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Scattering of neutral atoms by a periodic potential: 
the Morse corrugated potential

G. Armand (*) and J. R. Manson (**)

(*) Service de Physique des Atomes et des Surfaces, CEN Saclay, 91191 Gif-sur-Yvette Cedex, France
(**) Department of Physics and Astronomy, Clemson University, Clemson S.C. 29631, U.S.A.

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Abstract. — Within the two-potential formalism a general set of $t$ matrix integral equations is obtained which describes the scattering of a neutral particle by a periodic potential. Furthermore a projection method is developed which allows us in the case of resonance, to get a new set of equations in which the resonance singularities do not appear. This formalism is applied to the Morse corrugated potential. The integral equation set is solved by an iterative process and in this way an exact solution is obtained. The convergence of the iterative expansion is studied and an approximate convergence criterion is found. Results are compared with those given by an equivalent exponential corrugated potential which demonstrates the influence of the well and potential slope on the distribution of the intensities among the different diffracted beams. In order to have a precise determination of the corrugation function it is shown that it is necessary to use a realistic potential and also to avoid approximate methods for the calculation of intensities.

1. Introduction. — When neutral atoms of thermal energy are scattered by a clean and ordered surface the diffraction phenomenon is generally observed. The intensities of diffracted beams are measured and when the so-called resonance phenomenon is observed the energy levels of the potential are determined. The adjustment of these data with those calculated taking a given potential function gives, to a first approximation, the zeroth order Fourier component of the potential. Higher order Fourier components, suitably chosen, can be added and the diffracted beam intensity can be calculated. In this way more detailed information on the periodic potential can be obtained by fitting the calculated intensities to the experimental data.

On the other hand potential calculations from first principles could provide a good determination of the potential shape and could be of a great help in the choice of potential functions used in beam intensity calculations. Recently a great advance has been made in this way. Effectively, one has shown that to first order, the repulsive potential is proportional to the surface electronic density [1] and the electronic isodensity profile has been calculated [2]. For the domain of incident particle kinetic energy of interest, it appears that the repulsive part of the potential could be represented by an exponential corrugated function

$$V = V_0 \exp \left\{ - 2 \chi(z - \varphi(R)) \right\}$$

where $R$ is a vector orthogonal to $Oz$ the direction normal to the surface and $\varphi(R)$ is a function obviously
periodic with respect to the $R$ variable. The crest to trough amplitude of the corrugation should increase with the potential energy value.

By adding an attractive part to the repulsive potential given by (1) one obtains a potential function which can suitably describe the real interaction between the neutral atom and the surface. In this way the so-called Morse corrugated potential which is written

$$V = D \{ \exp[-2 \chi(z - \varphi(R)) - 2 \exp(-\chi z) \}$$

seems to be convenient in order to model the interaction except at large distances from the surface where the attractive potential part should vary as $z^{-3}$.

Using this potential and the corresponding $t$ matrix equation the scattering problem has been solved exactly. A brief description of the method and some results have already been published [3]. Comparison with experimental results shows that diffracted beam intensities are very well reproduced for different incident angles at a given incident energy [4]. For the same conditions the hard corrugated wall cannot give a good fit to the experimental data nor can the exponential corrugated potential (1), even if the latter gives a better representation of the measured intensities than the former.

In this paper we intend to describe some details of the calculation method which leads to an exact solution of the scattering equation. This is achieved by iteration of the $t$ matrix equation and the convergence of this process is studied. Some results are then presented which demonstrate the influence of the softness and of the well. Finally the domain of validity of different approximations is discussed.

Another way to obtain an exact solution of the scattering equation is the close coupling calculation method. It has been used with potentials similar to the Morse corrugated [5-8] or with different potentials given by summation of two-particle potentials [9-11]. Generally, in order to save computer time, the authors take only account of a few Fourier components of the potential. With this new potential the obtained results are exact. The $t$ matrix formalism allows to retain all the Fourier components of the potential without any increase of computer time. Thus the results obtained with these two methods can be different if the high order Fourier components of the potential are not negligible.

But one of the advantages of the $t$ matrix method is that it allows a deeper understanding of the scattering phenomena as we will see. In the case of resonance with bound states it directly gives some interesting physical quantities. Particularly with the result of the calculation for one incident angle one can easily get the resonance width and draw the resonance profile.

2. General theory. — In the framework of an elastic theory the Schrödinger equation can be transformed into a set of integral equations. The unknown functions are proportional to the $t$ matrix elements and the diffracted beam intensities can be deduced. In the particular case of resonance a singularity appears in these equations. In order to get around this difficulty a projection method is then used.

In this section the transformation and the projection method will be developed in the following sections.

In the two-potential formalism the integral form of the Schrödinger equation is:

$$|\psi_i^+\rangle = \frac{1}{\sqrt{2}} \left[ |\phi_i\rangle + \left( E_i - H - i\epsilon \right)^{-\frac{1}{2}} |V(R,z) - U(z)| \right] |\phi_i^+\rangle.$$  

Note that respectively a position vector $r$ and a wave vector $k$ are decomposed into components parallel $(R, K)$ and normal $(z, k_z)$ to the surface.

The distorted potential $U(z)$ is chosen as close as possible to $V(R,z)$, the potential to be treated, and in such a way that the eigenvalues and eigenvectors of $H$ with

$$H = -\frac{\hbar^2 V^2}{2m} + U(z)$$

are known.

This complete set is composed of bound states $(e_b; \exp(iK.R) \phi_b(z))$ and states in the continuum $(e_c; \exp(iK.R) \phi_c(z))$. We adopt the following normalization conditions:

$$\langle \exp iK'.R | \exp (iK.R) \rangle = 4 \pi^2 \delta(K - K')$$

$$\langle \phi_b(z) | \phi_b(z) \rangle = \delta_{bc}$$

$$\langle \phi_c(z) | \phi_c(z) \rangle = \delta(c - c').$$

Then the projection operator for this complete set is:

$$P = \frac{1}{4 \pi^2} \int \left[ \left| \sum_b | \phi_b(z) \rangle \langle \phi_b(z) | \right|^2 + \sum_c \left| | \phi_c(z) \rangle \langle \phi_c(z) | \right|^2 \int_{0}^{\infty} | \phi_c(z) \rangle \langle \phi_c(z) | \right] .$$

The potential $V(R,z)$ being periodic in $R$ the Floquet or Bloch theorem implies that the solution of (3) is equal to a sum of diffracted waves extended over all the reciprocal surface lattice vector $G$:

$$|\psi_i^+\rangle = \sum_{G} \chi_c(z) \exp(iK_i + G).R$$
where the subscript i refers to the incident condition. The partial wave $\psi_G(z)$ is expanded over the eigenvectors of $H$

$$
\psi_G(z) = \sum_b a_G b(z) + \int_0^\infty b_G(c) \phi_c(z) dc
$$

where the unknown coefficients $a_G$ and $b_G(c)$ are to be determined.

