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Dispersion relation for energy bands and energy gaps derived by the use of a phase-integral method, with an application to the Mathieu equation

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Abstract. The quantal problem of a particle moving in a one-dimensional periodic potential with one barrier per period is treated rigorously by means of a phase-integral method. A general dispersion formula, relating real energies to real or complex wavenumbers, valid for any conveniently chosen order of the phase-integral approximations used, is derived. The formula allows for the use of modified as well as unmodified phase-integral approximations, and different possibilities are discussed. For instance, a modification introduced by Floyd in the usual first-order JWKB approximation and applicable to the interior of high-energy bands can be utilised in our scheme for the generation of higher-order phase-integral approximations. This approach opens the possibility of using our phase-integral method in situations where the parameters of the problem are such that with unmodified approximations it would not work at all. The accuracy obtainable is illustrated by calculations on the Mathieu potential and comparison with available accurate numerical results.

1. Introduction

The results of a thorough analysis of the barrier transmission problem made by Fröman and Fröman (1970) will be used for treating the problem of a particle moving in a one-dimensional periodic potential (with one barrier per period) with the aid of the phase-integral method developed by the same authors (Fröman and Fröman 1965, 1974a, b, pp 126–31, Fröman 1966, 1970). Imposing on the wavefunction the conditions due to the periodicity of the potential, we obtain an exact dispersion relation determining the allowed energies (energy bands) corresponding to real values of the wavenumber k , as well as the forbidden energies (E real) corresponding to complex values of k . Neglecting in this exact relation certain correction quantities for which upper bounds are given (Fröman and Fröman 1970), we obtain an approximate dispersion relation which is in general very accurate when higher-order phase-integral approximations are used. For the numerical illustration of the accuracy of our results we consider the Mathieu equation, which is identical with the Schrödinger equation for the quantum pendulum, though for the latter only the solutions periodic with the same period as the potential are relevant. Besides the advantage, for our purposes, that accurate numerical information is available for comparison, the Mathieu equation is a convenient example because of its importance in many different branches of physics (see Meixner and Schäfer 1954, ch 4). For instance in quantum mechanics it is used for the analysis of band structures (see a thorough analysis by Slater (1952)), and recently it

has become of interest in field theory in connection with the extensively studied sine-Gordon model (see e.g. Neuberger 1978).

The application of the first-order JWKB approximation to the Mathieu equation was treated by Jeffreys (1925), who used the periodicity of the Mathieu functions to obtain the characteristic values well above the top of the barrier, and connection formulae to obtain those well below. Other early papers in which asymptotic methods were used are those by Goldstein (1928), Strutt (1929) and Wannier (1953). In this context we draw attention to the fact that the application of connection formulae to the case when the energy is well below the top of the barrier requires great caution with regard to their one-directedness. Otherwise insignificant terms appear in the resulting formulae. For instance, in a collection of solved problems (ter Haar 1964) in which that case is treated, one notices that only the leading term in the formula (3) on p 97, which determines the allowed energy bands, is correct, the next term being in error by a factor of two. One finds the same deficiency appearing also in recent standard JWKB calculations in the literature, for instance in Neuberger's paper (1978, equation (37)). Landauer (1951) considered energies above the top of the barrier and used a convergent expansion, the first term of which is the first-order JWKB approximation, while the next term accounts for reflections. Landauer's results were exploited by Buxton and Berry (1976) in an extensive analysis of Bloch wave degeneracies in high-energy electron diffraction. Dykhne (1961), considering the complex transition points, obtained the positions and widths of the energy gaps far above the top of the barrier. Balazs (1969) and Richardson (1971) obtained formulae which, except for missing a certain quantity (σ in our notation; see § 4 below) of importance in the neighbourhood of the top of the barrier, agree with the corresponding formulae in our treatment when the latter are specialised to the first-order approximation.

2. Formulation of the problem

Let the time-independent Schrödinger equation be

$$d^2\psi/dz^2 + Q^2(z)\psi = 0, \quad (1)$$

where

$$Q^2(z) = (2m/\hbar^2)(E - V(z)), \quad (2)$$

E being the energy of the particle and $V(z)$ a periodic, analytic potential with period a , which thus satisfies the relation

$$V(z + a) = V(z). \quad (3)$$

The periodicity of the potential implies that $Q^2(z)$ also is periodic, and hence (1) is the Hill equation. For a Floquet solution of (1) we have

$$\psi(z + a) = \lambda\psi(z), \quad (4a)$$

$$\psi'(z + a) = \lambda\psi'(z), \quad (4b)$$

where the Floquet factor λ is a constant (depending on E). It was shown by Liapunov (1902) that the quantity μ defined by

$$\mu = (\psi(z + a) + \psi(z - a))/2\psi(z) \quad (5)$$

is a function only of the energy and is independent of the choice of the solution $\psi(z)$. We

shall therefore write $\mu(E)$ instead of μ for the quantity (5). Letting $\psi(z)$ be a Floquet solution, we immediately obtain from (4a) and (5)

$$\mu(E) = \frac{1}{2}(\lambda + 1/\lambda), \quad (6)$$

i.e.

$$\lambda^2 - 2\mu(E)\lambda + 1 = 0. \quad (7)$$

Kramers (1935), in a well-known paper, derived this equation for λ but with $\mu(E)$ given by an expression alternative to (5). Expanding a Floquet solution in terms of two linearly independent basic solutions of (1), he obtained, in terms of those solutions and their derivatives at z and $z + a$, an expression for the quantity corresponding to $2\mu(E)$ in our notation, which he showed was independent of z and of the choice of the basic solutions. The properties of $\mu(E)$ for real values of E were also described by Kramers (1935). Studies of the analytic properties of $\mu(E)$ and $\lambda(E)$ in the complex energy plane were made by Kohn (1959) and by Kaus and Watson (1960).

