Quantum scattering by Wronskians

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We show that Wronskians between properly chosen linearly independent solutions of the Schrödinger equation greatly facilitate the study of quantum scattering in one dimension. They enable one to obtain the necessary relationships between the coefficients that determine the asymptotic behavior of the wavefunction. As illustrative examples we calculate the transmission probability for the penetration of a Gaussian barrier and the scattering resonances for a Gaussian well.

PACS numbers: 03.65.Nk, 03.65.Xp, 03.65.Ge

I. INTRODUCTION

Barrier penetration or tunnel effect is one of the most striking predictions of quantum mechanics and most textbooks discuss the few available exactly solvable one-dimensional models. In this journal there has been great interest in the subject as well as in one-dimensional potential scattering in general. Such interest has been focused not only on the analytical properties of potential scattering but also on the numerical calculation of transmission probabilities and other quantities that describe barrier penetration and potential scattering.

The purpose of this paper is to show that a straightforward application of Wronskians, which are well known in the study of ordinary linear differential equations, greatly facilitates the discussion of the analytical properties of potential scattering. They are also suitable for the numerical calculation of the transmission probability and any other quantity of interest in potential scattering. Present discussion is motivated by an earlier application of Wronskians to the analysis of one-dimensional models for resonance tunneling reactions.

In Sec. II we apply Wronskians to the Schrödinger equation for potential scattering in one dimension and derive matrix equations connecting the coefficients of the asymptotic forms of the wavefunction left and right of the scattering center. In Sec. III we specialize in a general short-range interaction and derive equations for the transmission probability. As illustrative nontrivial examples we consider a Gaussian barrier and a Gaussian well. By means of an exactly-solvable problem we discuss the origin of the scattering resonances in potential wells. In Sec. IV we summarize the main results and draw conclusions. In order to make this paper sufficiently self-contained we collect some well known mathematical properties of the Wronskians in an Appendix.

II. WRONSKIANS AND THE SCHÖDINGER EQUATION

The time-independent Schrödinger equation for a particle of mass \( m \) that moves in one dimension \((-\infty < X < \infty)\) under the effect of a potential \( V(X) \) is

\[
-\frac{\hbar^2}{2m} \psi''(X) + V(X)\psi(X) = E\psi(X)
\]  

(1)
If we define the dimensionless coordinate \( x = X/L \), where \( L \) is an appropriate length scale, then we obtain the dimensionless eigenvalue equation

\[
-\frac{1}{2} \varphi''(x) + v(x)\varphi(x) = \epsilon \varphi(x)
\]

\[
\varphi(x) = \sqrt{L}\psi(Lx), \quad v(x) = \frac{mL^2}{\hbar^2}V(Lx), \quad \epsilon = \frac{mL^2E}{\hbar^2}
\] (2)

The length unit \( L \) that renders both \( \epsilon \) and \( v(x) \) dimensionless is arbitrary and we can choose it in such a way that makes the Schrödinger equation simpler. We will see some examples in Sec. III.

In most cases of physical interest we can write the asymptotic behavior of the dimensionless wavefunction \( \varphi(x) \) as follows

\[
\varphi(x) \rightarrow \begin{cases} 
A_1 C_1(x) + B_1 S_1(x) \text{ for } x \to \infty \\
A_3 C_3(x) + B_3 S_3(x) \text{ for } x \to -\infty
\end{cases}
\] (3)

and in the intermediate region \(-\infty < x < \infty\) we have

\[
\varphi(x) = A_2 C_2(x) + B_2 S_2(x)
\] (4)

The form of the functions \( C_j(x) \) and \( S_j(x) \) depends on the problem and throughout this paper we choose all of them real. On the other hand, the coefficients \( A_j \) and \( B_j \) may be complex. We discuss some examples in Sec. III for the time being we assume that those functions satisfy the conditions (27) at a conveniently chosen point \( x_0 \). By means of the Eq. (29) given in the Appendix we can easily obtain matrix expressions connecting the coefficients \( A_i \) and \( B_i \) in the three regions:

\[
\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = R_1 \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \quad \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = R_2 \begin{pmatrix} A_3 \\ B_3 \end{pmatrix},
\]

\[
\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = R \begin{pmatrix} A_3 \\ B_3 \end{pmatrix}, \quad R = R_1 \cdot R_2
\] (5)

where

\[
R_1 = \begin{pmatrix} W(C_2, S_1) & W(S_2, S_1) \\ W(C_1, C_2) & W(C_1, S_2) \end{pmatrix},
\]

\[
R_2 = \begin{pmatrix} W(C_3, S_2) & W(S_3, S_2) \\ W(C_2, C_3) & W(C_2, S_3) \end{pmatrix}
\] (6)

In these equations \( W(f, g) \) denotes the Wronskian of the functions \( f(x) \) and \( g(x) \)\(^{5,22} \) already defined in the Appendix.

