski [3]).

The time evolution of a quantum system in presence of a sudden perturbation displays interesting behaviors, particularly in relation to quantum transients (for a general

[5] Authors to whom any correspondence should be addressed.

discussion of quantum transient the reader may refer to [4–6]). An example of this is the 'quantum shutter' studied by Moshinski [7], corresponding to a beam of particles of mass m and momentum p, initially confined in the negative semi-axis by a totally absorbing shutter located at the origin, after that the shutter is removed at $t > 0$.

The technological advances are making increasingly realistic the scenarios where a quantum particle, such as an atom, can be trapped by suitable attractive potential (corresponding for example to a tip of a needle in a scanning tunneling microscope or a highly focused laser beam in an optical tweezer) and thus be relocated in a different region [8–11]. As remarked by Granot and Marchewka, the quantum nature of this process leads to surprising results, as the possibility that the particle moves at twice the speed of the needle.

The idea that the Hamiltonian of a problem can change abruptly may of course be questioned, since the changes in the potential (or in the boundary conditions) will not be instantaneous in an experimental situation. With this motivation, the authors of [12] have modified the quantum shutter problem considering a time–dependent shutter potential, which vanishes asymptotically for $t \to \infty$. In our case, as for the case of [1], the transition probabilities calculated under the assumption of a sudden motion may be considered an approximation to an experimental situation only at small velocities. In a more realistic description the system should first accelerate, and then stabilize to a finite velocity. A more rigorous treatment of this process would require applying acceleration transformations to the quantum mechanical system (see for example [13]), whereas a simpler treatment could approximate the acceleration with a sequence of steps of increasing speed, up to a maximal speed. In this paper we discuss this second approach for the case of the simple harmonic oscillator (for which the complications arising from having to deal with a continuous part of the spectrum are absent), with just two times steps, showing that indeed the probabilities are sensibly affected.

Keeping in mind these limitations, the present paper has two different goals: first, to reproduce the analysis of [1] using a more direct approach based on a spectral decomposition rather than on the propagator; second, to extend this analysis to a wider class of problems, in one and three dimensions.

The paper is organized as follows: in section 2 we discuss the general framework, using spectral decomposition; in section 3 we consider several examples of potentials, with spectra which can be either mixed or discrete, and calculate *explicitly* the relevant probabilities for each case; finally in section 4 we draw our conclusions.

2. Spectral decomposition

Our starting point is the time dependent Schrödinger equation (TDSE)

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi + V(\vec{r} - \vec{v}t)\Psi(\vec{r}, t) \tag{1}$$

where $V(\vec{r} - \vec{v}t)$ is a potential moving with velocity $\vec{v}$.

Let us define $\vec{\xi}(\vec{r}, t) \equiv \vec{r} - \vec{v}t$ and let $\phi(\vec{\xi})$ be the solution of the time independent Schrödinger equation (TISE)

$$-\frac{\hbar^2}{2m}\Delta_\xi\phi + V(\vec{\xi})\phi(\vec{\xi}) = E\phi(\vec{\xi}) \tag{2}$$

It can be easily verified that

$$\Psi(\vec{r}, t) = e^{\frac{im\vec{v}\cdot\vec{r}}{\hbar} - \frac{im\vec{v}^2 t}{2\hbar}}\phi(\vec{\xi})e^{-\frac{iEt}{\hbar}} \tag{3}$$

is a solution to the time-dependent Schrödinger equation (1).

The physical situation studied by Granot and Marchewka amounts to having a quantum particle at the initial time in the ground state of the static potential and determining the probability at later times $t > 0$ that the particle can be found in any of the modes of the moving potential. Although the assumption of a sudden motion of the potential well over-simplifies the experimental conditions, it is expected to provide a better description for small velocities, while allowing one to obtain explicit (and simple enough) formulas.

For simplicity we will denote as $\psi_n(\vec{r}, t)$ and $\psi_{\vec{k}}(\vec{r}, t)$ the eigenmodes of the moving potential and $\phi_n(\vec{r})$ and $\phi_{\vec{k}}(\vec{r})$ the eigenmodes of the static potential, where n and $\vec{k}$ refer to bound an continuum states, respectively. We also call $\Phi(\vec{r})$ the initial wave function at $t = 0$ (for the specific case studied in [1] this is the wave function of the ground state).

Let $\Psi(\vec{r}, t)$ be the wave function solution to the TDSE with a moving potential at $t > 0$, subject to the condition $\Psi(\vec{r}, 0) = \Phi(\vec{r})$; this wave function can be naturally decomposed in the basis of the moving potential as

$$\Psi(\vec{r}, t) = \sum_n a_n\psi_n(\vec{r}, t) + \int\frac{d^3k}{(2\pi)^3}b(\vec{k})\psi_{\vec{k}}(\vec{r}, t) \tag{4}$$

where, using equation (3),

$$a_n = \int d^3r\psi_n^\star(\vec{r}, 0)\Phi(\vec{r}) = \int d^3r e^{-i\frac{m\vec{v}\cdot\vec{r}}{\hbar}}\phi_n^\star(\vec{r}, 0)\Phi(\vec{r})$$
$$b(\vec{k}) = \int d^3r\psi_{\vec{k}}^\star(\vec{r}, 0)\Phi(\vec{r}) = \int d^3r e^{-i\frac{m\vec{v}\cdot\vec{r}}{\hbar}}\phi_{\vec{k}}^\star(\vec{r}, 0)\Phi(\vec{r}).$$

In this way $\sum_n |a_n|^2$ is the probability that the particle remains in a bound state when the potential starts moving, whereas $\int\frac{d^3k}{(2\pi)^3}|b(\vec{k})|^2$ is the probability that the particle will escape to the continuum[6].