We can write λ in the form

$$\lambda = e^{ika}, \quad (8)$$

where, by virtue of (6), k is determined as a function of E by the equation

$$\cos(ka) = \mu(E). \quad (9)$$

In view of (4a) and (8), a Floquet solution of (1) can be expressed as

$$\psi(z) = e^{ikz}u(z), \quad (10)$$

where

$$u(z+a) = u(z). \quad (11)$$

For real values of the energy E the function $\mu(E)$ is real (Kramers 1935, p 484) and hence, as follows from (9), the wavenumber k is either real or is complex with the real part an integral multiple of π/a . For real values of k the solutions (10) are the well-known Bloch waves, and the energies, determined by (9), are the so-called allowed energies forming the energy bands. For complex values of k the solutions (10) have an exponential behaviour, and the corresponding energies satisfying (9) are the so-called forbidden energies, which form the energy gaps separating the energy bands. See the paper by Kramers (1935) for further details.

The problem of determining the structure of the energy bands and energy gaps is thus equivalent to the problem of obtaining a useful expression for $\mu(E)$.

3. Exact expression for $\mu(E)$ in terms of phase-integral quantities and an F matrix element

The explicit expressions for the phase-integral functions used in the present treatment are of the general form (Fröman 1966, 1970)

$$f_1(z) = q^{-1/2}(z) \exp\left(i \int^z q(z) dz\right), \quad (12a)$$

$$f_2(z) = q^{-1/2}(z) \exp\left(-i \int^z q(z) dz\right). \quad (12b)$$

The function $q(z)$ is, for the $(2N + 1)$ th-order phase-integral approximation, given by (Fröman and Fröman 1974a, b, pp 126–31)

$$q(z) = Q_{\text{mod}}(z) \sum_{n=0}^N Y_{2n}, \quad (13)$$

where, by analogy to (2), $Q_{\text{mod}}^2(z)$ is written as

$$Q_{\text{mod}}^2(z) = (2m/\hbar^2)(E - V_{\text{mod}}(z)), \quad (14)$$

and $V_{\text{mod}}(z)$ is a so-far unspecified modified potential with the same period as $V(z)$. We shall consider only real values of the energy E , and we assume that $V(z)$ and $V_{\text{mod}}(z)$ are real on the real axis. If $V_{\text{mod}}(z) = V(z)$ we speak of unmodified phase-integral approximations, and if $V_{\text{mod}}(z) \neq V(z)$ of modified approximations. We shall discuss the choice of $V_{\text{mod}}(z)$ in § 5. The first few functions Y_{2n} are (Fröman and Fröman 1970, equations (6a–c))

$$Y_0 = 1, \quad (15a)$$

$$Y_2 = \frac{1}{2}\epsilon_0, \quad (15b)$$

$$Y_4 = -\frac{1}{8}\epsilon_0^2 - \frac{1}{8}\epsilon_2, \quad (15c)$$

with

$$\epsilon_0 = \frac{Q^2(z) - Q_{\text{mod}}^2(z)}{Q_{\text{mod}}^2(z)} + Q_{\text{mod}}^{-3/2}(z) \frac{d^2}{dz^2} Q_{\text{mod}}^{-1/2}(z) \quad (16)$$

and

$$\epsilon_n = d^n \epsilon_0 / d\zeta^n, \quad n = 1, 2, \dots, \quad (17)$$

where

$$\zeta = \int^z Q_{\text{mod}}(z) dz. \quad (18)$$

The functions Y_{2n} can all be expressed in terms of $\epsilon_0, \epsilon_1, \epsilon_2, \dots$. Explicit expressions for the functions Y_{2n} up to Y_{20} can be found in a paper by Campbell (1972).

The connection problems for the arbitrary-order phase-integral approximations given by equations (12a, b)–(18) can be mastered by the same method as developed by Fröman and Fröman (1965) for the first-order JWKB approximation. Thus, according to the phase-integral method we are using, an exact solution of the differential equation (1) is expressed in terms of the functions $f_1(z), f_2(z)$ and a matrix $F(z, z_0)$, the elements of which are given by convergent series. The final approximate formulae are obtained by omitting certain correction quantities involving elements of the matrix F for which upper bounds are obtainable.

We assume, for each barrier, the complex z plane to be cut in the same way as in the paper by Fröman and Fröman (1970) on barrier transmission. Denoting real values of z on the first Riemann sheet and on the upper edge of the real axis by x , we let the points x_1 and x_2 in that paper be x_1 and $x_2 = x_1 + a$, lying to the left and to the right respectively of one of the barriers in our present problem (see our figure 1).

In order to obtain an expression for $\mu(E)$, we may utilise either (4a, b) or (5) and apply the phase-integral method just described in a straightforward way. In either case we shall need some phase-integral relations which we shall now derive.

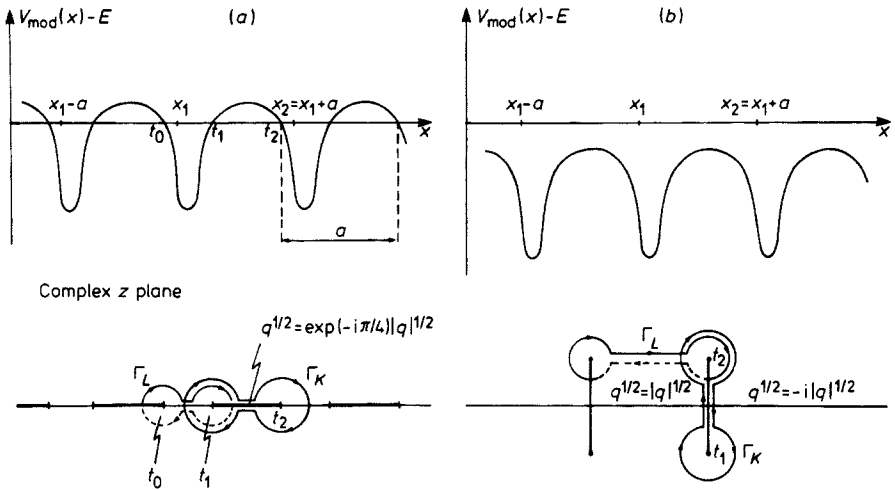


Figure 1. Schematic drawing of $V_{\text{mod}}(x) - E$ for a periodic potential with period a , and of the contours of integration Γ_K and Γ_L occurring in the definitions (23) and (24a) of K and L : (a) and (b) refer to the situation when the energy E lies below and above the barrier maxima respectively. The cuts in the complex z plane are indicated by heavy lines. Broken curves indicate parts of the contour of integration lying on the second Riemann sheet. The choice of phase for $q^{1/2}(x)$ on the upper edge of the real axis and on the first Riemann sheet is indicated. The contour integral of $q(z)$ along Γ_L in (b) can be replaced by the integral (24b), whereby the cuts crossing the real axis should be removed.

