Semianalytical approach to x-ray and neutron reflection from surface films

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In a paper by Xiao-Lin Zhou *et al.* [Phys. Rev. A **46**, 1839 (1992)] an approximate method for dealing with one-dimensional potentials is proposed. Here, we would like to demonstrate an alternative method that may be useful in these problems.

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In [1] the reflectance and transmittance of scalar plane waves undergoing specular reflection from a one-dimensional potential, characterizing a surface film and a semi-infinite substrate are considered. The method utilized the Green function and different approximations [small curvature approximation (SCA), distorted-wave Born approximation (DWBA), and Wentzel-Kramers-Brillouin (WKB) approximation] with some perturbation modifications.

Here we want to show that for one-dimensional potentials an alternative method exists, which seems to be unknown to a broad portion of the scientific community studying surface phenomena. This method is based on splitting a potential into independent parts by infinitesimal gaps with zero internal potential [2]. It is illustrated in Fig. 1.

The infinitesimal gap does not change the physics. This is because the tunneling through it is equal to unity. But, it considerably simplifies the mathematics. The introduction of gaps shows that every medium can be considered to be layered. For layered media there is an approach that is widely known as "invariant imbedding" (see, for instance, [3]). The proposed method is a generalization of it.

The reflection amplitude R_{12} of the whole potential is represented as a function of the amplitudes of reflection, R_i, and transmission, T_i, of both parts ($i = 1, 2$). For the moment we will not take the width of the gap ϵ to be zero. Taking into account the multiple reflections inside it, we get the relation

$$R_{12} = R_1 + \exp(2ik\epsilon)\frac{T_1^2 R_2}{1 - R_1 R_2 \exp(2ik\epsilon)}, \qquad (1)$$

where k is the wave number in vacuum.

In a similar way we obtain the transmission amplitude T_{12} of the whole potential:

$$T_{12} = \exp(ik\epsilon)\frac{T_1 T_2}{1 - R_1 R_2 \exp(2ik\epsilon)}. \qquad (2)$$

After substituting $\epsilon = 0$ we get

$$R_{12} = R_1 + \frac{T_1^2 R_2}{1 - R_1 R_2}, \qquad T_{12} = \frac{T_1 T_2}{1 - R_1 R_2}. \qquad (3)$$

The reflection amplitude R_2 corresponds to the potential which we call here the "substrate." It can be related, for example, to a layer with a smooth surface or a super-mirror on another substrate. In all the cases we suppose that an analytical expression for R_2 can be obtained [2].

The partial potentials may not be symmetrical. In that case the reflections from the left and from the right differ by a phase ϕ, and the relations (3) take the form

$$\overrightarrow{R}_{12} = \overrightarrow{R}_1 + T_1 \overrightarrow{R}_2 (1 - \overleftarrow{R}_1 \overrightarrow{R}_2)^{-1} T_1, \qquad (4)$$

$$T_{12} = T_2 (1 - \overleftarrow{R}_1 \overrightarrow{R}_2)^{-1} T_1, \qquad (5)$$

where $\overleftarrow{R} = \overrightarrow{R}\exp(i\phi)$ and T_i in both directions are identical.

We can treat any potential in this manner. Moreover, such an approach is applicable to any linear differential equation [4, 5] of mathematical physics. The relations are also applicable in the case when all the terms are matrices, and this paves the way for a generalization of the preceding formulas to the waves with any spin [6] and, consequently, to three-dimensional space [2, 7].

We have shown how to separate the film and the substrate. The latter can be composed of many different parts. In that case the formulas (3) should be applied several times recursively. This way we get a semianalytical approach to a potential of any form. Indeed, if one splits a potential by infinitesimal gaps in such a way that every part can be approximated by a curve admitting an analytical solution (see, for instance, [8]), then one finds the reflection and transmission amplitudes for every part. Then one obtains the resulting reflection and transmission amplitudes in the form of a finite continuous fraction [9]:

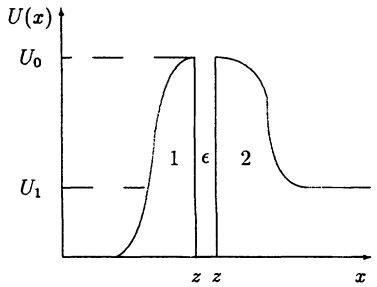

FIG. 1. Potential of a surface film on a substrate with smooth interfaces split by an infinitesimal gap at point z.

$$\vec{R} = \vec{r_1} + \cfrac{t_1^2}{-\overleftarrow{r_1} + \cfrac{1}{\vec{r_2} + \cfrac{t_2^2}{-\overleftarrow{r_2} + \cfrac{1}{\vec{r_3} + \cdots}}}}. \quad (6)$$

With such calculations no artificial oscillations appear in the solution.

To determine the potential by fitting the calculated reflection coefficient to the experimental data it may happen that it is most appropriate to first fit the partial amplitudes, i.e., the complex parameters t_i, $\overleftarrow{r_i}$, and ϕ_i of different parts of the potential, and after that solve the inverse problem for every part or to find the related parts by another fitting procedure.

When absorption can be neglected, the values t, $\overleftarrow{r}$, and ϕ depend only on three real parameters: $|r|$, the phase ϕ of r and, for example, the phase ϕ_1 of $\overleftarrow{r}$.

Of course, formula (6) is not very useful for analytical calculations in the case of a large number of layers. Its utility in this case is of the same value as the utility of the precise expressions for roots of algebraic equations of the third and fourth order. But for numerical calculations it has many advantages, because it gives the possibility of using different approximations for different parts of the potential and to treat some parts of it analytically.

For instance, such an approach has no advantage in the case of high energy when the WKB approximation applies. It is useful here only because of the possibility to safely separate the effect of a known substrate instead of dealing with DWBA. But in the case of low energies when a perturbation or WKB approach is questionable (it is here that you need SCA, DWBA, and other refinements) and if you need to specify only the parameters of some given part of the potential, the described approach can be of great help.

Indeed, suppose that in formula (6) parts 1,3,... are established and one needs to specify only part 2. In that case one finds a simple analytical dependence of the total reflection amplitude on characteristics of the unknown part, so one can deal directly and exclusively with it.

With respect to the widely used Parratt method [10] (see, for instance, [11]) the one discussed here seems to have an advantage. In the Parratt method one needs to match the wave functions at interfaces between neighboring layers and then to solve numerically recurrent relations. The action of every layer depends on characteristics of its neighbors.

In the proposed method one does not need (1) to match the wave function (it is matched automatically) and (2) to solve the recurrent relations. This is because (1) the action of every layer is taken independently of all others, as if this layer were singled out and placed in vacuum, and (2) the recurrent relations are taken in the solved form.

The computer experiment [12] shows that when finding the reflection amplitude from the potential shown in Fig. 1, when it is composed of two parts described by a hyperbolic tangent, the proposed method consumes time of an order of magnitude less than the Parratt method with its step approximation and matching of wave functions at boundaries.

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