Calling N the number of bound states of the potential, we define the physical amplitudes

$$\mathcal{Q}_{ij}(\vec{v}) \equiv \int_{-\infty}^{\infty} e^{-im\vec{v}\cdot\vec{r}/\hbar}[\phi_j(\vec{r})]^\star\phi_i(\vec{r})d^3r$$
$$\mathcal{P}_i(\vec{k}, \vec{v}) \equiv \int_{-\infty}^{\infty} e^{-im\vec{v}\cdot\vec{r}/\hbar}[\phi(\vec{k}, \vec{r})]^\star\phi_i(\vec{r})d^3r$$
$$\tilde{\mathcal{P}}_i(\vec{k}, \vec{v}) \equiv \int_{-\infty}^{\infty} e^{-im\vec{v}\cdot\vec{r}/\hbar}\phi_i^\star(\vec{r})\phi(\vec{k}, \vec{r})d^3r = \mathcal{P}_i^\star(\vec{k}, -\vec{v})$$

[6] We are discussing here the three dimensional case, but the modifications for the one and two dimensional cases are straightforward.

The wave function at later times for a particle initially in the ith state of the static potential will then be

$$\Psi(\vec{r}, t) = \sum_{j=1}^{N} \mathcal{Q}_{ij}\psi_j(\vec{r}, t) + \int_{-\infty}^{\infty} \mathcal{P}_i(\vec{k}, v)\psi(\vec{k}, \vec{r}, t)\frac{d^3k}{(2\pi)^3} \tag{5}$$

Clearly $|\mathcal{Q}_{ij}|^2$ represents the probability that the particle, initially in the *ith* bound state ends up in the *jth* bound state; similarly $|\mathcal{P}_i(\vec{k}, v)|^2 d^3k/(2\pi)^3$ represents the probability that the particle initially in the ith bound state ends up in the continuum with momentum in an infinitesimal volume about $\hbar\vec{k}$.

The conservation of total probability requires

$$\sum_{j=1}^{N}|\mathcal{Q}_{ij}|^2 + \int_{-\infty}^{\infty}|\mathcal{P}_i(\vec{k}, v)|^2\frac{d^3k}{(2\pi)^3} = 1 \tag{6}$$

Similarly we define the amplitude

$$\mathcal{R}(\vec{k}, \vec{k}', \vec{v}) \equiv \int_{-\infty}^{\infty} e^{-im\vec{v}\cdot\vec{r}/\hbar}[\phi(\vec{k}', \vec{r})]^\star\phi(\vec{k}, \vec{r})d^3r$$

which is related to the probability that a particle initially with momentum $\hbar\vec{k}$ ends up in a state with momentum $\hbar\vec{k}'$.

Of course these arguments can be generalized to the case that the initial wave function is not a stationary state of the static problem. In this case the time dependent wave function is

$$\Psi(\vec{r}, t) = \sum_{j=1}^{N} \bar{\mathcal{Q}}_j\psi_j(\vec{r}, t) + \int_{-\infty}^{\infty} \bar{\mathcal{P}}(\vec{k}, v)\psi(\vec{k}, \vec{r}, t)\frac{d^3k}{(2\pi)^3} \tag{7}$$

where

$$\bar{\mathcal{Q}}_j \equiv \int e^{-im\vec{v}\cdot\vec{r}/\hbar}[\phi_j(\vec{r})]^\star\Phi(\vec{r})d^3r = \sum_{i=1}^{N} a_i\,\mathcal{Q}_{ij} + \int b(\vec{k})\tilde{\mathcal{P}}_j(\vec{k}, \vec{v})\frac{d^3k}{(2\pi)^3}$$

$$\bar{\mathcal{P}}(k', v) \equiv \int e^{-im\vec{v}\cdot\vec{r}/\hbar}[\phi(\vec{k}', \vec{r})]^\star\Phi(\vec{r})d^3r$$

of which Equation (5) is a special case.

3. Applications

In this section we apply our general discussion to different examples.

3.1. Attractive dirac delta potential

We consider the attractive Dirac delta potential studied in [1]:

$$V(x, t) = \begin{cases} -\gamma\delta(x), & t \leqslant 0 \\ -\gamma\delta(x - vt), & t > 0 \end{cases} \tag{8}$$

To implement the procedure explained in section 2 we first write explicitly the eigenfunctions of the static potential, $V(x,0) = -\gamma\,\delta(x)$, reported in [14]

$$\phi_0(x) = \sqrt{\beta}e^{-\beta|x|} \tag{9}$$

$$\phi_p^{(e)}(x) = \frac{\sqrt{2}\,(p\cos(px) - \beta\sin(p|x|))}{\sqrt{\beta^2 + p^2}} \tag{10}$$

$$\phi_p^{(o)}(x) = \sqrt{2}\sin(px) \tag{11}$$

where $\beta = m\gamma/\hbar^2$. Damert [15] and Patil [16] have proved the completeness of the set of the energy eigenfunctions. Note that the spectrum of $V(x,0)$ is mixed with a single bound state of energy $E_0 = -\frac{\gamma^2 m}{2\hbar^2}$.

The orthonormality relations for this set of functions are

$$\int_{-\infty}^{\infty}\phi_0^\star(x)\phi_0(x)dx = 1$$

$$\int_{-\infty}^{\infty}\phi_0^\star(x)\phi_p^{(e)}(x)dx = \int_{-\infty}^{\infty}\phi_0^\star(x)\phi_p^{(o)}(x)dx = 0$$

$$\int_{-\infty}^{\infty}\phi_{p'}^{(e)\star}(x)\phi_p^{(e)}(x)dx = \int_{-\infty}^{\infty}\phi_{p'}^{(o)\star}(x)\phi_p^{(o)}(x)dx = 2\pi\delta(p - p')$$

$$\int_{-\infty}^{\infty}\phi_{p'}^{(o)\star}(x)\phi_p^{(e)}(x)dx = 0$$

Using the prescription (3) one can obtain the solutions to the time dependent problem for $t > 0$ corresponding to the static solutions of equations (9), (10) and (11):

$$\psi_0(x, t, v) = \sqrt{\beta}e^{-\beta|x-tv|+\frac{im(\gamma^2 t + v\hbar^2(2x-tv))}{2\hbar^3}}$$

$$\psi_k^{(e)}(x, t, v) = \frac{\sqrt{2}}{\sqrt{\beta^2 + k^2}}e^{-\frac{i(k^2t\hbar^2 + m^2v(tv-2x))}{2m\hbar}} \times (k\cos(k(x - tv)) - \beta\sin(k|x - tv|))$$

$$\psi_k^{(o)}(x, t, v) = \sqrt{2}\sin(k(x - tv))e^{-\frac{i(k^2t\hbar^2 + m^2v(tv-2x))}{2m\hbar}}$$