We consider a solution of (1) at the point x_1 expressed, together with its derivative, exactly in terms of the phase-integral functions $f_1(x_1)$ and $f_2(x_1)$ as (Fröman and Fröman 1965, equations (3.25a, b))

$$\psi(x_1) = a_1(x_1)f_1(x_1) + a_2(x_1)f_2(x_1) = f(x_1)\mathbf{a}(x_1), \tag{19a}$$

$$\psi'(x_1) = a_1(x_1)f_1'(x_1) + a_2(x_1)f_2'(x_1) = f'(x_1)\mathbf{a}(x_1), \tag{19b}$$

where f and \mathbf{a} denote the row vector and the column vector with elements f_1, f_2 and a_1, a_2 respectively. We note that, according to the phase-integral method we are using, the derivative of ψ is obtained by differentiating formally as if a_1 and a_2 were constants. For $\psi(x_1 \pm a)$ and $\psi'(x_1 \pm a)$ we obtain the expressions (Fröman and Fröman 1965, equation (3.26))

$$\psi(x_1 \pm a) = f(x_1 \pm a)\mathbf{a}(x_1 \pm a) = f(x_1 \pm a)\mathbf{F}(x_1 \pm a, x_1)\mathbf{a}(x_1), \tag{20a}$$

$$\psi'(x_1 \pm a) = f'(x_1 \pm a)\mathbf{a}(x_1 \pm a) = f'(x_1 \pm a)\mathbf{F}(x_1 \pm a, x_1)\mathbf{a}(x_1), \tag{20b}$$

where, and in the following, the upper signs yield one set of relations and the lower signs another, and where the matrix $\mathbf{F}(x_1 \pm a, x_1)$ is defined according to Fröman and Fröman (1965).

We shall next express the functions f_1 and f_2 at the points $x_1 \pm a$ in terms of f_1 and f_2 at the point x_1 , and in that context also give explicit expressions for certain quantities which will appear in our final formulae. We adhere to the same conventions as Fröman and Fröman (1970), and hence we choose the lower limit in the integral occurring in the exponents of the expressions (12a, b) for the functions $f_1(z)$ and $f_2(z)$ to be t_1 (see our figure 1) in the first-order approximation and the corresponding contour integral in the higher-order approximations (Fröman 1966), and we choose $q^{1/2}(z)$ to be real and

positive in the classically allowed region where x_1 is located. Because of the periodicity of the potential, we then have

$$f_1(x_1 \pm a) = \pm C f_2(x_1), \quad f_2(x_1 \pm a) = \mp(1/C) f_1(x_1), \quad (21a)$$

$$f'_1(x_1 \pm a) = \pm C f'_2(x_1), \quad f'_2(x_1 \pm a) = \mp(1/C) f'_1(x_1), \quad (21b)$$

where, for conciseness, we use the notation

$$C = \exp[K - i(L - \pi/2)], \quad (22)$$

with K and L defined as

$$K = \frac{1}{2i} \int_{\Gamma_K} q(z) dz, \quad (23)$$

$$L = \text{Re} \frac{1}{2} \int_{\Gamma_L} q(z) dz, \quad (24a)$$

the contours of integration Γ_K and Γ_L for both sub-barrier and super-barrier energies being shown in figure 1. For super-barrier energies the quantity L is most conveniently written as an integral along the real axis over an arbitrary period of the potential, whereby the cuts crossing the real axis should be disregarded and $q(x)$ chosen to be positive along the whole real axis. In this way formula (24a) can be written

$$L = \int_x^{x+a} q(x') dx', \quad \text{super-barrier case.} \quad (24b)$$

Let us now first obtain $\mu(E)$ by using (4a, b), putting $z = x_1$. Expressing the Floquet solution ψ and its derivative ψ' at the points x_1 and $x_1 + a$ by means of (19a, b) and (20a, b), and expressing in the resulting formulae $f(x_1 + a)$ and $f'(x_1 + a)$ in terms of $f(x_1)$ and $f'(x_1)$ respectively by means of (21a, b), we obtain, after some rearrangements, the equation

$$\begin{aligned} f_1(x_1) \{ &[-(1/C)F_{21}(x_1 + a, x_1) - \lambda] a_1(x_1) - (1/C)F_{22}(x_1 + a, x_1) a_2(x_1) \} \\ &+ f_2(x_1) [CF_{11}(x_1 + a, x_1) a_1(x_1) + (CF_{12}(x_1 + a, x_1) - \lambda) a_2(x_1)] \\ &= 0, \end{aligned} \quad (25)$$

and a similar equation with $f_1(x_1)$ and $f_2(x_1)$ replaced by $f'_1(x_1)$ and $f'_2(x_1)$ respectively. From these two equations we obtain, as a consequence of the fact that the Wronskian of f_1 and f_2 is different from zero, the system of equations

$$[-(1/C)F_{21}(x_1 + a, x_1) - \lambda] a_1(x_1) - (1/C)F_{22}(x_1 + a, x_1) a_2(x_1) = 0, \quad (26a)$$

$$CF_{11}(x_1 + a, x_1) a_1(x_1) + (CF_{12}(x_1 + a, x_1) - \lambda) a_2(x_1) = 0. \quad (26b)$$

Since $a_1(x_1)$ and $a_2(x_1)$ are not both equal to zero, the determinant of the system of equations (26a, b) must be equal to zero. This requirement yields, with the use also of the fact that $\det \mathbf{F}(x_1 + a, x_1) = 1$ (Fröman and Fröman 1965, equation (3.19)),

$$\lambda^2 - [CF_{12}(x_1 + a, x_1) - (1/C)F_{21}(x_1 + a, x_1)] \lambda + 1 = 0. \quad (27)$$

Comparing (27) with (7), and using the inversion relation for the \mathbf{F} matrix, i.e. equation (21) in the paper by Fröman and Fröman (1970), we realise that

$$\mu(E) = \frac{1}{2} [(1/C)F_{21}(x_1, x_1 + a) - CF_{12}(x_1, x_1 + a)]. \quad (28)$$

Noting that, since we are considering real energies, and since $V(z)$ and $V_{\text{mod}}(z)$ are assumed to be real on the real axis, we have the symmetry relation (Fröman and Fröman 1970, equation (22*b*))

$$F_{21}(x_1, x_1 + a) = -F_{12}^*(x_1, x_1 + a) e^{2K}, \tag{29}$$

and recalling the expression (22) for C , we can write (28) in the form

$$\mu(E) = |F_{12}| e^K \cos(L - 2\sigma), \tag{30}$$

where

$$\sigma = \frac{1}{2}(\arg F_{12} - \pi/2) \tag{31}$$

and F_{12} means $F_{12}(x_1, x_1 + a)$.

