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Scattering of Neutral Atoms by an Exponential Corrugated Potential

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The integral equation of the scattering is solved exactly for a one-dimensional exponential corrugated potential. Numerical results are presented for a sinusoidal and a triangular profile of small amplitude. As the "slope" of the exponential increases the intensities given by the hard corrugated wall are approached. The finite slope of the potential has the strong effect of forcing the particles into the specular peak and tends to reduce the effect of multiple scattering.

In the scattering of light neutral atoms by a crystalline surface the diffraction-peak intensities calculated with use of a hard-corrugated-wall potential (HCWP) are successfully[1] compared with the experimental data. The HCWP is written as

$$V=\infty, \quad z<\varphi(\vec{R}),$$

$$V=0, \quad z>\varphi(\vec{R}),$$

where $\varphi(\vec{R})$ is the corrugation function or the surface profile, $\vec{R}$ and z being the parallel and perpendicular components of the surface position vector. The HCWP with a potential well having an attractive long-range part[2,3] (z^{-3}) gives a good picture of the structures (minima or maxima) observed experimentally in the diffracted peaks in the vicinity of condition for which resonance with bound states can occur.

On the other hand, these observed resonances allow the determination of the potential energy levels. Then one usually tries to deduce a potential shape or more precisely its zero-order Fourier component which gives the best fit to the bound-state energies. One generally finds that this can be well represented by a Morse[4,5] or a 9-3 potential.[6] Recently, more elaborate forms have been proposed, for instance, the shifted Morse hybrid potential,[7] so called because it is given by a Morse form at short distances and by an attractive z^{-3} form far from the surface.

In spite of the uncertainty which arises in a potential shape determined only by a limited number of bound-state energies one would expect that the

repulsive region has a finite slope allowing a certain degree of wave penetration into the solid. This phenomenon, which is not allowed by the HCWP, has been modeled by introducing the so-called soft-wall potential [$V = V_0$, $z < \varphi(R)$].[8] However, a more realistic picture seems to be given by the exponential corrugated potential (ECP) defined by

$$V = C\exp\{-\chi[z - \varphi(\vec{R})]\}, \tag{1}$$

which in the limit $\chi \to \infty$ gives the HCWP. In the following we develop the one-dimensional solution to this potential and discuss some interesting numerical results pertaining to recent experiments in the scattering of atoms by metal surfaces.

We start with the integral form of the Schrödinger equation in the two-potential formalism:

$$\psi_i = \Phi_i + (E_i - H_0 + i\epsilon)^{-1}(V - v)\psi_i, \tag{2}$$

with $H_0 = -(\hbar^2/2m)\nabla^2 + v$ and $v = C\exp(-\chi z)$. The eigenvalues e_p and eigenfunctions $\Phi_p(z)$ of H_0 are well known[9]:

$$e_p = [(\hbar\chi)^2/8m]p^2, \quad k = \tfrac{1}{2}\chi p,$$

$$\Phi_p(z) = [p\sinh(\pi p)/\pi]^{1/2}K_{ip}(y),$$

$$y = [(8mC)^{1/2}/\chi\hbar]\exp(-\tfrac{1}{2}\chi z),$$

where K_{ip} is the modified Bessel function of the second kind with imaginary order ip. It is readily shown that $K_{ip} \to 0$ in the limit $z \to -\infty$ and for $z \to +\infty$,

$$\Phi_p = \sin(\tfrac{1}{2}\chi p z - \alpha_p),$$

$$\alpha_p = \arg[(2mC/\chi^2\hbar^2)^{ip/2}/\Gamma(1+ip)].$$

Also one can show that the normalization integral behaves like

$$\int_{-\infty}^{L}\Phi_{p'}(z)\Phi_p(z)dz = \Delta(L),$$

where for L large, $\Delta \to 0$ for $p' \neq p$ and $\Delta \to \frac{1}{2}L$ for $p' = p$. Therefore the corresponding projection operator is given by

$$P = \sum_n |\Phi_{p_n}\rangle\langle\Phi_{p_n}|(\tfrac{1}{2}L)^{-1}$$

with

$$\tfrac{1}{2}\chi p_n L - \alpha_p = n\pi.$$

Taking the limit $L \to \infty$ one finds

$$P = \frac{\chi}{\pi}\int_0^\infty |\Phi_p(z)\rangle\langle\Phi_p(z)|dp.$$

Then the condition $P|\Phi_p\rangle = |\Phi_p\rangle$ gives us the normalization factor

$$\int_{-\infty}^{+\infty}\Phi_{p'}(z)\Phi_p(z)dz = (\pi/\chi)\delta(p - p'). \tag{3}$$