The initial wave function is the bound state of the static delta potential

$$\Psi_0(x) = \sqrt{\beta}e^{-\beta|x|}$$

and it can be decomposed in the basis of the time-dependent potential as

$$\Psi_0(x) = \mathcal{Q}_{11}(v)\psi_0(x, 0) + \int_0^\infty\frac{dk}{2\pi}[\mathcal{P}_1^{(e)}(k, v)\psi_k^{(e)}(x, 0) + \mathcal{P}_1^{(o)}(k, v)\psi_k^{(o)}(x, 0)]$$

as explained in section 2.

The amplitude for transition to the bound state of the moving well is given by

$$\mathcal{Q}_{11}(v) = \int_{-\infty}^{\infty} e^{-imvx/\hbar}\phi_0^\star(x)\phi_0(x)dx = \frac{4}{\theta^2 + 4} \tag{12}$$

where $\theta \equiv \hbar v/\gamma$ is the adiabatic Massey parameter [1, 17].

Clearly, the probability that the particle remains in the bound state of the moving well is simply given by

$$P_{bound} = |\mathcal{Q}_{11}|^2 = \frac{16}{(\theta^2 + 4)^2} \tag{13}$$

in agreement with the equation (13) of [1].

Similarly we can calculate the coefficients $\mathcal{P}_1^{(e)}(k, v)$ and $\mathcal{P}_1^{(o)}(k, v)$, representing the amplitudes for transitions to a state in the continuum (even and odd states, respectively) with momentum $\hbar k$

$$\begin{aligned}\mathcal{P}_1^{(e)}(k, v) &= \int_{-\infty}^{\infty} e^{-imvx/\hbar}[\phi_k^{(e)}(x)]^\star \phi_0(x)dx \\ &= \frac{4\sqrt{2}\beta^{7/2}\theta^2 k}{\sqrt{\beta^2 + k^2}(\beta^4(\theta^2 + 1)^2 + k^4 - 2\beta^2(\theta^2 - 1)k^2)}\end{aligned} \tag{14}$$

$$\begin{aligned}\mathcal{P}_1^{(o)}(k, v) &= \int_{-\infty}^{\infty} e^{-imvx/\hbar}[\phi_k^{(o)}(x)]^\star \phi_0(x)dx \\ &= -\frac{4i\sqrt{2}\beta^{5/2}\theta k}{\beta^4(\theta^2 + 1)^2 + k^4 - 2\beta^2(\theta^2 - 1)k^2}\end{aligned} \tag{15}$$

where $\beta = mv/\hbar\theta$.

As a result the probability that the particle ends up in the continuum is

$$\begin{aligned}P_{continuum} &= \int_0^{\infty} [|\mathcal{P}_1^{(e)}(k, v)|^2 + |\mathcal{P}_1^{(o)}(k, v)|^2]\frac{dk}{2\pi} \\ &= \int_{-\infty}^{\infty} [|\mathcal{P}_1^{(e)}(k, v)|^2 + |\mathcal{P}_1^{(o)}(k, v)|^2]\frac{dk}{4\pi} \\ &= \int_{-\infty}^{\infty} \frac{16\beta^5\theta^2 k^2(\beta^2(\theta^2 + 1) + k^2)}{(\beta^2 + k^2)(\beta^4(\theta^2 + 1)^2 + k^4 - 2\beta^2(\theta^2 - 1)k^2)^2}\frac{dk}{2\pi}\end{aligned}$$

A straightforward integration of this expression using the residue theorem provides the final result

$$P_{continuum} = 1 - \frac{16}{(\theta^2 + 4)^2} \tag{16}$$

The total probability correctly sums to 1:

$$P_{total} = P_{bound} + P_{continuum} = 1$$

The solution at $t > 0$ is then obtained using equation (5): using this expression we were able to reproduce figure 3 of [1] performing a numerical integration of this equation (notice however a typo in the second equation of (15) of [1]).

3.2. Simple harmonic oscillator

The simple harmonic oscillator

$$V(x) = \frac{1}{2}m\omega^2 x^2 \tag{17}$$

is possibly the most important example of quantum mechanical problem for which exact solutions are known.

In this case the spectrum is discrete, with bound states of energy

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, \ldots \tag{18}$$

and with eigenfunctions

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{mx^2\omega}{2\hbar}} H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right) \tag{19}$$

where $H_n(x)$ is the Hermite polynomial of order n.

We define the dimensionless parameter

$$\kappa \equiv \frac{mv^2}{2\hbar\omega} \tag{20}$$

representing the ratio between the kinetic energy associated with the motion of the well and a quanta of energy $\hbar\omega$.