Solving equation (7) with respect to λ , when $\mu(E)$ is given by (30), we obtain

$$\lambda(E) = |F_{12}| e^K \cos(L - 2\sigma) \bullet i[1 - |F_{12}|^2 e^{2K} \cos^2(L - 2\sigma)]^{1/2}. \tag{32}$$

According to (9) and (30) we obtain the following exact formula determining the connection between the wavenumber k (real or complex) and the energy E (real):

$$\cos(ka) = |F_{12}| e^K \cos(L - 2\sigma). \tag{33}$$

The reason why (33) is valid only for real energies is that the symmetry relation (29) used in the derivation of (30) requires for its validity that $Q^2(z)$ and $Q_{\text{mod}}^2(z)$ are real on the real z axis. Since the quantities on the right-hand side of (33) are functions of the energy E , we see at once that (33) is consistent with the well-known relations

$$E(-k) = E(k), \tag{34a}$$

$$E(k + 2\pi/a) = E(k). \tag{34b}$$

If we put

$$k = k_r + ik_i, \tag{35}$$

it follows from what is said at the end of § 2 that k_i is equal to zero for allowed energies, while k_r is equal to an integral multiple (including zero) of π/a for forbidden energies.

As mentioned above, we may alternatively utilise (5) in order to derive the expression for $\mu(E)$. We thereby put $z = x_1$ in (5) and express $\psi(x_1)$, $\psi(x_1 + a)$ and $\psi(x_1 - a)$ in terms of phase-integral quantities by means of (19*a*) and (20*a*). We then express $f_1(x_1 \pm a)$ and $f_2(x_1 \pm a)$ in terms of $f_1(x_1)$ and $f_2(x_1)$ by means of (21*a*) with (22). Furthermore, we express the elements of $F(x_1 - a, x_1)$ in terms of those of $F(x_1, x_1 + a)$ by examining the structure of the formulae defining the elements of the F matrix (Fröman and Fröman 1965, equations (3.22*a-d*)), obtaining, because of the periodicity of the potential,

$$F_{11}(x_1 - a, x_1) = F_{22}(x_1, x_1 + a), \tag{36a}$$

$$F_{22}(x_1 - a, x_1) = F_{11}(x_1, x_1 + a), \tag{36b}$$

$$F_{21}(x_1 - a, x_1) = -C^2 F_{12}(x_1, x_1 + a), \tag{36c}$$

$$F_{12}(x_1 - a, x_1) = -(1/C^2) F_{21}(x_1, x_1 + a). \tag{36d}$$

Finally, we arrive in a straightforward way at the expression (28) for $\mu(E)$.

4. Approximate dispersion formula relating k (real or complex) to E (real)

For the quantity $|F_{12}|$ we have the estimate

$$|F_{12}| = (1 + e^{-2K})^{1/2} (1 + e^{-(|K| - K)/2}) O(\mu) + O(\mu^2), \quad (37)$$

where μ is the 'quantity of goodness' for the phase-integral approximations used (Fröman and Fröman 1970, equations (43*b*) and (44)), not to be confused with the quantity $\mu(E)$ considered in the previous section. The quantity μ in (37) is in general smaller the higher the order of the phase-integral approximation used (up to a certain optimal order).

The quantity σ , which is defined by (31), is of importance for energies near the top of the barrier. For the phase-integral approximation of order $2N + 1$, we have the approximate formula (Fröman *et al* 1972)

$$\sigma = \sum_{n=0}^N \sigma^{(2n+1)}, \quad (38)$$

with

$$\sigma^{(1)} = \frac{1}{2} [-\arg \Gamma(\frac{1}{2} + iK/\pi) + (K/\pi) \ln |K^{(1)}/\pi| - K^{(1)}/\pi], \quad (39a)$$

$$\sigma^{(3)} = \frac{1}{2} \frac{1}{24 K^{(1)}/\pi}, \quad (39b)$$

$$\sigma^{(5)} = \frac{1}{2} \left(\frac{7}{2880 (K^{(1)}/\pi)^3} - \frac{K^{(3)}/\pi}{24 (K^{(1)}/\pi)^2} + \frac{(K^{(3)}/\pi)^2}{2 K^{(1)}/\pi} \right), \quad (39c)$$

where K is the quantity defined by (23), pertaining to the actual order $2N + 1$ of the approximation being used, while $K^{(1)}$ and $K^{(3)}$ represent the first- and third-order contributions to K respectively. The formula (38) with (39*a-c*), the derivation of which will be presented in a forthcoming publication by Fröman and Fröman, approximates σ very satisfactorily for energies in the neighbourhood of the top of the barrier where σ is of decisive importance. The formula is less good for energies far away from the top, but this is no serious deficiency, since σ is then very small and may conveniently be omitted. In fact, if the energy is far below or far above the top of the barrier, somewhat improved results may be obtained by omitting σ instead of using the approximate expressions for σ given above (cf the comments on table 2 in § 6).