The solution of Eq. (2) with use of Eqs. (1) and (3) is obtained by expanding ψ_i as

$$\psi_i = \sum_G \exp[i(K_i + G)X]\psi_G(z),$$

$$\psi_G(z) = \int_0^\infty b_G(p)\Phi_p(z)dp.$$

One obtains

$$\psi_J(z) = \Phi_{p_i}(z)\delta_{J0} + \frac{8m}{\pi\hbar^2\chi}\sum_G(v_{J-G} - \delta_{JG})\int_0^\infty dp_n\, b_G(p_n)\int_0^\infty dp_l\frac{M(p_l, p_n)}{p_J^2 - p_l^2 + i\epsilon}\Phi_{p_l}(z), \tag{4}$$

where M is the matrix element $\langle\Phi_{p_l}v\Phi_{p_n}\rangle$, v_{J-G} is the Fourier component of the exponential corrugation

$$v_{J-G} = \frac{1}{a}\int_0^a \exp[\chi\varphi(X)]\exp[-i(J-G)X]dX,$$

and

$$p_J^2 = (4/\chi^2)[|\vec{k}_i|^2 - (K_i + J)^2] = (4/\chi^2)k_{Jz}^2.$$

As usual G and J are reciprocal-lattice vectors, and $\vec{k}_i$ is the incident wave vector with component K_i parallel to the surface.

The latter integral in Eq. (4) is readily solved analytically. Then one takes the limit $z \to \infty$ which gives

$$\psi_J(z \to \infty) = \delta_{J0}\sin(\tfrac{1}{2}\chi p_i z - \alpha_i) + A_J\exp[i(k_{Jz}z - \alpha_J)], \quad p_J^2 > 0,$$

$$\psi_J(z \to \infty) = 0, \quad p_J^2 < 0,$$

with

$$A_J = -\tfrac{1}{4}\pi\sum_G(v_{J-G} - \delta_{JG})\left(\frac{\sinh(\pi p_J)}{p_J}\right)^{1/2}\int_0^\infty dp\, b_G(p)[p\sinh(\pi p)]^{1/2}\frac{(p_J^2 - p^2)}{\cosh(\pi p_J) - \cosh(\pi p)},$$

and the diffracted intensities are given by

$$I_0 = |1 + 2iA_0|^2, \quad I_J = 4k_{Jz}(k_{iz})^{-1}|A_J|^2.$$

Then remains the task of determining the unknown functions b_G. This is achieved by taking the expectation value of Eq. (4) with the set of states $\{\Phi_{p_m}\}$. One obtains an infinite set of coupled integral equations, namely,

$$b_J(p_m) = \delta_{J0}\delta(p_m - p_i) + \frac{1}{2}\frac{[p_m \sinh(\pi p_m)]^{1/2}}{p_J^2 - p_m^2 + i\epsilon}\sum_G (v_{G-J} - \delta_{JG})\int_0^\infty dp\, b_G(p)[p\sinh(\pi p)]^{1/2}\frac{(p_m^2 - p^2)}{\cosh(\pi p_m) - \cosh(\pi p)}.$$

In order to get a numerical solution one conserves only a given number N_G of reciprocal-lattice vectors which obviously should include at least all the G vectors corresponding to the open diffraction channels. Further, one limits the integration to a value $p_{JM} = \beta p_{Jm}$ ($\beta > 1$), p_{Jm} being the maximum real value taken by any of the p_J. The segment $[0, p_{JM}]$ is then divided into N_p equal intervals $\Omega = p_{JM}(N_p)^{-1}$ and the continuous functions $b_G(p)$ are replaced by the discrete set

$$B_{G_n} = \int_{n\Omega}^{(n+1)\Omega} b_G(p)dp.$$

In this way we have a matrix equation, the matrix to be inverted being of size $N = N_G \times N_p$. As discussed below our numerical results verify that the obtained solution is convergent, that is to say that the calculated intensities are stable and the unitarity approaches 1 as N increases.

If we write the amplitude of the corrugation function $\varphi(x)$ as ha then the Fourier components v_{G-J} are increasing functions of the dimensionless variable χha. Therefore as this parameter increases it is necessary to increase N_G, and with the largest matrix size which can be inverted in our computer ($N = 225$) we are limited to χha values approximately equal to 0.1. A more efficient procedure is needed in order to increase the χha domain of obtainable solutions. However, within the range $\chi ha < 0.1$ the calculated precision of the diffracted intensities is better than 1% as shown by the results in Tables I and II.

Table I gives results for a sinusoidal profile. The h and a values have been chosen in such a way that the HCWP calculation displays approximately the observed, experimental upper limits on the intensities for Cu(100) in the 1 and $\bar{1}$ peaks. One sees that the introduction of a finite slope has the strong effect of forcing the particles into the specular peak. Particularly we notice that for given values of the intensities in the 1 and $\bar{1}$ peaks in the h value must be greater for the ECP than that used in the HCWP. One can notice that as χ increases the HCWP solution is approached.