Assuming that the particle is initially in the ground state of the static potential, the amplitudes can be obtained explicitly

$$\mathcal{Q}_{0,j}(\kappa) = \frac{e^{-\kappa/2} i^{-j}\kappa^{j/2}}{\sqrt{j!}} \tag{21}$$

The first few amplitudes are

$$\mathcal{Q}_{0,0}(\kappa) = e^{-\kappa/2}, \quad \mathcal{Q}_{0,1}(\kappa) = -ie^{-\kappa/2}\sqrt{\kappa}$$
$$\mathcal{Q}_{0,2}(\kappa) = -\frac{e^{-\kappa/2}\kappa}{\sqrt{2}}, \quad \mathcal{Q}_{0,3}(\kappa) = \frac{ie^{-\kappa/2}\kappa^{3/2}}{\sqrt{6}}$$

In this case the probability $|\mathcal{Q}_{0n}|^2$ of exciting the state n follows a Poisson distribution

$$|\mathcal{Q}_{0n}|^2 = \frac{\kappa^n}{n!}e^{-\kappa} \tag{22}$$

and it reaches a maximum for a velocity given by

$$\frac{mv^2}{2} = \hbar\omega n \tag{23}$$

or equivalently

$$\kappa = n \tag{24}$$

The probabilities of transition from the ground state of the SHO to an excited state, due to a sudden movement of the well, are plotted in figure 1. The vertical lines in the plot correspond to the condition (24). It is worth noticing that at $\kappa = n$, $|\mathcal{Q}_{0,n}(n)|^2 = |\mathcal{Q}_{0,n-1}(n)|^2$, for $n > 1$. The proof of this property can be found in appendix appendix.

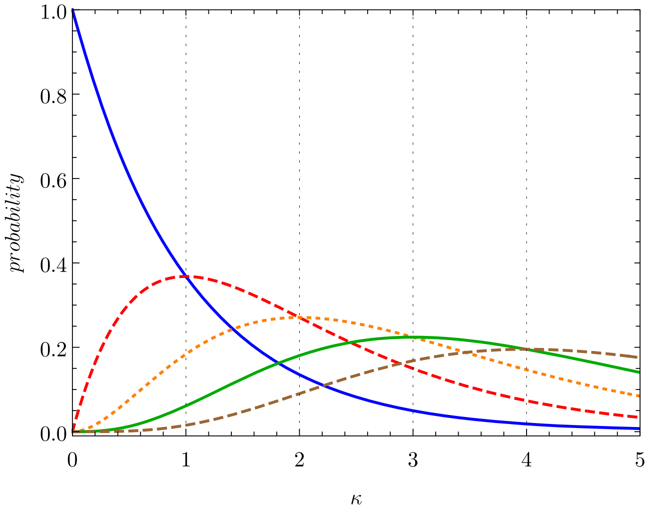

Figure 1. Probability of transition from the ground state to an excited state for the simple harmonic oscillator, due to a sudden movement. The vertical lines correspond to the condition (24).

As we already mentioned in the Introduction, a better description of the physical process would require a smooth transition from zero velocity up to a maximal velocity. Ideally, this should be done using an acceleration transformation (see for instance [13]), but a simpler approach could involve a sequence of time steps where the velocity takes a constant value at each step. We briefly discuss this approach for the simple harmonic oscillator, where the complications of the continuum part of the spectrum are absent, and for the special case of just two time steps. We assume that the particle is in the ground state at time $t = 0$, when suddenly the potential starts moving with velocity $v_1 = \eta\, v$ (with $0 < \eta < 1$) up to $t = t_1$, and for $t > t_1$ finally moves with velocity v. The probability that the particle will be in the ground state at $t > t_1$ can be calculated as

$$\mathcal{P}_{0\to 0}(\kappa) = \sum_{j=0}^{\infty} |\mathcal{Q}_{0,j}(\kappa_1)\,\mathcal{Q}_{j,0}(\kappa_2)|^2 \tag{25}$$

where $\kappa_1 \equiv m v_1^2/2\hbar\omega$ and $\kappa_2 \equiv m(v - v_1)^2/2\hbar\omega$.

A simple calculation yields the result

$$\mathcal{P}_{0\to 0}(\kappa) = e^{-2\eta^2\kappa + 2\eta\kappa - \kappa} I_0(2(\eta - 1)\eta\kappa) \tag{26}$$

where $I_n(x)$ is the Bessel function modified Bessel function of the first kind (notice that this expression correctly reduces to the previously considered case for $\eta = 0$ or $\eta = 1$).

Taking into account the asymptotic behaviour of $I_0(x)$ for $x \to -\infty$ (and assuming $\eta \neq 0$ and $\eta \neq 1$), one obtains

$$\mathcal{P}_{0\to 0}(\kappa) \approx \frac{e^{-(1-2\eta)^2\kappa}}{2\sqrt{\pi}\sqrt{(1-\eta)\eta\kappa}} \tag{27}$$

which decays more weakly than in the original case (observe in particular that for $\eta = 1/2$ the exponential decay disappears). Notice also that the probability is maximal for $\eta = 1/2$: for this value, the condition $\mathcal{P}_{0\to 0}(\kappa) > 1/2$ is met for $\kappa \lesssim 1.75$.

This example shows that the probabilities of excitation depend crucially on the details of the movement of the potential and therefore any realistic description of the experiments should first start with a good modeling of the acceleration stage.

3.3. Pöschl-Teller potentials

The second example that we want to consider is the Pöschl-Teller (PT) potential

$$V(x) = -\frac{\hbar^2\lambda(\lambda+1)}{2a^2 m}\,\mathrm{sech}^2\left(\frac{x}{a}\right) \tag{28}$$

for which exact solutions are available.

The potential (28) provides a nice generalization of our discussion for the attractive delta potential, both because it has a mixed spectrum, with λ bound states (λ integer), and because it is known to be reflectionless [18].

The eigenfunctions of the bound states read

$$\phi_j(x) = \frac{\mathcal{N}_j}{\sqrt{a}}\, P_\lambda^j\left(\tanh\left(\frac{x}{a}\right)\right),\quad j = 1,\ldots,\lambda \tag{29}$$

where $P_\lambda^j(x)$ is the associated Legendre polynomial; the corresponding eigenenergies are $E_j = -\frac{j^2\hbar^2}{2a^2 m}$. Here $\mathcal{N}_j$ is a (dimensionless) normalization constant.

As an example we consider the case $\lambda = 1$, for which

$$\phi_1(x) = -\frac{\sqrt{1 - \tanh^2\left(\frac{x}{a}\right)}}{\sqrt{2}\,\sqrt{a}} \tag{30}$$

$$\phi_k(x) = \frac{\left(-\tanh\left(\frac{x}{a}\right) + iak\right)}{1 + iak}\, e^{ikx} \tag{31}$$

and assume that the particle is in the ground state of the static potential at $t = 0$.