With the error terms in the estimate (37) for $|F_{12}|$ omitted, we obtain from (33) the following approximate dispersion formula, determining the relation between k (real or complex) and E (real):

$$\cos(ka) = (1 + e^{2K})^{1/2} \cos(L - 2\sigma), \quad (40)$$

where K and L are given by (23) and (24*a, b*) respectively, and σ is given by (38) and (39*a-c*). It may be worth emphasising that the formula (40) is valid for allowed and forbidden energies below and above the top of the barrier, as well as in the important intermediate-energy range near the top of the barrier, where neither the tight-binding model nor the nearly-free-electron model is adequate. We recall that σ is of decisive importance for energies in the neighbourhood of the top of the barrier, in which region the approximate expression (38) with (39*a-c*) is very accurate.

In particular, for the band edges we have, according to (40),

$$\cos(L - 2\sigma) = \pm(1 + e^{2K})^{-1/2}. \tag{41}$$

Thus the energies at the band edges satisfy

$$L - 2\sigma = (\nu - 1)\pi + \tan^{-1} e^K = (\nu - \frac{1}{2})\pi - \tan^{-1} e^{-K}, \text{ lower edge of } \nu\text{th band,} \tag{41a}$$

and

$$L - 2\sigma = \nu\pi - \tan^{-1} e^K = (\nu - \frac{1}{2})\pi + \tan^{-1} e^{-K}, \text{ upper edge of } \nu\text{th band,} \tag{41b}$$

where $0 < \tan^{-1} e^{\pm K} < \pi/2$, and ν is a positive integer. Thus the ν th band comprises energies between those satisfying

$$L - 2\sigma = (\nu - \frac{1}{2})\pi \mp \tan^{-1} e^{-K}, \quad \nu = 1, 2, \dots, \tag{42a}$$

while the ν th gap, which corresponds to energies between the upper edge of the ν th band and the lower edge of the $(\nu + 1)$ th band, comprises energies between those satisfying

$$L - 2\sigma = \nu\pi \mp \tan^{-1} e^K, \quad \nu = 1, 2, \dots \tag{42b}$$

When the energy is far below the top of the barrier, we have $e^{2K} \gg 1$, and σ is very small (and may possibly be omitted). We realise from (42a) that the energy bands are very narrow, the centre of the ν th band being conveniently defined by the condition

$$L - 2\sigma = (\nu - \frac{1}{2})\pi, \quad \nu = 1, 2, \dots \tag{43}$$

We realise that this relation, as is to be expected, determines the quasi-stationary energy levels in the wells of the periodic potential.

When the energy is far above the top of the barrier, we have $e^{2K} \ll 1$, and also in this case σ is very small (and may possibly be omitted). The allowed energy bands become broad and are separated by narrow gaps of forbidden energies, the centres of which, as is seen from (42b), may be defined by the condition

$$L - 2\sigma = \nu\pi, \quad \nu \text{ positive integers.} \tag{44}$$

If the first-order expression for L with $V_{\text{mod}}(z) = V(z)$, i.e. with $Q_{\text{mod}}(z) = Q(z)$, is used, and if σ is neglected, formula (44) becomes simply

$$\int_x^{x+a} \left(\frac{2m}{\hbar^2} (E - V(x)) \right)^{1/2} dx = \nu\pi. \tag{45}$$

This formula agrees with the formula for the centres of the energy gaps lying far above the barrier top given by Dykhne (1961); see also a paper by Richardson (1971).

In connection with formulae (43)–(45), we would like to emphasise that the accurate determination of the position of a narrow band or a narrow gap, to within a few half-widths or so, is a very delicate problem, which in general requires the use of phase-integral approximations of a rather high order; otherwise the result may correspond to a displacement by a great number (several powers of 10) of half-widths (see Fröman and Fröman 1970, pp 620–1. Drukarev *et al* 1979, p 184).

When a band or a gap, as the case may be, is sufficiently narrow, we can expand $L - 2\sigma$ around the energy corresponding to the centre of the band or of the gap,

respectively, obtaining from (42a, b)

$$[\partial(L - 2\sigma)/\partial E]\Delta E \approx 2 \tan^{-1} e^{\mp K} \approx 2 e^{\mp K}, \quad (46)$$

where ΔE is the width of the band (upper sign) or of the gap (lower sign), respectively. The energy derivative $\partial L/\partial E$ can, for phase-integral approximations of arbitrary order, be obtained in a simple form (Fröman 1974, equation (6)). However, in view of the approximations made to obtain (46), the first-order expression may suffice for determining the width, and in that approximation formula (46) yields

$$\Delta E \approx 2\hbar e^{\mp K}/(T - 2\hbar\partial\sigma/\partial E), \quad (47)$$

where, for a sub-barrier band, we have, according to (24a) with $q(z) = Q_{\text{mod}}(z)$,

$$T = \hbar \frac{\partial L}{\partial E} = \frac{m}{\hbar} \int_{t_0}^{t_1} \frac{dx}{Q_{\text{mod}}(x)}, \quad (47a)$$

while, for a super-barrier gap, we have, according to (24b) with $q(x) = Q_{\text{mod}}(x)$,

$$T = \hbar \frac{\partial L}{\partial E} = \frac{m}{\hbar} \int_x^{x+a} \frac{dx'}{Q_{\text{mod}}(x')}. \quad (47b)$$

The quantity $\partial\sigma/\partial E$ is obtained approximately by differentiating (39a) with K put equal to $K^{(1)}$. The resulting expression is given explicitly in the paper by Drukarev *et al* (1979). According to (47a), the quantity T is, in the sub-barrier case, the classical time a particle would need to travel across the well from t_0 to t_1 . (It should be noticed that in decay problems one usually introduces the classical time for a whole oscillation in the well, i.e. twice the quantity (47a) (cf Drukarev *et al* 1979).) In the super-barrier case, the quantity T is, according to (47b), the time a particle would need to travel one whole period in the potential $V_{\text{mod}}(z)$. For the first-order approximation now under consideration, the quantity σ is equal to $\sigma^{(1)}$, which is approximately given by (39a) when the energy lies in the neighbourhood of the top of the barrier. In view of the expansion made to obtain (47), we cannot expect this formula to be very accurate unless the band or the gap is narrow. However, we may still use the formula for energies close to the top of the barrier, and we then realise that, when the energy approaches the top of the barrier, T and $\partial\sigma/\partial E$ tend to infinity, while the difference $T - 2\hbar\partial\sigma/\partial E$ tends to a finite value. This demonstrates the decisive importance of retaining the quantity σ for energies near the top of the barrier; see also the discussion in the paper by Drukarev *et al* (1979). If we delete the term $2\hbar\partial\sigma/\partial E$ in the denominator of (47) and put $V_{\text{mod}} = V$, formula (47) with (47b) becomes the same as a formula given by Dykhne (1961) for the case of a narrow gap.

