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1981 J. Phys. A: Math. Gen. 14 1513

(http://iopscience.iop.org/0305-4470/14/6/025)

J. Phys. A: Math. Gen. 14 (1981) 1513–1518. Printed in Great Britain

Asymptotic expressions for the widths of low-lying energy bands in one-dimensional periodical potentials

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Received 15 September 1980

Abstract. The motion of a quantum particle in a one-dimensional, slowly varying periodical potential is considered. By using the comparison equation method, the asymptotic expression for exponentially small bandwidths of the low-lying energy bands is obtained. In the special case of a sinusoidal potential (corresponding to the Mathieu differential equation), the general formula reduces to an already existing result. Potentials, symmetrical and non-symmetrical, within the elementary period are discussed.

1. Introduction

One-dimensional models have been used many times in the past, at least for the qualitative description of the motion of a particle in a periodical field. Besides the calculations of the band structure (Kronig and Penney 1931), such models were used when treating more complicated phenomena such as surface states (Davison and Levine 1970), tunnelling transitions in solids (Burstein and Lundqvist 1969) and so on. One of the most simple methods for band structure calculations is the WKB approximation (Brillouin 1950, Balazs 1969). It is usually assumed that the WKB method applies only in the case of high-lying bands. Nevertheless, with the help of the comparison equation method, one can derive the asymptotic expansions for the widths of low-lying bands. The large parameter in the theory is defined by the slowness of the variation of the potential with respect to the characteristic scale.

In the present work we derive the asymptotic formulae for the width and the position of the low-lying bands in a periodical, slowly varying potential. It is also assumed that the overlapping of the wavefunctions corresponding to neighbouring cells is small. Section 2 contains the formulation of the problem and the derivation of general formulae defining the spectra. In §3 the asymptotic expressions for the wavefunctions and the bandwidths are derived for the case of a symmetrical potential.

Section 4 contains the bandwidth calculations in the case of a non-symmetrical potential, and a concluding discussion. The bandwidths are exponentially small with respect to the large parameter. The greater part of the calculations has a formal character, but the final results can be rigorously justified, at least in the symmetrical case, by using the method proposed by Alenitzyn (1981). We also mention here the work of Kuni and Storonkin (1977) where derivations similar to ours were performed for the diffusion problem.

2. Formulation of the problem and derivation of spectral equations

We shall study the band structure of the one-dimensional Schrödinger equation

$$u''(x)+(h\lambda-h^2q(x))u(x)=0 \tag{2.1}$$

where h is the large parameter ($h \gg 1$) and λ is the spectral parameter, such that for the low-lying bands one has $\lambda = 0(1)$. With respect to the potential $q(x)$ we make the following assumptions: (i) $q(x)$ is a periodical function with the period $2e$ ($q(x+2e)=q(x)$), (ii) $q(x)$ is regular at the real axis (to obtain the leading term of the asymptotic expansion it is sufficient to assume that $q(x)$ is twice continuously differentiable), (iii) $q(x)\geqslant 0$ and $q(x)=0$ only for $x=0$ on $[-e, e]$, (iv) $q'(0)=0$. Hereafter we call the potential that satisfies (v) $q(x)=q(-x)$ symmetrical. It is also convenient to introduce the function $p(x)$: $q(x)=p^2(x)$; $p(-e)<0$, $p(e)>0$.

It is well known that the allowed bands are the intervals $[\lambda_0^p, \lambda_0^a]$, $[\lambda_1^a, \lambda_1^p]$, $[\lambda_2^p, \lambda_2^a], \ldots$ where λ_n^p are the eigenvalues of the periodical boundary problem

$$u(-e)=u(e), \qquad u'(-e)=u'(-e) \tag{2.2}$$

and λ_n^a are the eigenvalues of the antiperiodical boundary problem

$$u(-e)=-u(e), \qquad u'(-e)=-u'(-e) \tag{2.3}$$

for equation (2.1).