The amplitudes for the transition to the bound state and to the continuum states of the moving potential can then be calculated explicitly as

$$\begin{aligned}
\mathcal{Q}_{11} &\equiv \int_{-\infty}^{\infty} e^{-imvx/\hbar}[\phi_1(x)]^\star \phi_1(x)\,dx \\
&= \frac{1}{2}\pi\kappa\,\mathrm{csch}\left(\frac{\pi\kappa}{2}\right) \\
\mathcal{P}_1(k, v) &\equiv \int_{-\infty}^{\infty} e^{-imvx/\hbar}[\phi(k, x)]^\star \phi_1(x)\,dx \\
&= \frac{\pi\sqrt{a}\,\kappa}{\sqrt{2}\,(ak + i)}\,\mathrm{sech}\left(\frac{1}{2}\pi(ak + \kappa)\right)
\end{aligned}$$

where $\kappa \equiv amv/\hbar$.

Similarly to what done for the simple harmonic oscillator, we see that for $\kappa < 0.95$, the probability that a particle would stay in the ground state, after the well starts to move, will be higher than $1/2$.

In the left plot of figure 2 we plot the probability that a particle initially in the bound state of the Poschl-Teller potential with $\lambda = 1$ stays trapped as the well starts to move with constant velocity (blue curve), $P_{bound}(\kappa) = |\mathcal{Q}_{11}|^2$, and the probability that the particle ends up in the continuum (red curve), $P_{continuum}(\kappa) = \int_{-\infty}^{\infty} |\mathcal{P}_1(k, v)|^2 \frac{dk}{2\pi}$. The integral over momentum is performed numerically and it is verified within the numerical accuracy that $P_{bound}(\kappa) + P_{continuum}(\kappa) = 1$.

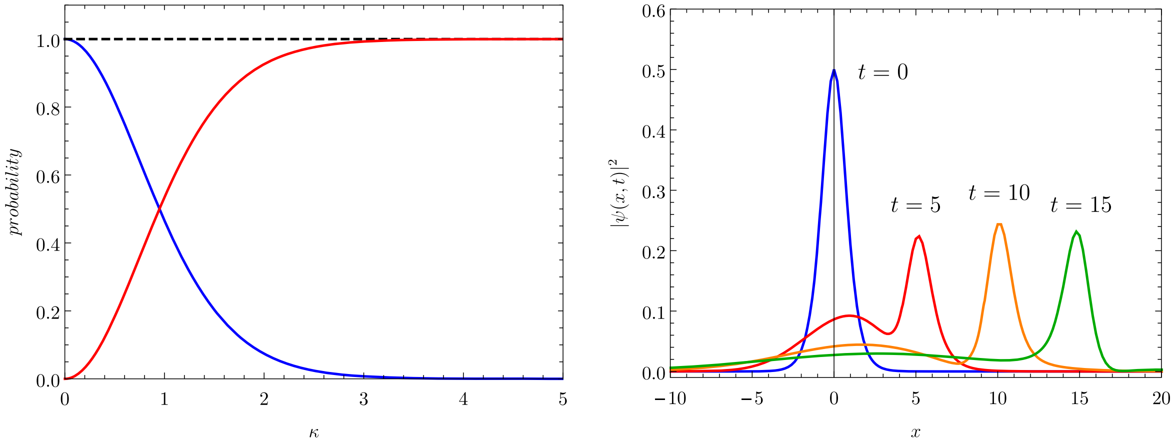

Figure 2. Left plot: Probability that a particle initially in the bound state of the Poschl-Teller potential with $\lambda = 1$ stays trapped as the well starts to move with constant velocity (blue curve); the red curve is the probability that the particle ends up in a state of the continuum. Right plot: Probability density at four different times $t = 0, 5, 10, 15$ for a particle initially in the bound state of the static potential with $\lambda = 1$. We have used $a = m = \hbar = \kappa = 1$.

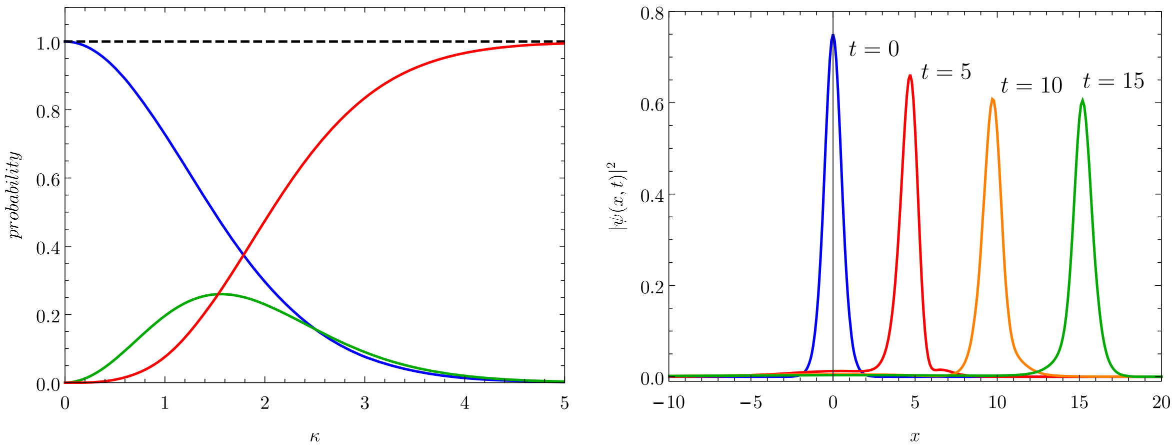

Figure 3. Left plot: Probability that a particle initially in the bound state of the Poschl-Teller potential with $\lambda = 2$ stays trapped as the well starts to move with constant velocity (blue and green curves); the red curve is the probability that the particle ends up in a state of the continuum. Right plot: Probability density at four different times $t = 0, 5, 10, 15$ for a particle initially in the bound state of the static potential with $\lambda = 2$. We have used $a = m = \hbar = \kappa = 1$.