For super-barrier energies, reflections are in our treatment accounted for by taking the complex transition points properly into account, from which the appearance of the quantity e^{2K} in formula (40) derives. For the energy gaps, reflections are important even for energies far above the top of the barrier. Hence the quantity e^{2K} in (40), although small, remains important and gives rise to the decisive factor e^K in the formula (47) for the width of a gap. However, for energies in the *interior* of an energy band far above the top of the barrier, reflections are negligible, and each one of the phase-integral functions $f_1(x)$ and $f_2(x)$ represents an approximate wavefunction along the whole real axis. Thus, for the special situation of energies in the interior of a band far above the top of the barrier, we can represent $\psi(x)$ by either (12a) or (12b), choosing

$q(x)$ to be positive and imagining for the moment that the cuts crossing the real axis have been removed. Using (4a) and recalling (24b), we then obtain

$$\begin{aligned}\lambda &= \psi(x+a)/\psi(x) \\ &= q^{-1/2}(x+a) \exp\left(\pm i \int^{x+a} q(x') dx'\right) / q^{-1/2}(x) \exp\left(\pm i \int^x q(x') dx'\right) \\ &= \exp\left(\pm i \int_x^{x+a} q(x') dx'\right) \\ &= e^{\pm iL},\end{aligned}\tag{48}$$

where the alternative signs in the exponent correspond to the two possible directions of propagation of the Bloch waves. From (8) and (48) we obtain the dispersion formula

$$ka = \pm L,\tag{49}$$

which it may possibly be advantageous to use instead of (40) in the interior of high-energy bands, i.e. when L is not close to an integer multiple of π (cf (42b)). Obviously, the use of (49) instead of (40) is equivalent to neglecting both σ and e^{2K} in (40). Recalling that the quantities σ and e^{2K} decrease with increasing energy, we may thus consider (49) as a limiting case of (40), appropriate for the interior of high-energy bands and possibly sometimes more accurate than (40) in that situation. Both formulae are, however, very accurate for the interior of a high-energy band, especially when higher-order approximations are used, and in practice it may not be important to know whether the use of (49) would yield greater accuracy than the use of the general formula (40).

5. On the choice of $V_{\text{mod}}(z)$

The arbitrary-order phase-integral approximations, described at the beginning of § 3, were originally derived in unmodified form (Fröman 1966, 1970), i.e. with $Q_{\text{mod}}(z) = Q(z)$. Later the problem of consistent modification in any order was solved (Fröman and Fröman 1974a,b pp 126–31). As displayed in our formulae (12)–(18), the unmodified case presents itself as a special case of the general formulae. By using a convenient modification with $Q_{\text{mod}}(z) \neq Q(z)$, one may, for instance, achieve the result that the phase-integral approximations become good at certain singular points where the unmodified approximations would fail, or one may achieve improvements in accuracy in other respects, e.g. in the respect that, with increasing order, the modified phase-integral approximations tend faster than the unmodified ones towards the optimal result. Because of the flexibility yielded by the procedure of consistent modification, it may even be possible to apply the phase-integral method in situations where the parameters of the problems are such that with unmodified approximations it would not be useful at all (see table 4).

In the present problem $Q^2(z)$ has no singular points on the real axis, and hence, from that point of view, the unmodified phase-integral approximations are useful, apart from in the neighbourhood of transition points. Thus it is very natural to choose $Q_{\text{mod}}(z) = Q(z)$, i.e. $V_{\text{mod}}(z) = V(z)$. If the condition for the usefulness of the first-order phase-integral approximation, i.e. the usual JWKB approximation, is fulfilled (Fröman

and Fröman 1965, equations (2.3)–(2.5)), the higher-order phase-integral approximations can be expected to yield very accurate results. If, however, the parameters of the problem are unfavourable for the usefulness of the unmodified phase-integral approximations, we may, above the top of the barrier, obtain useful approximations by choosing as the modified potential the function W introduced by Floyd (1976) in a first-order JWKB treatment. We remark, however, that Floyd's assertion in connection with the motivation for his treatment—that phase-integral approximations have the deficiency of ignoring the effects of reflections and hence the existence of band gaps in energy—when applied to an electron with sufficient energy to preclude the existence of classical turning points, is irrelevant, as our present paper demonstrates explicitly. Within our framework the derivation of the modified potential obtained by Floyd proceeds as follows. If, in the differential equation (1), one puts

$$\psi = Q_{\text{mod}}^{-1/2} \exp\left(\pm i \int^z Q_{\text{mod}} dz\right), \quad (50)$$

it is found that Q_{mod}^2 satisfies the differential equation

$$Q^2 = Q_{\text{mod}}^2 - \frac{1}{16Q_{\text{mod}}^4} \left[5 \left(\frac{d}{dz} Q_{\text{mod}}^2 \right)^2 - 4 Q_{\text{mod}}^2 \frac{d^2}{dz^2} Q_{\text{mod}}^2 \right], \quad (51)$$

which is the same as equation (3.6) with (3.5a) in the work by Fröman and Fröman (1965), though in the latter work the notation q^2 replaces Q_{mod}^2 in (51). Inserting expressions (2) and (14) for Q^2 and Q_{mod}^2 respectively into (51), and assuming that $|V_{\text{mod}}(z)/E| \ll 1$, we may linearise the resulting equation, obtaining

$$(\hbar^2/8mE)V''_{\text{mod}} + V_{\text{mod}} = V, \quad (52)$$

where the double prime denotes differentiation with respect to z . Formula (52) is identical with Floyd's (1976) equation (8) satisfied by W . From (52) it follows that $V_{\text{mod}} \rightarrow V$ as $E \rightarrow \infty$. For sufficiently high energies we can therefore replace V''_{mod} by V'' in (52), obtaining

$$V_{\text{mod}}(z) = V(z) - (\hbar^2/8mE)V''(z). \quad (53)$$

This expression for V_{mod} can also be obtained in the following alternative way from the unmodified third-order expression for $q(z)$. Assuming that $|V(z)/E| \ll 1$, we may expand the square of our unmodified third-order expression for $q(z)$, given by (13), (14) with $V_{\text{mod}} = V$, (15a, b) and (16), retaining only linear terms in V/E . In this way we obtain

$$q^2 = [Q(1 + \frac{1}{2}\epsilon_0)]^2 \approx Q^2(1 + \epsilon_0) \approx \frac{2m}{\hbar^2} \left(E - V + \frac{\hbar^2}{8mE} V'' \right). \quad (54)$$

Choosing now $Q_{\text{mod}}^2(z)$ to be equal to the last member of (54) and recalling (14), we arrive at the expression (53) for $V_{\text{mod}}(z)$.