If we repeat the procedure and obtain the inverse relations we appreciate that

\[
R_1^{-1} = \begin{pmatrix} W(C_1, S_2) & -W(S_2, S_1) \\ -W(C_1, C_2) & W(C_2, S_1) \end{pmatrix},
\]

\[
R_2^{-1} = \begin{pmatrix} W(C_2, S_3) & -W(S_3, S_2) \\ -W(C_2, C_3) & W(C_3, S_2) \end{pmatrix}
\] (7)
from which it follows that
\[ R_j^t J = J R_j^{-1}, \quad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \]  
(8)

where the superscript \( t \) stands for transpose. Since the skew–symmetric matrix \( J \) satisfies \( J^t = J^{-1} = -J \) we conclude that
\[ R_j^t J = J R_j^{-1} \]  
(9)

which resembles the symplectic condition for a canonical transformation in classical mechanics. Any matrix that satisfies Eq. (9) is said to be symplectic. Besides, Eq. (7) tells us that the determinant of every symplectic matrix \( R_1, R_2 \) and \( R \) is unity.

If the potential is parity–invariant \((v(-x) = v(x))\) then \( C_2(-x) = C_2(x), S_2(-x) = -S_2(x) \) and
\[
W(C_2, S_1) = W(C_2, S_3), \\
W(S_2, S_1) = W(S_3, S_2) \\
W(C_1, C_2) = W(C_2, C_3) \\
W(C_1, S_2) = W(C_3, S_2)
\]
(10)

so that we need to calculate half the number of Wronskians. It is worth noting that Wronskians containing \( C_1 \) and \( S_1 \) are constant for \( x \to \infty \) and those with \( C_3 \) and \( S_3 \) are constant for \( x \to -\infty \).

III. POTENTIAL SCATTERING

We assume that
\[
\lim_{x \to -\infty} v(x) = v_- \\
\lim_{x \to \infty} v(x) = v_+
\]  
(11)

where \( v_\pm \) are finite constants. If \( v(x) \) approaches those limits sufficiently fast then we know that the asymptotic behavior of the solution is
\[
\varphi(x) \to \begin{cases} 
A_1'e^{ik_1x} + B_1'e^{-ik_1x} & \text{for } x \to -\infty \\
A_3'e^{ik_3x} + B_3'e^{-ik_3x} & \text{for } x \to \infty
\end{cases}, \\
k_1 = \sqrt{2(\epsilon - v_-)}, \quad k_3 = \sqrt{2(\epsilon - v_+)}
\]  
(12)

provided that \( \epsilon > \max\{v_+, v_-\} \).

If we choose
\[
C_j = \cos(k_j x), \quad S_j(x) = \frac{\sin(k_j x)}{k_j}, \quad j = 1, 3
\]  
(13)
in Eq. (8) and compare it with Eq. (12) we obtain
\[
A'_j = \frac{1}{2} \left( A_j - i \frac{B_j}{k_j} \right), \quad B'_j = \frac{1}{2} \left( A_j + i \frac{B_j}{k_j} \right)
\]  
(14)
Suppose that we want to study the scattering of a particle that comes from the left \((x < 0)\). In such a case \(B_3' = 0\) and the transmission probability is given by

\[ T = \frac{k_3|A_3'|^2}{k_1|A_1'|^2} \quad (15) \]

Noting that \(B_3 = i k_3 A_3\) we can easily rewrite the transmission probability in terms of the coefficients \(A_j\) and \(B_j\) because

\[ \frac{A_3'}{A_1'} = \frac{2k_1A_3}{k_1A_1 - iB_1} \quad (16) \]

In the intermediate or scattering region we write \(\varphi(x)\) as in Eq. (1), where \(C_2(x)\) and \(S_2(x)\) are two solutions of the dimensionless Schrödinger equation that satisfy Eq. (27). In order to obtain them we may resort to any available numerical integration method, like, for example, Runge–Kutta\(^{25}\) (see also [http://en.wikipedia.org/wiki/Runge–Kutta](http://en.wikipedia.org/wiki/Runge–Kutta)). Let \(y(x)\) be either \(C_2(x)\) or \(S_2(x)\). Typical numerical integration methods yield \(y(x)\) at a set of coordinate points \(x_0 \pm jh\) where \(j = 0, 1, \ldots\) and \(h\) is the step size. They simultaneously provide the derivative of the function \(y'(x)\) at the same set of points so that the numerical calculation of the Wronskians between the intermediate solutions and the asymptotic ones is straightforward. Numerical integration methods like Runge–Kutta are available in many commercial and free softwares so that it is unnecessary to write a computer program for that purpose. In the present case we resorted to the fourth–order Runge–Kutta method built in the computer algebra system Derive ([http://www.chartwellyorker.com/derive.html](http://www.chartwellyorker.com/derive.html)). The starting point of the integration process requires \(y(x_0)\) and \(y'(x_0)\) that are already known for the functions \(C_2(x)\) and \(S_2(x)\). We propagate the solution left and right till the Wronskians appearing in the matrices \(13\) are constant within a given error. Then we calculate the coefficients \(A_1\) and \(B_1\) in terms of \(A_3\) by means of Eq. (5) and finally the transmission coefficient from equations \(16\) and \(16\). Note that the application of the numerical integration method is straightforward because all the functions \(C_j(x)\) and \(S_j(x)\) are real.