The situation is qualitatively similar to the case treated in [1], but with $P_{bound}(\kappa)$ decaying now exponentially for $\kappa \gg 1$.

The wave function at $t > 0$ can be then obtained as

$$\Psi(x, t) = \frac{1}{2}\pi\kappa \operatorname{csch}\left(\frac{\pi\kappa}{2}\right)\psi_1(x, t) + \int_{-\infty}^{\infty} \frac{\pi\sqrt{a}\,\kappa}{\sqrt{2}\,(ak + i)} \operatorname{sech}\left(\frac{1}{2}\pi(ak + \kappa)\right) \times \psi(k, x, t)\frac{dk}{2\pi} \tag{32}$$

where

$$\psi_1(x, t) = e^{\frac{imvx}{\hbar} - \frac{imv^2 t}{2\hbar}}\phi_1(x - vt)e^{-\frac{iE_1 t}{\hbar}}$$
$$\psi(k, x, t) = e^{\frac{imvx}{\hbar} - \frac{imv^2 t}{2\hbar}}\phi(k, x - vt)e^{-\frac{i\hbar k^2 t}{2m}}$$

Since the Pöschl-Teller potential is reflectionless we expect that the wave function would be qualitatively different from the wave function of the moving delta well, due to the absence of a peak moving with velocity $2v$. The time evolution of a wave function for a particle initially in the bound state of the PT potential, which suddenly starts to move with constant velocity, is displayed in the right plot figure 2. We have used $a = m = \hbar = \kappa = 1$; the probability density is plotted at four different times $t = 0, 5, 10, 15$. In this case it is evident the absence of the reflected wave, as expected, given the nature of the potential. We also appreciate that the peak is moving at velocity v, and the corresponding wave function is not dispersing.

The plots in figures 3 are the analogous of the plots in figures 2, but for a potential with $\lambda = 2$; in this case the potential possess two bound states and, as the potential starts to move, the probability of exciting the first excited state of the well grows up to a maximum (for $\kappa \approx 1.5$) and then decreases (see the left plot in figure 3). The conservation of total probability is verified numerically to hold.

The location of the maximum of the probability of exciting a different bound state approximately corresponds to absorbing the kinetic energy of the particle and make a

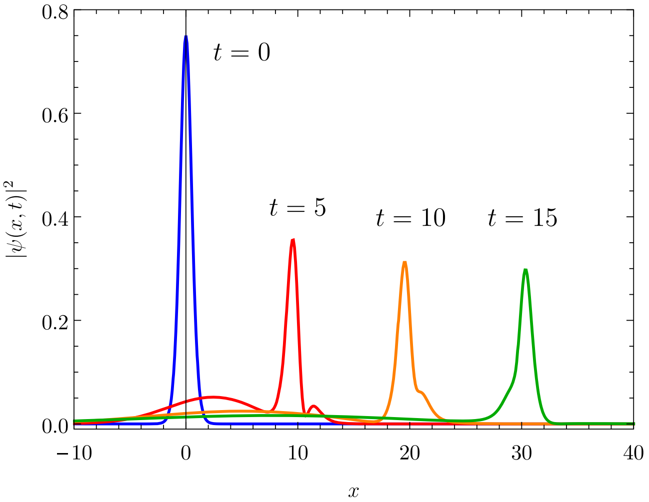

Figure 4. Probability density at four different times $t = 0, 5, 10, 15$ for a particle initially in the bound state of the static potential with $\lambda = 2$. We have used $a = m = \hbar = 1$ and $\kappa = 2$.

transition to the other bound state

$$-\frac{\hbar^2}{2ma^2}(\mu^2 - \lambda^2) = \frac{1}{2}mv^2 \tag{33}$$

or equivalently

$$\kappa = \sqrt{\lambda^2 - \mu^2} \tag{34}$$

For the case in the left plot of figure 3, $\lambda = 2$ and $\mu = 1$, and therefore the maximum corresponds to $\kappa = \sqrt{3}$.

In figure 4 we display the time evolution of the wave function for $\lambda = 2$ but for $\kappa = 2$, at which the components of the bound states are comparable: in this case one can appreciate the asymmetric time-dependent shape of the peak, which reflects the fact that the particle is not in a stationary state.

3.4. Hydrogen atom

Let us now consider a hydrogen atom, initially at rest in the ground state, which is suddenly kicked and the proton starts to move with constant velocity $\vec{v}$.

The wave function of the bound states of the (static) hydrogen atom read

$$\begin{aligned}\psi_{nlm}(r, \theta, \phi) &= R_{nl}(r)Y_l^m(\theta, \phi)\\ &= 2^{l+1}e^{-\frac{r}{a_0 n}}\sqrt{\frac{(-l+n-1)!}{a_0^3 n^4 (l+n)!}}\left(\frac{r}{a_0 n}\right)^l\\ &\times L_{-l+n-1}^{2l+1}\left(\frac{2r}{na_0}\right)Y_l^m(\theta, \phi)\end{aligned} \tag{35}$$

with $n \geqslant 1$, $0 \leqslant l \leqslant n{-}1$ and $|m| \leqslant l$.

Based on our general discussion, the amplitude for the transition from the ground state to any excited state reads[7]

$$\mathcal{Q}_{1,0;n,l} = \int e^{-i\frac{\mu v r\cos\theta}{\hbar}}\psi^\star_{n,l,0}(\vec{r})\psi_{1,0,0}(\vec{r})d^3r \tag{36}$$

where μ here is the mass of the electron.