6. Numerical results for the Mathieu potential

The results obtained by the analysis of the barrier transmission problem (Fröman and Fröman 1970), on which the treatment in the present paper is based, have proved to be extremely accurate for energies both below and above, as well as close to the top of, the

barrier, especially when higher-order phase-integral approximations are used (Karls-son 1975, Lundborg 1977), and our main result, formula (40), as well as the formulae derived therefrom, is therefore expected to be very accurate. For the *interior* of a high-energy band, the alternative dispersion relation (49) is also expected to yield very accurate results. Since it is worthwhile to illustrate the accuracy quantitatively, numerical results obtained by the application to the Mathieu potential will be compared with available tabulated results (National Bureau of Standards (NBS) 1967, McLachlan 1964, Floyd 1976).

We write the Mathieu equation in the form (1) with

$$Q^2(z) = A - 2B \cos(2z), \quad (55)$$

which, according to (2), means that

$$(2m/\hbar^2)E = A, \quad (56a)$$

$$(2m/\hbar^2)V(z) = 2B \cos(2z), \quad (56b)$$

with the period equal to π . The notations used in McLachlan's book correspond to $Q^2(z) = a - 2q \cos(2z)$, and those used in the NBS tables correspond to $Q^2(z) = a - \frac{1}{2}s \cos(2z)$. The lower and the upper edge of the ν th band, $\nu = 1, 2, \dots$, will be denoted by $a_{\nu-1}$ and b_ν respectively, in accordance with the notation in table 25 on p 371 in McLachlan's book. The values given in the NBS tables denoted by $be_{\nu-1}$ and bo_ν correspond to $a_{\nu-1} + 2B$ and $b_\nu + 2B$ respectively. With the aid of the NBS tables, the values of $a_{\nu-1}$ and b_ν are obtained with one more figure than given by McLachlan.

As mentioned in § 5, under semi-classical conditions it is most natural to use unmodified phase-integral approximations, i.e. to choose

$$(2m/\hbar^2)V_{\text{mod}}(z) = (2m/\hbar^2)V(z) = 2B \cos(2z). \quad (57)$$

As concerns the modifications discussed in § 5, we obtain, by choosing $V_{\text{mod}}(z)$ as a solution of (52),

$$(2m/\hbar^2)V_{\text{mod}}(z) = (1 - 1/A)^{-1} 2B \cos(2z), \quad (58)$$

while from (53) and (56a, b) we obtain

$$(2m/\hbar^2)V_{\text{mod}}(z) = (1 + 1/A) 2B \cos(2z). \quad (59)$$

If $|1/A| \ll 1$, the modifications (58) and (59) differ only with respect to terms involving higher powers of $1/A$, and hence they are then expected to yield essentially the same result. However, if semi-classical conditions are violated, the modification (58) may still be useful, while the modification (59) cannot be used.

Table 1 shows, as an illustrative example of the approach towards a very accurate result of the successive orders of approximation, the values for the upper edge of the 8th band, pertaining to the Mathieu potential with $B = 1$, calculated from (41b) with $V_{\text{mod}}(z) = V(z)$ and with σ neglected. The figures given in the 13th-order approximation may be expected to be correct, apart from a couple of units in the last figure.

The results for band edges displayed in table 2 demonstrate the importance of including σ for energies in the neighbourhood of the top of the barrier, i.e. for energies in the neighbourhood of $A = 8$, since B was chosen to be equal to 4. With σ included, accurate values of the band edges are obtained from (41a, b) for all energies. We also note that, for the bands close to the top of the barrier, i.e. the 3rd band and the lower part of the 4th band, the inclusion of σ is essential for obtaining accurate values, while

Table 1. $B = 1$, $V_{\text{mod}}(z) = V(z)$. Upper edge b_8 of the 8th energy band calculated from (41b) to illustrate the approach of the phase-integral results towards a very high degree of accuracy. The value obtained from the NBS tables, $b_8 = bo_8 - 2B = bo_8 - 2$, is also given.

Order of approximation	Band edge b_8 obtained from (41b) with σ neglected
1	64·0078
3	64·007 935
5	64·007 937 16
7	64·007 937 1887
9	64·007 937 189 24
11	64·007 937 189 251 5
13	64·007 937 189 251 7

Value obtained from the NBS tables: 64·007 937 19

Table 2. $B = 4$, $V_{\text{mod}}(z) = V(z)$. Band edges $a_{\nu-1}$ and b_ν of the ν th band calculated from (41a, b) in the 5th-order approximation with σ included as well as with σ neglected. The values obtained from the NBS tables, $a_{\nu-1} = be_{\nu-1} - 2B = be_{\nu-1} - 8$ and $b_\nu = bo_\nu - 2B = bo_\nu - 8$, are also given.