Then the usual procedure is used [12]: in the right hand side of (3) the Green operator is multiplied on the left by the projector, $|\psi_+^i\rangle$ is replaced by its expansion (6) taking account of (7) and the potential is expanded into Fourier components:

$$
V(R, z) = \sum_\mathcal{G} v_G(z) \exp(iG \cdot R)
$$

with

$$
v_G(z) = S^{-1} \int_{\mu, c} V(R, z) \exp(-iG \cdot R) dR
$$

where $S$ is the unit cell $(\mu, c)$ area. In this way one gets an expression for $|\psi_+^i\rangle$ which is identified with the expansion (6). One obtains the wave function corresponding to each channel:

$$
\psi_j(z) = \phi_j(z) \delta_{j0} + \int_0^\infty dc \phi_c(z) E_{j-1}^{-1} L_j(c) + \sum_b \phi_b(z) E_{j-1}^{-1} L_j(b)
$$

with

$$
E_{j-1} = e_i - \frac{\hbar^2}{2m} |K_i + J|^2 - e_c + i\epsilon \quad E_{j-1} = e_i - \frac{\hbar^2}{2m} |K_i + J|^2 - e_b
$$

$$
L_j(c \mid b) = \sum_\mathcal{G} \sum_b a_G b M_{j-1} \phi_j(c \mid b) + \int_0^\infty dc' b_G(c') M_{j-1} \phi_j(c \mid c')
$$

with

$$
M_{j-1} \phi_j(c \mid b') = \langle \phi_k(z) \mid v_{j-1}(z) \mid \phi_b(z) \rangle - \delta_{jG} \langle \phi_k(z) \mid U(z) \mid \phi_b(z) \rangle
$$

$$
M_{j-1} \phi_j(c \mid c') = \langle \phi_k(z) \mid v_{j-1}(z) \mid \phi_c(z) \rangle - \delta_{jG} \langle \phi_k(z) \mid U(z) \mid \phi_c(z) \rangle
$$

The expectation value with the state $\phi_b(z)$ or $\phi_c(z)$ gives respectively the unknown dimensionless coefficients $a_G$ and $b_G(c)$:

$$
a_G = E_{j-1}^{-1} L_j(b), \quad b_G(c) = E_{j-1}^{-1} L_j(c) + \delta(c_i - c) \delta_{j0} .
$$

Then putting into (10) the expression of these coefficients one gets the following set of coupled integral equations:

$$
L_j(c \mid b) = M_{j-1} \phi_j(c \mid b) + \sum_\mathcal{G} \left\{ \sum_b M_{j-1} \phi_j(c \mid b') E_{j-1}^{-1} L_j(b') + \int_0^\infty M_{j-1} \phi_j(c \mid c') E_{j-1}^{-1} L_j(c') dc' \right\} .
$$

If $n$ is the number of bound states of the distorted potential $U(z)$ there are $n + 1$ sets of integral equations each of them being extended to the infinite set of reciprocal lattice vectors.

Once the $L_j$ functions are known the expression of the partial wave $\psi_j(z)$ is determined by formula (9). It is of particular interest to calculate its asymptotic form when $z$ is large and positive. At this limit the $\phi_k(z)$ functions go to zero and only the integrals over continuum states remain. As the asymptotic form of $\phi_k(z)$ is known the calculation can be done giving the wave amplitude and therefore the beam intensity.

It is interesting to note that equations (11) are equivalent to the so-called CCGM equations [13].

The $L_j(c \mid b)$ functions are proportional to the $t$ matrix elements. This could be proved by looking at their definition

$$
t_j(c \mid b) = \langle \exp \{ i(K_i + J) \cdot R \} \phi_b(z) \mid V(R, z) - U(z) \mid \psi_+^i \rangle
$$
and performing the corresponding integrals. Therefore equations (11) could be written in a more compact form:

\[ t_{ci} = v_{ci} + \sum_{c, b} \frac{v_{cb} t_{c1}}{E_i - E_b} + \sum_{c, e} \frac{v_{ce} t_{c1}}{E_i - E_e + i\epsilon} \] (12a)

\[ t_{bi} = v_{bi} + \sum_{b, b'} \frac{v_{b'b} t_{b1}}{E_i - E_b} + \sum_{b, e} \frac{v_{be} t_{b1}}{E_i - E_e + i\epsilon} \] (12b)

which depicts the scattering phenomena more clearly. From the initial state one goes into a continuum or bound state through a t matrix element which contains in itself multiple scattering effects, and from this state one goes to the final state f or b by the corresponding matrix element v.

In equation (11) it can happen that one or several quantities, like \( E_{GR} \), are simultaneously small or equal to zero. If we label a corresponding state by subscript R we then have for each of them

\[ E_{GR} = e_i - \frac{\hbar^2}{2m} |K_i + G|^2 - e_R = E_i - E_b = 0 \] (13)

which is the kinematic condition for a resonance. This yields a singularity in the set of equations to be solved. In order to reduce this difficulty a particular method is used, called the projection method [14]. We rewrite the t matrix equation

\[ t = v + vPG^+ t \]

in which we have introduced the projection operator \( P \). It can be decomposed into two parts \( P = P_1 + P_2 \) and one gets

\[ (1 - vP_2 G^+) t = v + vP_1 G^+ t . \]

Then defining a new matrix \( h \) by the relation

\[ h = (1 - vP_2 G^+)^{-1} v \]

this relation gives a set of two coupled equations

\[ h = v + vP_2 G^+ h \]
\[ t = h + hP_1 G^+ t . \] (14)

One can notice immediately that, if \( P_1 \) or \( P_2 \) contains only bound states, the \( t \) or \( h \) matrix equation (14), respectively, reduces to a set of linear algebraic equations. This fact can be of great help in the choice of partition of the projector.

Among the numerous possibilities, two partitions are interesting in order to solve the problem at hand. A first choice consists in putting into \( P_2 \) the states which contribute to the appearance of the singularity. The \( t \) matrix equation (14) is written as:

\[ t_{ci} = h_{ci} + \sum_{b'} h_{cb'} t_{b1} + \sum_{c} \frac{h_{ce} t_{c1}}{E_i - E_c + i\epsilon} \]

\[ t_{bi} = h_{bi} + \sum_{b'} h_{b'b} t_{b1} + \sum_{c} \frac{h_{be} t_{b1}}{E_i - E_e + i\epsilon} . \] (15)

This system is equivalent to the set (12). But here we have renormalized matrix elements \( h \) in place of \( v \) and the resonant states are excluded from the summation (\( \sum' \)). The \( h \) matrix elements are determined from a set of linear equations. For instance, with one resonant state the \( h_{ci} \) matrix element becomes

\[ h_{ci} = v_{ci} + \frac{v_{cb} v_{bR}}{E_i - E_R - v_{bR}} . \]