In the simplest case of a parity–invariant potential we need half the Wronskians in order to obtain the matrix \(R\) in equations \(15\) and \(16\) as discussed at the end of Sec. \(11\). The transmission probability reads

\[ T = \frac{k_1^2}{[(W(C_2, C_3)^2 + k_1^2 W(C_2, S_3)^2) (W(C_3, S_2)^2 + k_1^2 W(S_3, S_2)^2)]} \quad (17) \]

and we only have to integrate the differential equations for \(C_2(x)\) and \(S_2(x)\) from \(x_0 = 0\) to the right: \(x_j = jh, j = 0, 1, \ldots, N\).

As an illustrative example we choose the Gaussian barrier

\[ V(X) = V_0 e^{-\alpha X^2}, \ V_0, \alpha > 0 \quad (18) \]

If we set \(L = 1/\sqrt{\alpha}\) then \(v(x) = v_0 e^{-x^2}\) and the dimensionless Schrödinger equation depends on just one potential parameter \(v_0 = mV_0/(\hbar^2 \alpha)\). Since \(v_- = v_+ = 0\) then \(k_1^2 = 2\epsilon\), where \(\epsilon = mE/(\hbar^2 \alpha)\) is the dimensionless energy.

Throughout this paper we choose the integration step size \(h = 0.01\) and \(N = 500\) integration points so that the maximum coordinate value is \(x_{500} = 5\). Fig. \(1\) shows the behaviour of the functions \(C_2(x)\) and \(S_2(x)\) for \(\epsilon = 1\) and the Gaussian barrier with \(v_0 = 2\). In Fig. \(2\) we appreciate that the Wronskians approach constants as \(|x| \to \infty\) and that \(x = 5\) is large enough for an accurate estimation of those limits. We thus calculated the transmission coefficients shown in Fig. \(3\) for three values of \(v_0\). As expected there is tunneling for all \(\epsilon > 0\) and \(\lim_{x \to \infty} T = 1\). It is clear that
the oscillatory behavior of $T(\epsilon)$ found by Chalk is due to the truncation of the Gaussian potential with the purpose of connecting the power-series solution for the intermediate region with the asymptotic plane waves. We appreciate that the necessary truncation of the integration interval does not produce any undesirable effect on the transmission probabilities calculated in terms of Wronskians. In fact, the great advantage of the Wronskian method is that we calculate the constant asymptotic limit of each Wronskian with a given desired accuracy as shown in Fig. 2.

In passing we point out that there is no trace of the questionable tunneling condition derived by Nandi for the Gaussian barrier.

Another simple, nontrivial, and most interesting problem is the Gaussian well

$$V(X) = -V_0 e^{-\alpha X^2}, V_0, \alpha > 0$$

(19)

Proceeding as in the preceding example we obtain the dimensionless potential $v(x) = -v_0 e^{-x^2}$ and the same expressions for $v_0$ and $\epsilon$. In this case it is most instructive to calculate the transmission probability $T$ in terms of $v_0$ for fixed values of $\epsilon$ in order to reveal the scattering resonances as shown in Fig. 4. Note that the maxima of the transmission probability $T = 1$ that occur at some particular values of $v_0$ are roughly independent of the energy $\epsilon$. This well known phenomenon is better understood by means of an exactly solvable model.