Table II gives results for a triangular profile of height ha. The apex of the triangle is located at $0.75a$. The χ value has been put equal to the value which is usually found in the coupled-channel calculation.[10] As in the preceding case the comparison to HCWP calculation indicates that the diffracted peak intensities are reduced and the specular one is increased.

From these two examples one may conclude that the finite slope of the repulsive part of the potential and the consequent wave penetration tend to reduce the effect of multiple scattering. However,

TABLE I. Results for the scattering of He by a sinusoidal profile, $ha\sin(2\pi x/a)$, $k_i = 0.11\times 10^{10}$ cm^{-1}, $a = 2.55\times 10^{-8}$ cm, $h = 0.002$, with an incident angle 45°.

	χ (cm^{-1})			
G channel	0.1×10^9	0.3×10^9	0.5×10^9	HCWP
-7	0.22×10^{-33}	0.2×10^{-25}	0.24×10^{-24}	0.11×10^{-21}
-6	0.15×10^{-26}	0.16×10^{-20}	0.55×10^{-20}	0.73×10^{-19}
-5	0.93×10^{-21}	0.11×10^{-16}	0.25×10^{-16}	0.51×10^{-17}
-4	0.39×10^{-17}	0.26×10^{-13}	0.66×10^{-13}	0.65×10^{-13}
-3	0.51×10^{-14}	0.58×10^{-10}	0.19×10^{-9}	0.4×10^{-9}
-2	0.68×10^{-11}	0.14×10^{-6}	0.51×10^{-6}	0.12×10^{-5}
-1	0.42×10^{-6}	0.41×10^{-3}	0.10×10^{-2}	0.19×10^{-2}
0	1.000 002 1	1.000 58	1.001 33	0.997 243
1	0.14×10^{-9}	0.31×10^{-4}	0.21×10^{-3}	0.81×10^{-3}
Unitarity	1.000 002 5	1.001 04	1.002 56	1.000 000 00

TABLE II. Results for He scattered by a triangular profile of height ha and perpendicular incidence. The apex of the triangle is located at $0.75a$. χ labels the exponential corrugated potential with $\chi = 0.2 \times 10^{9}$ cm^{-1}, $k_i = 0.11 \times 10^{10}$ cm^{-1}, $a = 1.93 \times 10^{-8}$ cm.

	$h = 0.01$		$h = 0.015$	
G channel	HCWP	χ	HCWP	χ
-3	0.22×10^{-4}	0.1×10^{-10}	0.36×10^{-4}	0.72×10^{-10}
-2	0.54×10^{-3}	0.13×10^{-4}	0.11×10^{-2}	0.195×10^{-4}
-1	0.65×10^{-2}	0.4×10^{-2}	0.15×10^{-1}	0.85×10^{-2}
0	0.9860	0.99945	0.96892	0.99875
1	0.59×10^{-2}	0.38×10^{-2}	0.128×10^{-1}	0.77×10^{-2}
2	0.78×10^{-3}	0.37×10^{-4}	0.19×10^{-2}	0.95×10^{-4}
3	0.57×10^{-4}	0.32×10^{-9}	0.153×10^{-3}	0.115×10^{-8}
Unitarity	1.000 00	1.007 34	1.000 00	1.0150

before being considered as a general rule this conclusion should be supported by a more extended set of numerical calculations. The most closely related method of determining the wave function (4) is the close-coupling method which has been applied to the surface scattering problem by Wolken.[11] The close-coupling calculation consists of a step-by-step direct integration in real space for determining the perpendicular wave function $\psi_G(z)$. In order to make the calculations tractable the close-coupling methods have been restricted to relatively small numbers of Fourier components in the potential. Hence, it is difficult to compare directly with the calculations presented here since the corrugated exponential potential contains all Fourier components. Therefore the potentials used in these two calculations are substantially different. The method developed in this paper, although specially applied to the corrugated exponential potential, is quite general and can, in principle, be applied to any form for the interaction. The perpendicular wave function $\psi_G(z)$ is projected onto the space defined by the solutions of the zero-order Fourier component of the potential and then the problem is solved in that transform space. In many cases, expansion in such a basis set will be much more convenient and faster than direct numerical integration.

As a final remark we mention that the corrugated exponential potential (1) was chosen because of its simplicity, and no less importantly, because all of its matrix elements can be readily evaluated. In order to introduce an attractive well at the surface the same methods can be used for the Morse potential since the corresponding matrix elements are also known. Of course, as mentioned in the above paragraph, the techniques applied here are good in principle for any general form of the potential and it appears that under certain conditions such calculations could be carried out with quite a reasonable amount of numerical work.

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