In this way the singularity is shifted provided the matrix element \( v_{bR} \) is not too small, which can extend the domain of convergence. Note that this procedure is equivalent to the elimination of the resonant state. It is in fact equivalent to calculating \( t_{bi} \) from equation (12b) and to putting its value into the remaining equations (12).
A second choice which appears certainly more interesting is to include in $P_1$ the resonant states alone. The diffracted intensities being proportional to the squared modulus of $t_{fi}$ this is the matrix element one should calculate. It is given by

$$t_{fi} = h_{fi} + \sum_{p=1}^{n} \frac{h_{Rpi} t_{Rpi}}{E_i - E_{Rp}}$$

where $n$ is the number of resonant states. The unknown matrix elements $t_{Rpi}$ are solutions of a system of $n$ linear equations:

$$t_{Rpi} = h_{Rpi} + \sum_{q=1}^{n} \frac{h_{Rpi} h_{Rqi} t_{Rqi}}{E_i - E_{Rq}} \quad p = 1, \ldots, n.$$ 

The different quantities $h$ needed in order to completely solve the problem are solutions of a set of coupled integral equations like (15) but in which respectively $t$ and $h$ are replaced by $h$ and $v$. There is one system giving $h_{fi}$ and $h_{fi}$ and consequently $h_{Rfi}$; and one system for each resonant state giving $h_{Ri}$ and $h_{Ri}$ and therefore $h_{RR}$. As a whole we have $n + 1$ systems of coupled integral equations to be solved. This is the price to be paid for getting interesting physical information on the resonance line as we will see from the following simple example. Let us consider the simple case $n = 1$ then

$$t_{Ri} = h_{Ri} + \frac{h_{RR} t_{Ri}}{E_i - E_R}$$

and therefore

$$t_{fi} = h_{fi} + \frac{h_{Ri} h_{Ri}}{E_i - E_R - h_{RR}}.$$ 

The diffracted intensity will be proportional to

$$|h_{fi}|^2 \left|1 - \frac{iB}{x - i}\right|^2$$

with

$$B = i \frac{2 h_{Ri} h_{Ri}}{h_{Ri}} \Gamma, \quad x = [E_i - E_R - \text{Re}(h_{RR})] \frac{\Lambda}{\Gamma}$$

and

$$\frac{\Gamma}{2} = \text{Im}(h_{RR}).$$

The resonance shape is contained in this expression. $\Gamma$ is the line width and the extremum is given by the zero of $x$ provided the imaginary part of $B$ is not too important. One notices that this extremum is shifted from the kinematic condition, and its value can be readily determined. Furthermore if we suppose that the different quantities $h$ do not vary strongly with $K_i$ close to $K_{ip}$, the point for which the numerical calculation has been done, one can obtain to a good approximation the resonance line shape.

Therefore this last choice seems to be more powerful since with just one calculation point one gets a complete set of information about the resonance line.

3. Morse corrugated potential. — For the purpose of numerical calculation it is more convenient to write the Morse corrugated potential (hereafter referred to as MCP) in a form slightly different from expression (2), namely

$$V(R, z) = D \left[ \frac{1}{v_o \beta} \exp \left\{ - 2 \chi z - \varphi(R) \right\} - \frac{2}{\beta^{1/2}} \exp \left\{ - \chi z \right\} \right], \quad (16)$$

$\beta$ is a parameter which can be written as $\exp \{ 2 \chi z \}$ and obviously yields a translation of the whole potential along the normal to the surface. $v_o$ is the mean value of $\exp \{ - 2 \varphi(R) \}$ over the unit cell and consequently the Fourier components of the MCP are

$$V_c = 0 \quad V_\phi(z) = D \frac{v_o}{v_0 \beta} \exp \left\{ - 2 \chi z \right\}$$

$$G \neq 0 \quad V_c(z) = D \frac{v_o}{v_0 \beta} \exp \left\{ - 2 \chi z \right\}$$
with 
\[ v_G = \frac{1}{S} \int_{\mu,c} \exp \{- iG \cdot R \} \exp \{- 2 \varphi(R) \} \, dR \]

\( S \) is the unit cell \((\mu, \sigma)\) area.

The corrugation of the repulsive part extends into the well. Effectively the potential minimum \( V_{\text{min}} \) and the locus of this minimum \( z_{\text{min}} \) as \( R \) varies are given by

\[ V_{\text{min}} = -Dv_0 \exp \{- 2 \varphi(R) \} \]

\[ z_{\text{min}} = -Z - \frac{1}{\chi} \log (v_0) + 2 \varphi(R) \]

showing clearly that at this point the corrugation is \( 2 \varphi(R) \). One can demonstrate that the attractive part is also corrugated, the amplitude of the modulation being smoothly attenuated as \( z \) increases. As far as the repulsive part is concerned the true corrugation is equal to \( 2 \varphi(R) \) for \( V = 0 \) and \( \varphi(R) \) for \( V \) large. Therefore the true corrugation decreases with energy. This trend is in contradiction with that predicted by electronic density calculations and with the interpretation of the experimental data. Thus the MCP can be considered as a step on the way which leads to a good potential representation. In any case it is a good test for calculation methods and will give, as discussed later, physical results which will remain valid for any soft potential.

It is particularly convenient to take for the distorted potential \( U(z) \) a Morse potential

\[ U(z) = C \{ \exp(-2 \chi z) - 2 \exp(-\chi z) \}. \]  

(17)

Note that it may be translated from the zeroth order Fourier component of the MCP \((\beta \neq 1)\) and also may have a different well depth. This difference may be used in order to improve the convergence domain of the iterative process as will be discussed in the next paragraph. The eigenvalues and eigenvectors of \( U(z) \) are very well known since the work of Morse [15] as well as the matrix element of \( \exp \{-2 \chi z\} \) after the work of Lennard-Jones and co-workers [16]. These different quantities are given in appendix 1.

The matrix elements are introduced in equation (11) and the unknown quantities \( L_j \) are transformed into dimensionless functions \( F_j \) by the relations:

\[ F_j(r) = 4 A^2 L_j(c) \]

\[ F_j(n) = 4 A^2 \pi (-1)^n L_j(b) \]

where \( n \) is the quantum number labelling the bound state \( b \) and \( A^2 = 2m/\hbar^2 \chi^2 \) with \( m \) the mass of the incident particle. One gets:

\[ F_j(r, p_i) = f(r, p_i) \lambda_{j,0}(r, p_i) + \frac{1}{4} \sum \frac{F_{j}(n')}{\pi} \frac{l(r, n')}{p_G + \Omega(n')} \lambda_{jG}(r, n') + \int_0^{\infty} dq \frac{F_{j}(q)}{p_G - q^2 + \frac{i}{\chi}} \lambda_{jG}(r, q) \]  

(18)

\[ F_j(n, p_i) = l(p_i, n') \xi_{j0}(p_i, n) + \frac{1}{4} \sum \frac{F_{j}(n')}{\pi} \frac{s(n, n')}{p_G + \Omega(n')} \omega_{jG}(n, n') + \int_0^{\infty} dq \frac{F_{j}(q)}{p_G - q^2 + \frac{i}{\chi}} \xi_{jG}(n, q) \]

with

\[ \lambda_{jG}(r, q) = V_{jG} + \delta_{jG} A \sqrt{C} ax(r, q)/f(r, q) \]

\[ \xi_{jG}(n, q) = V_{jG} + \delta_{jG} A \sqrt{C} ax(n, q)/l(n, q) \]

\[ \omega_{jG}(n, n') = V_{jG} + \delta_{jG} A \sqrt{C} ax(n, n')/s(n, n') \]  