The scattering resonances appearing in Fig. 4 are similar to the ones exhibited by the exactly solvable well

$$V(X) = -\frac{V_0}{\cosh(\alpha X)^2}, V_0, \alpha > 0$$

(20)

that we easily transform into the dimensionless potential $v(x) = -v_0 / \cosh(x)^2$. Both the dimensionless potential parameter $v_0$ and energy $\epsilon$ have the same expressions as in the preceding examples. In this case the transmission probability reads

$$T = \frac{\sinh \left( \pi \sqrt{2\epsilon} \right)^2}{\sinh \left( \pi \sqrt{2\epsilon} \right)^2 + \sin(\pi \lambda)^2}, \lambda = \frac{1}{2} \left( 1 + \sqrt{1 + 8v_0} \right)$$

(21)

The family of curves $T$ vs. $v_0$ for constant $\epsilon$ resembles the one shown in Fig. 4. Note that there is full transmission $T = 1$ when $\sin(\pi \lambda) = 0$; that is to say, when $\lambda$ is an integer. In order to understand the origin of these resonances we pay attention to the bound states

$$\epsilon_n = -\frac{1}{2}(\lambda - 1 - n)^2, n = 0, 1, \ldots \leq \lambda - 1$$

(22)

We appreciate that full transmission takes place when one of the excited bound–state energies ($n > 0$) lies exactly at the rim of the well $\epsilon_n = 0$ in which case $\lambda = n + 1$ (the ground–state energy $\epsilon_0 = -(\lambda - 1)^2/2$ is negative for all $v_0 > 0$).

This exactly solvable problem also proved to be useful for testing the accuracy of our programs for the calculation of the transmission probability.

### IV. CONCLUSIONS

In this paper we propose an alternative way of approaching quantum scattering in one dimension. We think that the method based on the Wronskians between linearly independent solutions to the Schrödinger equation is preferable to
other approaches. The relatively light effort necessary to master a few mathematical properties of the Wronskians pays generously when attacking the scattering problem either analytically or numerically. In this paper we focused mainly on the latter because we are interested in nontrivial problems that are not so widely discussed in most textbooks on quantum mechanics.[1–4]

The derivation of all the necessary scattering equations in terms of Wronskians is straightforward as well as their practical application by means of extremely simple computer programs. The calculation of the transmission probability is quite reliable if one simply checks for constant Wronskians before truncating the propagation of the solutions towards left and right in the numerical integration routine. Thus, the error due to a finite integration interval is simply the error in the lack of constant Wronskians that is easily bounded to the desired accuracy. In this way we avoid any spurious oscillations in the transmission probability as discussed in Sec. [11]

In addition to all that, the Wronskians have proved to be most useful for the estimation of the complex energies that describe tunnel resonances as discussed in the paper on which we based present pedagogical presentation[23]. One can also apply the Wronskian method to bound states and calculate their energies by simply taking into account the appropriate asymptotic behavior of the wavefunction and requiring that it be square integrable. It is clear that the approach exhibits a wide variety of useful applications and for that reason we think that it is worth teaching in advanced undergraduate or graduate courses on quantum mechanics.

V. APPENDIX

In order to make this paper sufficiently self–contained in this appendix we outline some well known results about the Wronskians that are useful for the study of ordinary differential equations in general[22] and also for the treatment of the Schrödinger equation in particular[5,23]. To this end, we consider the ordinary second–order differential equation

\[ L(y) = y''(x) + Q(x)y(x) = 0 \] (23)

If \( y_1 \) and \( y_2 \) are two linearly independent solutions to this equation then we have

\[ y_1 L(y_2) - y_2 L(y_1) = \frac{d}{dx}W(y_1, y_2) = 0 \] (24)

where

\[ W(y_1, y_2) = y_1 y_2' - y_2 y_1' \] (25)

is the Wronskian (or Wronskian determinant[22]). Two obvious properties are:

\[ W(f, g) = -W(g, f), \quad W(f, f) = 0 \] (26)

By linear combination of \( y_1(x) \) and \( y_2(x) \) we easily obtain two new solutions \( C(x) \) and \( S(x) \) satisfying

\[ C(x_0) = S'(x_0) = 1, \quad C'(x_0) = S(x_0) = 0 \] (27)

at a given point \( x_0 \) so that \( W(C, S) = 1 \) for all \( x \). If we write the general solution to Eq. (23) as

\[ y(x) = AC(x) + BS(x) \] (28)
then

\[ A = W(y, S), \quad B = W(C, y) \]  

(29)

This equation is quite useful for deriving relationships between the coefficients of the asymptotic expansions of the wavefunction in different regions of space as shown in sections III and IV. A more detailed discussion of the Wronskians is available in Powell and Crasemann’s book on quantum mechanics.\(^5\)

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FIG. 1: Functions $C_2(x)$ (solid line) and $S_2(x)$ (dashed line) for $\epsilon = 1$ and the Gaussian barrier with $v_0 = 2$ (solid line).

FIG. 2: Wronskians for $\epsilon = 1$ and the Gaussian barrier with $v_0 = 2$.

FIG. 3: Transmission probability for three Gaussian barriers.
FIG. 4: Transmission probability for the Gaussian well as a function of the well depth for three values of the energy.