Using the partial wave decomposition of a plane wave

$$e^{i\frac{\mu v r\cos\theta}{\hbar}} = \sum_{l=0}^{\infty}(2l+1)\ i^l\ j_l\left(\frac{\mu v r}{\hbar}\right)P_l(\cos\theta)$$

one can reduce the expressions to a one dimensional integral

$$\begin{aligned}\mathcal{Q}_{1,0;n,l}(\kappa) &= \sqrt{2l+1}\, i^l \int_0^\infty j_l\left(\frac{\mu v r}{\hbar}\right)\\ &\times R_{10}(r)R_{nl}(r)r^2dr\end{aligned} \tag{37}$$

We have calculated explicitly the amplitudes for $1 \leqslant n \leqslant 10$; their expressions (not reported here) depend uniquely on the dimensionless parameter $\kappa \equiv \frac{\hbar v}{e^2/4\pi\epsilon_0} = \mu v a_0/\hbar$ (a_0 is the Bohr radius). Just to get an idea, $\kappa = 1$ corresponds to a speed $v \approx 0.007892c$; using the root mean square speed for hydrogen gas $v_{rms} = \sqrt{3k_B T/M}$ we can associate a temperature $T \approx 2.2 \times 10^8 K$. To obtain a sizeable ionization effect on the atoms of a gas trapped in a container by means of the elastic collisions of the individual atoms with the walls of the container, one should reach incredibly high temperatures[8].

Using these expressions we can calculate exacly the probability of a transition $(1, 0) \to (n, l)$, with $n \leqslant N$, due to a sudden movement with velocity $\vec{v}$[9]

$$P_{n\leqslant N} = \sum_{n=0}^{N}\sum_{l=0}^{n-1}|\mathcal{Q}_{1,0;n,l}(v)|^2 \tag{38}$$

Of course the probability of not ionizing the atom corresponds to using $N \to \infty$ in the expression above. Repeating the qualitative estimate done for the simple harmonic oscillator and for the Pöschl-Teller potentials, we see that $P_{n=1} < 1/2$ implies $\kappa < 0.87$.

At small velocities ($\kappa \ll 1$) we may obtain the leading behavior of this probability

$$\begin{aligned}P_{n\leqslant 6} &\approx 1 - 0.302617\kappa^2 - 0.576334\kappa^4 + \dots\\ P_{n\leqslant 7} &\approx 1 - 0.297702\kappa^2 - 0.572154\kappa^4 + \dots\\ P_{n\leqslant 8} &\approx 1 - 0.294468\kappa^2 - 0.569285\kappa^4 + \dots\\ P_{n\leqslant 9} &\approx 1 - 0.292225\kappa^2 - 0.567241\kappa^4 + \dots\\ P_{n\leqslant 10} &\approx 1 - 0.290603\kappa^2 - 0.565735\kappa^4 + \dots\end{aligned} \tag{39}$$

The coefficients of the contribution of order κ^2 form a nice monotonic sequence, so that one can use extrapolation to estimate its value for $N \to \infty$ accurately. Moreover, since these coefficients receive contributions only from the transition $(1, 0) \to (n, 1)$, a larger number of coefficients can be calculated with limited effort.

[7] Since the quantum number for the third component of angular momentum needs to vanish, $m = 0$, we express the amplitudes as functions of n and l alone.

[8] Of course, this argument is only qualitative since the boundary conditions for that problem would be different and the wave functions for the moving and static systems would not be related by equation (3).

[9] Notice that for the hydrogen atom there is an infinite number of bound states.

We have used Richardson extrapolation on the sequence of the first 20 coefficients obtaining

$$-0.283\,412\,215\,955\,169\,520\,94 \\ -0.78146725925265723860\ \frac{1}{N^2} \\ +0.781\,467\,259\,252\,511\,902\,51\ \frac{1}{N^3} + \ldots \qquad (40)$$

showing that the ionization probability for the hydrogen atom goes as $0.283\,412\,215\,955\,169\,520\,94\kappa^2$ for $\kappa \to 0$.

This result can be confirmed by using the wave functions of the continuum, $\Psi_{klm}(\vec{r})$. In this case

$$\mathcal{P}(k) = \int e^{-i\frac{\mu v r \cos\theta}{\hbar}} \Psi^{\star}_{klm}(\vec{r}) \psi_{1,0,0}(\vec{r}) d^3 r \qquad (41)$$

is the amplitude for the transition from the ground state to the continuum (i.e. its modulus square is the probability of ionizing the atom).

The direct calculation of the ionization probability requires using the continuum wave functions. These wave functions are reported for instance in [19] and read:

$$\Psi_{klm}(r,\theta,\phi) = Y_{lm}(\theta,\phi)\,\frac{\phi_{kl}(r)}{r} \equiv Y_{lm}(\theta,\phi)\,R_l(k,r) \qquad (42)$$

where (note that the radial wave functions $R_l(k, r)$ obey the $k/(2\pi)$ normalization)

$$\phi_{kl}(r) = \frac{2^{l+1}(kr)^{l+1}}{a_0 r(2l+1)!} e^{\frac{\pi}{2a_0 k} - ikr} \left| \Gamma\left(l - \frac{i}{ka_0} + 1\right) \right| \\ \times {}_1F_1\left(l + \frac{i}{ka_0} + 1;\, 2(l+1);\, 2ikr\right) \qquad (43)$$

Using these wave functions we obtain the exact expression for the leading behavior of the ionization probability as $\kappa \to 0$

$$\int_0^\infty |\mathcal{P}(k)|^2 \frac{dk}{2\pi} \\ \approx \kappa^2 \int_0^\infty \frac{256\pi u\left(\frac{u+i}{-u+i}\right)^{-i/u}\left(-1+\frac{2i}{u+i}\right)^{i/u}\left(\coth\left(\frac{\pi}{u}\right)+1\right)}{3(u^2+1)^5}\frac{du}{2\pi} + O(\kappa^4) \\ \approx 0.283\,412\,215\,955\,169\,520\,89\ \kappa^2 \qquad (44)$$

The value obtained using the extrapolation of the complementary probabilities provides a very accurate estimate (with an error approximately of 4.7×10^{-20}).