(19)

\[ J = G, \quad V_{jG} = \frac{D}{C} \frac{1}{\beta} - 1; \quad J \neq G, \quad V_{jG} = \frac{v_{jG} D}{v_0} \frac{1}{C} \beta^{-1/2} \]

\[ \alpha = 1 - \frac{D}{C} \beta^{-1/2} \]

\[ f, l, s, \text{are respectively the matrix elements between continuum-continuum, bound-continuum and bound-bound states of } \exp \{-2 \chi z\}, \text{and } g, k, j \text{the same quantities but of } \exp \{- \chi z\} \text{ (see appendix 1).} \]

\[ p_G^2 = \frac{1}{\chi} [k_i^2 + (K_i + G)^2] = \left( k_G \chi \right)^2, \]

\[ \Omega(n) = A^2 C - A \sqrt{C} (2n + 1) + \left( n + \frac{1}{2} \right)^2. \]
When resonant states are projected out of the set of integral equations (referred to in section 2 above as the second choice) the \( h_j(r, p) \) and \( h_j(n, p) \) matrix elements corresponding respectively to \( h_f \) and \( h_R \) when \( n = R \), are given by exactly the same set of integral equations as (18). As outlined above in this case the summation over bound states does not contain the resonant states. They are also excluded from the equations giving the \( h_{JR}(r, n) \) and \( h_{JR}(n, n) \) elements corresponding respectively to \( h_{fR} \) and \( h_{RR} \) when \( n = n_R \), which appears as:

\[
 h_{JR}(r, n_R) = \frac{l(r, n_R)}{p^2} \gamma_{JR}(r, n_R) + \\
 + \frac{1}{4} \sum_{n'} \int \frac{L(r, n')}{p^2 + \lambda_{JR}(r, q)} h_{GR}(n', n_R) + \int_0^\infty dq \frac{h_{GR}(q, n_R) l(n, q) \gamma_{JR}(q, q)}{p^2 - q^2 + i\epsilon}. 
\]

All these systems of integral equations are very similar and therefore can be solved by the same method.

As \( z \) goes to infinity the partial wave function \( \psi_J(z) \) can be written using equation (9) and bearing in mind that \( \phi_J(z) \) goes to zero:

\[
 \psi_J(z) \rightarrow \phi_J(z) \delta_{30} + \frac{1}{4} \int_0^{\infty} dq \frac{\phi_J(q) F_J(q)}{p^2 - q^2 + i\epsilon}
\]

with

\[
 \phi_J(q) = \sqrt{\frac{2}{\pi}} \left[ \exp i(qxz - \varphi_q) + \exp - i(qxz - \varphi_q) \right].
\]

The integration is readily done taking a thin rectangular contour a side of which is the positive \( q \) axis and located in the upper and lower half planes for the first and second exponentials of \( \phi_J(q) \) respectively. The former contour contains a pole and one gets:

\[
 \psi_J(z) \rightarrow \left[ \exp i(k_{iz} z - \varphi_i) + \exp - i(k_{iz} z - \varphi_i) \right] \frac{i\pi F_J(p_J)}{4p_J} \exp i(k_{iz} z - \varphi_i)
\]

for an open channel and \( \psi_J(z) \rightarrow 0 \) for a closed one.

The ratio of diffracted intensity to incident intensity in an open channel \( J \), say \( R_J \), is then

\[
 R_J = \left| \delta_{30} - \frac{i\pi}{4(p_i p_J)^{1/2}} F_J(p_J) \right|^2.
\]

4. Numerical solution. Convergence. — The set of integral equations to be solved is not very much different from the set of equations solved in the case of the exponential corrugated potential. With the MCP there is a slight modification of the kernel and the addition of linear terms due to bound states.

As this addition does not change substantially the nature of the problem and its difficulty, the procedures which can be used to get a numerical solution are the same in the two cases. They have been described and discussed in previous publications [12, 17] and will not be reproduced here. It has been demonstrated that with computers available to date the only practical way of getting a solution is to use the Neumann iterative process. If it converges it is well known that it converges to the correct solution [18].

With the exponential corrugated potential it has been shown that a translation of the distorted potential could increase to a large extent the convergence domain and a solution for high corrugation amplitudes has been obtained in this way [17]. With the MCP the same translation could be used \( (\beta \neq 1) \) and furthermore the distorted potential well depth \( C \) could be different. Particularly it is interesting from the point of view of numerical calculation to choose these two parameters in such a way that the coefficient \( \alpha = 1 - \frac{D}{C} \beta^{1/2} \) is equal to zero. In this case each of the different functions \( \gamma, \xi \) or \( \omega \) (see Eqs. (19)) reduces to a number \( V_{JC} \) equal to

\[
 J = G, \quad V_{JG} = \frac{C}{D} - 1; \quad J \neq G, \quad V_{JG} = \frac{v_J - q}{v_0} \frac{C}{D}.
\]

In the summation over reciprocal lattice vectors these numbers are the coefficients which multiply the sum over bound and continuum states. For a given corrugation function \( \varphi(R) \) and a given \( D \) value if we take \( C = D \)
they are equal to $V_{jj} = 0$, $V_{jG} = e_{j-G/V_0}$. When the corrugation height increases the $V_{jG}$ increase also and eventually the iterative process will diverge. Then it is clear that one has an interest from the point of view of convergence properties to lower the $V_{jG}$ coefficient values. This can be achieved by taking $C$ less than $D$. In this way the $V_{jG}$ coefficients are reduced and $V_{jj}$ becomes negative, a fact which can yield cancellations between some terms of the iterative expansion. In this manner the convergence domain can be extended to higher corrugation amplitude.

In order to discuss this problem on a quantitative basis, equations (18) (or (20)) are written in a matrix form:

$$
\begin{align*}
F_1'(r, p_1) &= f(r, p_1) V_{j0} + \sum_n M_1 V_{jG} S(r, q) F_1(q) \\
F_2'(n, p_1) &= l(p_1, n) V_{j0} + \sum_n M_n V_{jG} S(n, q) F_1(q)
\end{align*}
$$

(21)

where the notations $\| \|$ label a vector and a square matrix respectively. The different matrices are defined by:

$$
\begin{align*}
\| M_1 \| &= \frac{1}{4 \pi^2} l(r, n') \| V_{jG} \| p_G^2 + \Omega(n') \\
\| M_m \| &= \frac{1}{4} s(n, n') \| V_{jG} \| p_G^2 + \Omega(n')
\end{align*}
$$

and

$$
\| V_{jG} \| = \frac{V_{jG}}{4}.
$$

The operators $\int_0^\infty dq f(r, q) p_G^2 - q^2 + i\epsilon \| l(n, q) \|$ are written symbolically as $\| S(r, q) \|$ and $\| S(n, q) \|$. The matrix $p_G^2 - q^2 + i\epsilon \| l(n, q) \|$ is diagonal.