Band edge	Values obtained from the NBS tables	Results obtained from (41a, b) in the 5th-order approximation	
		σ included	σ neglected
a_0	-4·280 518 82	-4·2798	-4·2802
b_1	-4·259 182 90	-4·2587	-4·259 06
a_1	2·318 008 17	2·318 07	2·321
b_2	2·746 88103	2·746 895	2·750
a_2	6·829 074 84	6·829 10	6·4
Top of barrier = 8			
b_3	9·261 446 10	9·261 4457	9·8
a_3	10·671 027 10	10·671 034	10·8
b_4	16·452 035 29	16·452 034	16·450
a_4	16·649 818 91	16·649 8179	16·648
b_5	25·330 544 87	25·330 5441	25·330 45
a_5	25·343 757 63	25·343 7569	25·343 66
b_3	36·229 411 42	36·229 4111	36·229 4011
a_6	36·229 952 51	36·229 9522	36·229 9422
b_7	49·167 067 63	49·167 0675	49·167 065
a_7	40·167 082 82	49·167 0827	49·167 080 68
b_8	64·127 159 14	64·127 159 10	64·127 158 52

by neglecting σ the tabulated results are somewhat improved only for the lowest-energy band. Neglecting σ would possibly yield somewhat improved results for still higher energies than those tabulated in table 2.

Table 3 shows results obtained by using formulae (41a, b), still with $V_{\text{mod}}(z) = V(z)$, for the calculation of band edges $a_{\nu-1}$ and b_ν , pertaining to the Mathieu potential with $B = 1$. For the higher bands the band edges obtained from (41a, b) are given in table 3

Table 3. $B = 1$, $V_{\text{mod}}(z) = V(z)$. Band edges $a_{\nu-1}$ and b_{ν} of the ν th band calculated from (41a, b). The values obtained from the NBS tables, $a_{\nu-1} = be_{\nu-1} - 2B = be_{\nu-1} - 2$ and $b_{\nu} = bo_{\nu} - 2B = bo_{\nu} - 2$, are also given.

Band edge	Values obtained from the NBS tables	Values calculated from (41a, b)	
a_0	-0.455 138 60	-0.450	} band width = 0.34 } band gap = 1.75
b_1	-0.110 248 82	-0.1108	
a_1	1.859 108 07	1.859 4	
		Top of barrier = 2	} 5th-order approximation, σ included
b_2	3.917 024 77	3.916 99	
a_2	4.371 300 98	4.371 297	
b_3	9.047 739 26	9.047 734	
a_3	9.078 368 85	9.078 364	
b_4	16.032 970 08	16.032 970 03	
a_4	16.033 832 34	16.033 832 29	
b_5	25.020 840 82	25.020 840 823	
a_5	25.020 854 34	25.020 854 345	
b_6	36.014 289 91	36.014 289 897 87	
a_6	36.014 290 05	36.014 290 058 79	
b_7	49.010 418 25	49.010 418 249 894	
a_7	49.010 418 25	49.010 418 249 894	
b_8	64.007 937 19	64.007 937 189 251 7	

with more figures than the NBS values quoted. The reason is that, by studying the results obtained from (41a, b) in successive orders of the phase-integral approximations (cf table 1), one may judge the accuracy, and on this basis all the figures in the 13th-order approximation given in table 3 may be expected to be correct, apart from a few units in the last figure.

Table 4 illustrates a situation where semi-classical conditions do not prevail, and the parameters are thus quite unfavourable for the use of unmodified phase-integral approximations. In fact, the ratio of the local de Broglie wavelength $2\pi/Q$ and the period π of the potential varies between limits of approximately 5 and 12. Neither is the modification (59) useful, since at the extrema of the potential we have $|V/E| \approx 0.7$, and thus the condition $|V/E| \ll 1$ is not fulfilled for all values z . However, for the modification (58) we have $|V_{\text{mod}}/E| \leq 2B/|A - 1| \approx 0.07$, and hence the condition

Table 4. $B = 0.03$. Values of A for $k = 0.3$ (in the interior of the 1st band) obtained in successive orders of approximation from (49) with the use of the modification (58). The value calculated numerically by Floyd (1976) is quoted for comparison.

Order of approximation	Values of A obtained from (49) $V_{\text{mod}}(z) = (1 - 1/A)^{-1} V(z)$
1	0.0900
3	0.089 505 505
5	0.089 540
7	0.0910
Numerically calculated value (Floyd 1976): 0.089 505 558 48	

$|V_{\text{mod}}/E| \ll 1$ is fulfilled for all values of z . Thus the modification (58) is expected to be useful. In table 4 we give values of A obtained from (49) in successive orders of phase-integral approximations for the value $k = 0.3$ in the interior of the first band. We should note that, when specialised to the first-order approximation, and with the notation $V_{\text{mod}}(z)$ in (14) replaced by $W(z)$, formula (49) becomes the same as a formula given by Floyd (1976, equation (12)), and hence the *first-order* result in our table 4 is the same as that obtained by Floyd. The value calculated numerically by Floyd (1976) is also quoted for comparison.

In table 5 the application of unmodified phase-integral approximations (cf (57)), as well as phase-integral approximations modified according to (58) and (59), is illustrated for a situation where these modifications are expected to be almost equivalent. The values of A for $k = 5.5$ in the interior of the 6th band, pertaining to the Mathieu potential with $B = 1$, were calculated from (49) in various orders of approximation. The use of (58) or (59) is seen to yield essentially the same results. Furthermore, it is confirmed that a faster approach towards a very accurate value is achieved when those modifications are used than when $V_{\text{mod}}(z) = V(z)$. We remark that here A is large enough that (49) yields almost the same result as (40) with σ neglected.

Table 5. $B = 1$. Values of A for $k = 5.5$ (in the interior of the 6th band), obtained from (49) with the use of the expressions (57), (58) and (59) respectively for $V_{\text{mod}}(z)$, are given in various orders of the phase-integral approximations used. The value calculated numerically by Floyd (1976) is also quoted.

Order of approximation	Values of A obtained from (49)		
	$V_{\text{mod}}(z) = V(z)$	$V_{\text{mod}}(z) = (1 - 1/A)^{-1} V(z)$	$V_{\text{mod}}(z) = (1 + 1/A) V(z)$
1	30.2665	30.267 68	30.267 65
3	30.267 08	30.267 101 42	30.267 101 40
5	30.267 1009	30.267 101 540	30.267 101 539
7	30.267 101 53	30.267 101 5559	30.267 101 5557
9	30.267 101 5568	30.267 101 558 00	30.267 101 557 99
11	30.267 101 558 21	30.267 101 558 315	30.267 101 558 313
13	30.267 101 558 35	30.267 101 558 365	30.267 101 558 364

Numerically calculated value (Floyd 1976): 30.267 101 56

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