4. Conclusions

We have extended the one dimensional model of Granot and Marchewka in [1] for an atom displacing with a moving tip (represented by a Dirac delta function) to a number of potentials with different spectrum (both discrete and mixed) and in one and three dimensions. Our calculations are based on a spectral decomposition, rather than on the direct use of the propagator (as done in [1]) and, for the case discussed in [1] we reproduce the probability that the particle stays trapped calculated by Granot and Marchewka.

The remaining examples that we discuss present new and interesting features, not found in the example considered in [1]: for instance, for the case of Pöschl-Teller potentials we show that the reflected peak moving with velocity $2v$ found in [1] is absent, due to the reflectionless nature of PT potentials; moreover, for the case of potentials with more than one bound state, there is a probability that the particle gets to an excited bound state, rather than to the continuum and we have found a simple criterium based on energy conservation to identify the maxima of this probability. Finally, we have calculated *exactly* the leading contribution in the velocity v to the probability that a hydrogen atom gets ionized due to a sudden movement of the proton.

For the case of a simple harmonic oscillator, we have calculated the probability that a particle initially in the ground state will be found in the ground state at $t > t_1$, after that the potential suddenly starts to move with velocity $v(t) = \theta(t)\, v_1 + \theta(t-t_1)\,(v-v_1)$, with $t_1 > 0$. Our calculation shows that this probability is strongly affected, particularly for large velocities. Future extensions of the present work should take into account the effects of an acceleration, to allow a more realistic description of the physical process.

Acknowledgments

The research of P.A. was supported by Sistema Nacional de Investigadores (México).

Appendix A. Amplitudes for the simple harmonic oscillator

We can understand this result in terms of the creation and annihilation operators $\hat{a}$ and $\hat{a}^\dagger$; calling $|n\rangle$ an eigenstate of the Hamiltonian of the simple harmonic oscillator we have

$$\hat{a}^\dagger \hat{a}|n\rangle = n|n\rangle \\ \hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle \\ \hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle.$$

Following [20] we define

$$I_{mn} \equiv \langle m|U|n\rangle$$

where $\hat{U} = e^{-\alpha\hat{x}}$ and $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^{\dagger})$.

Then

$$I_{0,n} = \langle 0|\hat{U}|n\rangle = \langle 0|\hat{U}\frac{\hat{a}^{\dagger}}{\sqrt{n}}|n-1\rangle = \frac{1}{\sqrt{n}}\langle 0|\left(\hat{a}^{\dagger} - \alpha\sqrt{\frac{\hbar}{2m\omega}}\right)\hat{U}|n-1\rangle \quad \text{(A.1)}$$

$$= -\frac{\alpha}{\sqrt{n}}\sqrt{\frac{\hbar}{2m\omega}}\langle 0|\hat{U}|n-1\rangle = -\frac{\alpha}{\sqrt{n}}\sqrt{\frac{\hbar}{2m\omega}}I_{0,n-1}. \quad \text{(A.2)}$$

On the other hand $I_{0,0} = e^{\alpha^2\hbar/4m\omega}$ and for $\kappa/2 = -\frac{\hbar}{4m\omega}\alpha^2$ we obtain

$$I_{0,n}(\kappa) = -i\sqrt{\frac{\kappa}{n}}I_{0,n-1}(\kappa) \quad \text{(A.3)}$$

from which the property

$$|I_{0,n}(n)|^2 = |I_{0,n-1}(n)|^2 \quad \text{(A.4)}$$

follows.

ORCID iDs

Paolo Amore https://orcid.org/0000-0002-1321-9437
Francisco M Fernández https://orcid.org/0000-0003-0393-790X

References

[1] Granot E and Marchewka A 2009 *EPL* **86** 20007
[2] Doescher S W and Rice M H 1969 *Am. J. Phys.* **37** 1246–9
[3] Makowski A J and Dembinski S T 1991 *Phys.Lett.* A **154** 217–20
[4] del Campo A, Garcia-Calderon G and Muga J G 2009 *Phys. Rep.* **476** 1–50
[5] Del Campo A and Boshier M G 2012 Shortcuts to adiabaticity in a time-dependent box *Sci. Rep.* **2** 648
[6] Sebastian D, Jarzynski C and del Campo A 2014 Classical and quantum shortcuts to adiabaticity for scale-invariant driving *Phys. Rev.* X **4** 021013
[7] Marcos M 1952 Diffraction in time *Phys. Rev.* **88** 625
[8] Arthur A *et al* 1986 *Opt. Lett.* **11** 288–90
[9] Block S M, Goldstein S L B and Schnapp B J 1990 *Nature* **348** 348 6299
[10] Phillips D B *et al* 2014 *Nat. Photonics* **8** 400
[11] Moffitt J R *et al* 2008 *Annu. Rev. Biochem.* **77** 205–28
[12] Scheitler G and Kleber M 1988 On the adiabaticity of continum states: tunnelling through a time-dependent barrier *Zeitschrift für Physik D Atoms, Molecules and Clusters* **9** 267–71
[13] Klink W H 1997 Quantum mechanics in nonintertial reference frames *Ann. Phys.* **260** 27–49
[14] Blinder S M 1988 *Phys. Rev.* A **37** 973
[15] Damert W C 1975 *Am. J. Phys.* **43** 531
[16] Patil S H 2000 *Am. J. Phys.* **68** 712
[17] Elberfeld W and Kleber M 1988 Time-dependent tunneling through thin barriers: a simple analytical solution *Am. J. Phys.* **56** 154–9
[18] Kay I and Moses H E 1956 Reflectionless transmission through dielectrics and scattering potentials *J. Appl. Phys.* **27** 1503–8
[19] Peng L and Gong Q 2010 *Comp. Phys. Comm.* **181** 2098–101
[20] Fernández F M and Castro E A 1995 *Algebraic Methods in Quantum Chemistry and Physics* vol. 3 (Boca Raton, FL: CRC Press)
[21] Voigtländer B 2015 *Scanning Probe Microscopy* (Heidelberg: Springer)