Starting the iteration process with given vectors $| F_1'(r, p_1) \rangle_{(0)}$ and $| F_2'(n, p_1) \rangle_{(0)}$ which can be different from $f(r, p_1) V_{j0}$ and $l(p_1, n) V_{j0}$ respectively one has:

$$
\begin{align*}
| F_1'(r, p_1) \rangle_{(1)} &= | F_1'(r, p_1) \rangle_{(0)} + | A_1'(r', p_1) \rangle_{(1)} \\
| A_1'(r', p_1) \rangle_{(1)} &= \sum_n M_1 V_{jG} | F_1(n', p_1) \rangle_{(0)} + \| V_{jG} \| \| S(r', q) \| | F_1(q) \rangle_{(0)}
\end{align*}
$$

and for the $p$ iteration step:

$$
\begin{align*}
| F_1'(r, p_1) \rangle_{(p)} &= | F_1'(r, p_1) \rangle_{(p-1)} + \| A_1'(r', p_1) \rangle_{(p)} \\
| A_1'(r', p_1) \rangle_{(p)} &= \sum_n M_1 V_{jG} | A_1(n', p_1) \rangle_{(p-1)} + \| V_{jG} \| \| S(r', q) \| | A_1(q, p_1) \rangle_{(p-1)}
\end{align*}
$$

Therefore the quantity $| A_1 \rangle_{(p)}$, which is added to $| F_1 \rangle_{(p-1)}$ at each iteration step is composed of a sum of product of $p$ operators like $\| M_1 \|$, $\| M_m \|$ or $\| V_{jG} \|$ $\| S \|$. Each product acts finally on the starting vectors $| F_1 \rangle_{(0)}$. This demonstrates that the convergence does not depend upon the starting point but on the operator structure. For instance let us consider the terms which are composed exclusively of products of $| M_1 \|$ or $\| M_m \|$. It is easy to prove that such a product will converge as $p$ increases if the corresponding matrix eigenvalues have their modulus less than 1, and this is a necessary condition for the convergence of the iteration process. Unfortunately we have not succeeded in obtaining a convergence criterion for the $\| S \|$ operator and a fortiori for the mixed product containing $\| M \|$. 

and \(\| S \|\). From the convergence study done in the case of an exponential corrugated potential \([17]\) where the integral equations contain only the \(\| S \|\) operator, one can say that the convergence will be achieved by lowering the eigenvalues of the \(\| V_{JG} \|\) matrix (which is Hermitian) in such a way that their values are evenly distributed about zero.

Therefore in the absence of an absolute criterion it seems that the maxima of the modulus of the eigenvalue of matrices \(\| M \|\) and \(\| V_{JG} \|\) are two quantities which have a great importance in the convergence of the iterative expansion. The parameters \(\beta\) and \(C\) should be chosen in such a way that these two maximum eigenvalue moduli would be simultaneously minimum.

When the choice of the parameters leads to an \(\alpha\) value not equal to zero the same quantities seem to be significant. Effectively one can show that the ratio of the functions which multiply \(\alpha\) in \(\lambda_{JG}^{\xi}, \xi_{JG}, \omega_{JG}\) (see Eqs. (19)) are less than or equal to \((2 A \sqrt{C})^{-1}\). Then the maximum value of these quantities for \(J = G\) are the same and equal to \(V_{JG} + 2 \alpha\). To a first approximation the matrix eigenvalues could be calculated by replacing in the diagonal term \(V_{JG}\) by \(V_{JG} + 2 \alpha\). The same empirical criterion defined above would apply.

Numerous numerical calculations have been done in order to test these conclusions, with different systems and conditions. It appears that the convergence is achieved when the maxima of the eigenvalue moduli are simultaneously less than 0.4-0.5 for \(\| M \|\) matrices and 0.12-0.15 for the \(\| V_{JG} \|\) matrix. Of course, these limiting values giving the convergence domain depend upon the system. For instance it seems that for given conditions an increase of the incident wave vector tends to slightly reduce this domain. Also it is important to notice that the number of iterations which are necessary in order to get a good unitarity increases for systems having large unit cells and/or high corrugation. Thus the problem of convergence remains an open question.

A typical example of the convergence limit is given in the next section.

5. Results and discussion. — Physical results will be discussed by considering successively and separately the effects on diffracted beam intensities out of resonance conditions of the following: the influence of the softness (which in the repulsive part of the potential depends mainly upon the range parameter \(2 \chi\)), the influence of the well depth \(D\), and amplitude of the corrugation function \(e J / e i\) is a convenient parameter which allows us to scale the wave penetration of the different beams.

The exponential corrugated potential (ECP) is very well suited for looking at the influence of the range parameter \(2 \chi\) and consequently the influence of the potential slope and wave penetration. This has been thoroughly discussed in previous publications \([12, 17]\) and the conclusions are briefly summarized here. For a given corrugation of small or medium crest to trough amplitude, increasing \(2 \chi\) yields an increase of diffracted beam intensities except that of the specular which decreases. For high \(2 \chi\) value these intensities tend to that given by the hard corrugated wall potential (HCWP). The relative difference between ECP and HCWP solutions is small for beams having \(E_{2s}\) value much greater than one and increases as \(E_{2s}\) decreases to become important for beams of low \(E_{2s}\) value. This illustrates the effect of wave penetration which modifies the distribution of beam intensities. The diffracted beams loose intensity to the benefit

\[
\psi_J(z) = \psi_J(0) \exp\left\{ i(K_J + J)z - E_J \right\}.
\]

The normal component \(\psi_J(z)\) is the only one which is affected by the wave penetration into the potential region and the importance of this phenomenon can be appreciated by looking at the potential slope at an energy equal to the normal kinetic energy of the beam \(J\). In this way each wave \(\psi_J(z)\) feels a potential region of different slope and the wave penetration will be higher for beams of lower normal kinetic energy. The ratio of this quantity to that of the specular beam \(E_{2s} = e_J/e_i\) is a convenient parameter which allows us to scale the wave penetration of the different beams.

The exponential corrugated potential (ECP) is very well suited for looking at the influence of the range parameter \(2 \chi\) and consequently the influence of the potential slope and wave penetration. This has been thoroughly discussed in previous publications \([12, 17]\) and the conclusions are briefly summarized here. For a given corrugation of small or medium crest to trough amplitude, increasing \(2 \chi\) yields an increase of diffracted beam intensities except that of the specular which decreases. For high \(2 \chi\) value these intensities tend to that given by the hard corrugated wall potential (HCWP). The relative difference between ECP and HCWP solutions is small for beams having \(E_{2s}\) value much greater than one and increases as \(E_{2s}\) decreases to become important for beams of low \(E_{2s}\) value. This illustrates the effect of wave penetration which modifies the distribution of beam intensities. The diffracted beams lose intensity to the benefit
of the specular and this loss is greater as the wave penetration increases.

We think that the same qualitative behaviour should happen with the MCP as $2\chi$ increases. Note that with this potential the HCWP is also recovered as $2\chi$ goes to infinity. But we do not make any numerical calculations which can support this fact because the range of $2\chi$ values of physical interest is limited. Effectively by adjustment of a Morse or a shifted Morse potential to bound state energy levels determined experimentally but looking at the resonance line positions, one finds that the $2\chi$ value is constrained to lie between 2 and 2.6 Å$^{-1}$ for alkali-halide crystals [19] and equal to 1.8 Å$^{-1}$ for the helium copper potential. Therefore we take $2\chi = 1.94$ Å$^{-1}$ and calculations with the same system as in the case of ECP have been made, in order to be able to make a fruitful comparison. We consider then a copper (100) face and an incident hydrogen molecule ($|k_i| = 8.6$ Å$^{-1}$, $E_i = 77$ meV). The incident plane contains the [100] direction and the incident angle $\theta_i = 31^\circ$. The corrugation function is taken to be:

$$\varphi(R) = \frac{1}{2}\hbar a \left[ \cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{2\pi y}{b}\right) \right]$$

with $a = 2.55$ Å the side of the square unit cell.

In these conditions the iteration process converges up to an $h$ value equal to 0.1. Let us recall that for the MCP the true corrugation varies with the energy and also varies with well depth value for a given energy. The true corrugation is accounted for by an $h$ value labelled $h^*$. For the preceding limit we have $h^* = 0.15$ which gives a corrugation crest to trough equal to 0.768 Å.

Turning now our attention to the well depth influence, $D$ is considered as a parameter. The solid lines in figures 1 and 2 give respectively the variation of specular beam intensity and those of the most intense diffracted beams as a function of the well depth with $h$ equal to 0.04. On figure 1 the variation of $I_{00}$ for $h = 0.024$ has been added.

The specular peak intensity decreases rapidly as $D$ increases, the variation being the steepest for the highest corrugation parameter $h$. On the diffracted beam intensities a rainbow effect is apparent on the $\bar{T}_0$, $\bar{T}_1$ and $01$ beams. In the case discussed here $h^*$ varies from 0.04 for $D = 0$ to 0.069 for $D = 44$ meV at $E_i = 77$ meV. Simultaneously, the potential slope increases as $D$ increases. These two facts could explain the intensity variation depicted by the two figures. However it is interesting to see if there is an influence of the well itself. With this in mind, for a given $D$ value the true $h^*$ value has been calculated and the well depth $D$ is added to that part of the energy associated with motion normal to the surface. Keeping $2\chi = 1.94$ Å$^{-1}$ one calculates the intensities with the ECP and these new parameters. Doing so we define an equivalent exponential corrugated potential (EECP) which takes account of the true corrugation exhibited by the MCP and of the particle acceleration due to the potential attractive part. It remains that the MCP slope at a given energy is a little greater than the corresponding quantity for the EECP, by a factor varying from 1 to 1.6 in the whole range of variation of $D$ for $E_i = 77$ meV. The EECP results are given by dashed lines on figures 1 and 2.

If the remaining difference between MCP and EECP results could be accounted for by the different potential slopes, the diffracted beam intensities should be greater in the MCP case. This is true except for the $10$ beam and the $01$ beam at $D$ greater than 31 meV. Also the relative difference should be dependent upon the $E_{13}$ value as explained above. Here it seems that there is no correlation between the intensity difference and this parameter. Therefore the observed variation in diffracted beam intensities from one potential to another could not be ascribed to the variation of potential slope and is consequently an effect of the well. It certainly yields a deformation of the wave function in the potential region which modifies the distribution of intensities among the different open channels.

As far as the determination of the corrugation parameter is concerned it is interesting to make the following observation. Let us suppose that from an

![Fig. 2. — Variation of the main diffracted peak intensities as a function of the well depth $D$ value for corrugation parameter $h = 0.04$; solid line, with the MCP; dashed line, with the EECP. Other parameters are the same as in Fig. 1.](image-url)

Table I. — Value of the corrugation parameter $h$ and the true corrugation $h^*$ determined with different potentials for $I_{00} = 0.578$. The experimental conditions are given in the text.

<table>
<thead>
<tr>
<th>Potential</th>
<th>$2\chi$ Å$^{-1}$</th>
<th>$D$ meV</th>
<th>$h$</th>
<th>$h^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCWP</td>
<td>$\infty$</td>
<td>0</td>
<td>0.04</td>
<td>0.04</td>
</tr>
<tr>
<td>ECP</td>
<td>1.94</td>
<td>0</td>
<td>0.058</td>
<td>0.058</td>
</tr>
<tr>
<td>MCP</td>
<td>—</td>
<td>4</td>
<td>0.04</td>
<td>0.046</td>
</tr>
<tr>
<td>EECP</td>
<td>—</td>
<td>4</td>
<td>0.051</td>
<td>0.051</td>
</tr>
<tr>
<td>MCP</td>
<td>—</td>
<td>18</td>
<td>0.024</td>
<td>0.034</td>
</tr>
</tbody>
</table>
experiment one knows the $2 \chi$ and $D$ values and that one intends to determine the $h$ value which gives a specular intensity equal to 0.578 (horizontal line on figure 1). Table I gives the obtained results for different potentials. It is clearly apparent that the corrugation found depends upon the chosen potential. The MCP could give a corrugation lower than that given by the HCW depending upon the $D$ value and in any case lower than that of the ECP. If one disregards the proper effect of the well discussed above these results can be qualitatively understood in terms of potential slope or wave penetration. Going from HCWP to ECP it is necessary to increase the corrugation in order to have the same specular intensity, the finite slope yielding an increase of this quantity. Now going from the ECP to the MCP an increase of $D$ produces an increase of the repulsive potential slope (see formula (22)) and the corrugation parameter should be reduced. One can notice the difference between the true corrugation given by the MCP and ECP. It is mainly an effect of the wave deformation produced by the well. But due to the small well depth value this effect is not very important.

The same determination could be done with a diffraction peak. Obviously one should not find the same $h^*$ value except with the MCP which is taken here as a reference. This remark and the results discussed above outline clearly the fact that a good potential model should be used in order to get a good corrugation function. However a good approximation can be given by the ECP or better by the EECP in the case of very small well depth values.

We consider the last point of our discussion, that is to say the influence of the corrugation height. As a function of the true corrugation parameter $h^*$ the variation of the specular intensity for the MCP and

![Fig. 4.](image)

**Variation of most intense diffraction peaks as a function of the true corrugation parameter $h^*$ for the MCP.** Same conditions as Fig. 3.

![Fig. 5.](image)

**Same as Fig. 4 but for the EECP.**

EECP is given in figure 3. Figures 4 and 5 give the variation of the most intense diffracted peaks for the MCP and EECP, respectively. These calculations have been carried out with $D = 21.6$ meV and $2 \chi = 1.94$ Å$^{-1}$. Rainbow effects are clearly apparent on these figures. Table II gives the positions and intensities of the rainbow maxima which are located

<table>
<thead>
<tr>
<th>Bean</th>
<th>$E_{jk}$</th>
<th>$h^*$</th>
<th>$I$</th>
<th>MCP</th>
<th>$h^*$</th>
<th>$I$</th>
<th>EECP</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>1.344</td>
<td>0.07</td>
<td>0.143</td>
<td>0.092</td>
<td>0.143</td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>1.24</td>
<td>0.114</td>
<td>0.129</td>
<td>&gt; 0.12</td>
<td>&gt; 0.14</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>1.172</td>
<td>0.048</td>
<td>0.149</td>
<td>0.062</td>
<td>0.153</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.776</td>
<td>0.085</td>
<td>0.097</td>
<td>0.12</td>
<td>0.076</td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>0.725</td>
<td>0.011</td>
<td>0.112</td>
<td>&gt; 0.12</td>
<td>&gt; 0.06</td>
<td></td>
<td></td>
</tr>
<tr>
<td>01</td>
<td>0.604</td>
<td>0.055</td>
<td>0.07</td>
<td>0.075</td>
<td>0.063</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.208</td>
<td>≥ 0.13</td>
<td>≥ 0.07</td>
<td>&gt; 0.12</td>
<td>&gt; 0.024</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

![Fig. 3.](image)

**Variation of specular intensity as a function of true corrugation parameter $h^*$; solid line, MCP value; dashed line, EECP value.** The calculation is done with the same system as in Fig. 1, with $D = 21.6$ meV.
at a higher $h^*$ value for the EECP. The shift produced by the MCP is greater than 0.014 and no correlation can be detected between the shift value and the $E_{jz}$ parameter. However this parameter seems to indicate the manner in which the intensity maxima vary. The beams for which $E_{jz}$ is greater than unity have a maximum higher in the EECP case (or equal for the 11 beam). The converse is true for beams of $E_{jz}$ value less than unity.

The same behaviour is observed when one compares the results given by the ECP ($2 \chi = 3 \text{Å}^{-1}$) and the HCWP [17]. The HCWP yields a shift of the rainbow maximum towards lower $h$ values and the intensity maxima variation is correlated in the same way as above to $E_{jz}$ a fact which has been interpreted in terms of slope variation of the potential. As the HCWP results can be recovered with an ECP of high $2 \chi$ value (say $2 \chi = 15 \text{Å}^{-1} [17]$) the slope variation of the potential in the ECP-HCWP case is considerably greater than that yielded by passing from the EECP to the MCP. Thus it seems that the slope variation could not be responsible for the whole effect observed here. The modification of the wave functions certainly produces the main effect and acts in the same way as a substantial slope variation in the potential.

The presence of the well induces a change in the wave function shape of the continuum states and introduces the bound states. It is not possible to know which of these two effects is predominant in the new distribution of diffracted intensities. However at resonance conditions the effect of the resonant state is to yield strong variations in beam intensities apparent as a resonance line. As an example figure 6 gives the variation of specular intensity as a function of incident angle. Five deep and sharp resonance lines are visible corresponding to the resonance of the 10 and 01 beams with the five different levels of the potential. These two beams are symmetric with respect to the incident plane and consequently there is no splitting of the resonance lines. In order of increasing quantum number $n$, their calculated widths are respectively 0.039 5, 0.075 4, 0.081 9, 0.056 5, 0.009 2 meV a quantity which is maximum for $n = 2$.

The differences in width are a reflection of the variation of the matrix elements $\langle \phi_n | \exp (-2 \chi x) | \phi_i \rangle = l(n, p_i)$, which are mainly influenced by the shape and spread of the bound state wave function $\phi_n$. In this way the range of the attractive part of the potential plays an important role and should be of a realistic form. However, some important features can be drawn from calculations with the MCP. This will be the subject of a forthcoming paper in which we intend to discuss the resonance phenomena in detail.

6. Approximations. — The iterative process used in order to solve the scattering integral equations could be stopped after a low number of iterations and approximate intensity values could be obtained by a normalization of the results; i.e. by dividing each intensity by the sum of all calculated intensities.

In this way a first approximation consists in the normalization of the first order iteration result which is the well known normalized distorted wave Born approximation (NDWBA). The intensity calculation is then very simple once the matrix elements are known. Multiple scattering effects are completely neglected and therefore the resonance phenomena cannot be described.

Another approximate solution is obtained in neglecting in the CCGM equations (Eqs. (11)) the principal part of each integral. This is called the CCGM approximation. In this way one gets a system of linear algebraic equations for the unknown $t$ matrix elements and therefore the intensities are readily calculated. One can prove that the result is always unitary which shows that the unitarity condition is not sufficient to warrant the exactness of the solution. Due to the suppression of the principal part integrals only the continuum states which conserve energy are taken into account and therefore multiple scattering is partly kept in the solution. However, the sum over bound states being included, the resonance phenomenon is apparent in the results.

It is now interesting to compare the results obtained with these two approximations and the exact solution. Calculations have been done with the system used in this paper for increasing value of $h$ (table III). When $h$ is small the CCGM approximation is good for all the most intense peaks but the NDWBA is only valuable for the 00 and 10 beams. As $h$ increases the difference with the exact result increases also and the approximations give increasingly worse intensity values.

This demonstrates that this kind of approximation should be used only for very small corrugation. As the corrugation amplitude increases their validity should be verified before extensive use by comparing with an exact solution.
Table III. — Calculated beam intensities with the MCP. The column labelled $E$ gives the exact result. In the column labelled $B$, for each line the upper and lower number gives respectively the NDWBA and CCGM approximation results. $k_i = 8.6 \text{ Å}^{-1}$, $\theta_i = 31^\circ$, $2 \chi = 1.94 \text{ Å}^{-1}$, $D = 21.6 \text{ meV}$. $h$ is the corrugation function parameter (see text).

<table>
<thead>
<tr>
<th>$h$</th>
<th>$E$</th>
<th>$B$</th>
<th>$C$</th>
<th>$E$</th>
<th>$B$</th>
<th>$C$</th>
<th>$E$</th>
<th>$B$</th>
<th>$C$</th>
<th>$E$</th>
<th>$B$</th>
<th>$C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.895 0</td>
<td>0.900 6</td>
<td>0.036 40</td>
<td>0.141 3</td>
<td>0.316 2</td>
<td>0.015 9</td>
<td>0.000 03</td>
<td>0.012 8</td>
<td>0.000 01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.02</td>
<td>0.637 0</td>
<td>0.693 8</td>
<td>0.108 9</td>
<td>0.459 7</td>
<td>0.419 6</td>
<td>0.202 6</td>
<td>0.000 43</td>
<td>0.184 7</td>
<td>0.000 16</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.03</td>
<td>0.351 7</td>
<td>0.501 8</td>
<td>0.148 0</td>
<td>0.727 1</td>
<td>0.682 3</td>
<td>0.692 8</td>
<td>0.001 57</td>
<td>0.784 6</td>
<td>0.000 61</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.04</td>
<td>0.144 7</td>
<td>0.361 5</td>
<td>0.123 6</td>
<td>0.770 5</td>
<td>0.874 2</td>
<td>1.235 0</td>
<td>0.003 5</td>
<td>1.946</td>
<td>0.001 40</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.338 3</td>
<td>0.157 9</td>
<td>0.420 3</td>
<td>0.426 33</td>
<td>0.216 0</td>
<td>0.216 0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

7. Conclusions. — For a periodic potential the Schrödinger equation has been transformed into a set of integral equations. The unknown functions are proportional to the reduced $t$ matrix element of the two-potential formalism. When a kinematic resonance condition is satisfied singularities appear in these equations. Then by a projection method a new set of integral equations is obtained which does not contain the singularities. The new unknown functions are linearly related to the $t$ matrix elements and the problem can be solved without difficulty.

This general formalism has been applied to the case of a Morse corrugated potential and the integral equation set is solved by an iterative process. The convergence domain can be enlarged by using a distorted potential slightly different from the zero order Fourier component of the Morse corrugated potential. The former could have a different well depth and could be translated with respect to the latter. However the convergence domain is not sufficiently large to cover all experimental situations. For system of large unit cell and high corrugation amplitude the process diverges. Therefore the convergence of the iterative process remains an open mathematical question.

The addition of a well to a soft potential yields a different distribution of the diffracted peak intensities. This is due to the acceleration of the incident particle by the attractive part of the potential and mainly to the modification of the wave function shape in the continuum and the addition of bound state effects. Therefore this implies that the so-called Beeby correction which introduces in the Debye-Waller factor the increase of incident energy by the well depth, is a very approximate correction.

As a practical point it has been shown that the use of a hard corrugated wall or even an exponential corrugated potential in order to determine the corrugation function, could lead to erroneous results. A realistic potential should be used for all case in which the well depth is not too small.

On the other hand, it is demonstrated that approximate solutions of the scattering equations such as the normalized distorted wave Born approximation or the so-called CCGM approximation could give acceptable results only for small corrugation. Thus they can be used with confidence in only a limited range of corrugation amplitudes.

Acknowledgments. — It is a pleasure to thank Dr C. Manus for his constant support and Dr J. Lapujoulade, Dr Y. Lejay, B. Salanon and J. Perreau for numerous fruitful discussions.

This work was supported in part by the NATO Research Grant RG86.81.

Appendix 1. — With $A^2 = 2 m h^2 \chi^2$ ($m$ the incident particle mass) and $x = 2 A \sqrt{C} \exp \{- \chi z \}$, and using the normalization by $\delta$ function, the eigenvalues $e$ and eigenvectors $\phi$ of a Morse potential

$$U(z) = C[\exp \{- 2 \chi z \} - 2 \exp \{- \chi z \} ]$$

are:

— Bound state:

$$A^2 e_n = y_n^2, \quad y_n = A \sqrt{C} - n - \frac{1}{2}$$

$$\phi_n(x) = \left[ \frac{n! 2^{y_n} \chi}{\Gamma(2 y_n + n + 1) \Gamma(2 y_n)} \right]^{1/2} x^{y_n} \exp - \frac{x}{2} L_n^{2 y_n}(x)$$

with $L_n^{2 y_n}$ the modified Laguerre polynomial and $\Gamma$ the gamma function.
Continuum state:

$$\phi_p(x) = \left(\frac{x}{2\pi}\right)^{1/2} \left| \frac{\Gamma\left(\frac{1}{2} - A\sqrt{C} - ip\right)}{\Gamma\left(2ip\right)} \right| x^{-1/2} W_{\lambda_1 \lambda_2, ip}(x)$$

with $p = A(e_p)^{1/2}$ and $W_{\lambda_1 \lambda_2, ip}$ the Whittaker function.

If we write $e_p = \frac{h^2 k^2}{2m}$ we have $p = \frac{kz}{\chi}$.

The asymptotic form of $\phi_p$ as $z$ goes to infinity is given by $2\left(\frac{x}{2\pi}\right)^{1/2} \cos(p\chi z + \varphi_p)$.

$\varphi_p$ being a phase factor well defined.

The dimensionless matrix elements relative to equations (17) are:

Continuum-continuum state

$$f(p, q) = \left[\frac{2p \sinh(2\pi p) 2q \sinh(2\pi q)}{\cosh(2\pi p) - \cosh(2\pi q)}\right]^{1/2} \left[\left(p^2 - q^2\right) \lambda^+ + 2A\sqrt{C}\lambda^- \right]$$

with

$$\lambda^\pm = \left| \frac{\Gamma(-A\sqrt{C} + \frac{1}{2} + ip)}{\Gamma(-A\sqrt{C} + \frac{1}{2} + ip)} \right| \pm \left| \frac{\Gamma(-A\sqrt{C} + \frac{1}{2} + ip)}{\Gamma(-A\sqrt{C} + \frac{1}{2} + ip)} \right|$$

$$\frac{\varphi(p, q)}{f(p, q)} = \left[\left(p^2 - q^2\right) \lambda^+ + 2A\sqrt{C}\lambda^- \right]^{-1} \times \lambda^-.$$

If $p = q$

$$f(p, p) = \frac{4p}{\pi} \left[p + A\sqrt{C} \Im(\psi(-A\sqrt{C} + \frac{1}{2} + ip))\right]$$

$\psi$ being the logarithmic derivative of $\Gamma$.

Bound-continuum state

$$l(n, q) = \left(\frac{q \sinh(2\pi q)(2A\sqrt{C} - 2n - 1)}{\Gamma(2A\sqrt{C} - n)}\right)^{1/2} \left| \frac{\Gamma(-A\sqrt{C} + \frac{1}{2} + iq)}{\Gamma(A\sqrt{C} + \frac{1}{2} + iq)} \right|^2 \times$$

$$\times \left[\gamma_n^2 + q^2 + 2A\sqrt{C}\right]$$

$$k(n, q)/l(n, q) = \left[\gamma_n^2 + q^2 + 2A\sqrt{C}\right]^{-1}$$

Bound-bound state

$$s(n, n') = \left(\frac{n! n'! 2\gamma_n 2\gamma_{n'}}{\gamma_n + n + 1 \gamma_{n'} + n' + 1}\right)^{1/2} \frac{\Gamma(2\gamma_n + n + 1)}{n'!} \times$$

$$\times \left(\frac{n'!}{\Gamma(2\gamma_{n'} + n' + 1)}\right)^{1/2} \frac{\Gamma(2\gamma_n + n + 1)}{n'!} \times$$

$$\times (n - n')(2A\sqrt{C} - (n + n') - 1) + 2A\sqrt{C})$$

for $n' \leq n$. If $n' > n$, $n$ is put in place of $n'$ and vice versa.

$$f(n, n')/s(n, n') = \left[(n - n')(2A\sqrt{C} - (n + n') - 1) + 2A\sqrt{C}\right]^{-1}.$$

References