We introduce two linearly independent solutions of equation (2.1): $u_1(\lambda, x)$ and $u_2(\lambda, x)$. For the case of the symmetrical potential we choose $u_2(\lambda, x)\equiv u_1(\lambda, -x)$. Expanding the eigenfunctions $u_n^{p,a}(x)$ of the periodical and antiperiodical problems (2.1), (2.2), (2.3) in terms of the basis functions

$$u_n^{p,a}(x)=A^{p,a}u_1(\lambda, x)+B^{p,a}u_2(\lambda, x)$$

we obtain from boundary conditions (2.2) and (2.3) the spectral equation for the determination of eigenvalues $\lambda_n^{p,a}$

$$\begin{aligned}&[u_1(\lambda, -e)u_2'(\lambda, e)+u_1(\lambda, e)u_2'(\lambda, -e)]\\ &\qquad -[u_2(\lambda, -e)u_1'(\lambda, e)+u_2(\lambda, e)u_1'(\lambda, -e)]=\pm 2W(u_1, u_2)\end{aligned} \tag{2.4}$$

where $W(u_1, u_2)\equiv u_1u_2'-u_1'u_2$ is the Wronsky determinant of the solutions $u_1(\lambda, x)$ and $u_2(\lambda, x)$; the signs + and − correspond to the periodical and antiperiodical problems, respectively. In the case of the symmetrical potential, equation (2.4) can be factorised

$$[u_1(\lambda, e)\pm u_1(\lambda, -e)][u_1'(\lambda, e)\pm u_1'(\lambda, -e)]=0. \tag{2.5}$$

Consider the auxiliary boundary problem

$$\begin{aligned}&\tilde{u}(x)+(h\lambda-h^2\tilde{q}(x))\tilde{u}(x)=0\\ &\tilde{u}(x)\to 0\\ &x\to\pm\infty\end{aligned} \tag{2.6}$$

where $\tilde{q}(x)$ is equal to $q(x)$ on $[-e, e]$, and outside that interval is smoothly continued in such a way that $\tilde{q}(x)\to+\infty$ when $x\to\pm\infty$. It was shown by one of the authors (Slavyanov 1969) that the asymptotic expansion of the eigenvalues $\tilde{\lambda}_n(h)$, when $h\to+\infty$, of the boundary problem (2.6), is determined by the local behaviour of the potential $\tilde{q}(x) \equiv p^2(x)$ in the vicinity of $x = 0$. Let the following expansion hold:

$$p(x) = \sum_{k=0}^{\infty} p_k x^{k+1}, \qquad p_k \equiv \frac{p^{(k+1)}(0)}{(k+1)!}, \qquad k \geqslant 1 \quad p_0 = 1;$$

then $\tilde{\lambda}_n \sim \Sigma_{k=0}^{\infty} Q_{k+1}(\mu_n) h^{-k}$, where $\mu_n = 2n+1$ $(n = 0, 1, 2, \ldots)$ and $Q_{k+1}(\mu_n)$ are polynomials of degree $k+1$ with the coefficients depending on $p_{2k}, p_{2k-1}, \ldots, p_0$. The first three terms of the asymptotic expansion are

$$\tilde{\lambda}_n = \mu_n + h^{-1}[\mu_n^2(\tfrac{3}{4}p_2 - \tfrac{3}{2}p_1^2) + (\tfrac{3}{4}p_2 - \tfrac{1}{2}p_1^2)] + h^{-2}[\mu_n^3(\tfrac{5}{8}p_4 - \tfrac{15}{4}p_3p_1 - \tfrac{3}{4}p_2^2 + \tfrac{69}{8}p_2p_1^2 - \tfrac{17}{4}p_1^4)$$
$$+ \mu_n(\tfrac{25}{8}p_4 - \tfrac{35}{4}p_3p_1 - \tfrac{21}{8}p_2^2 + \tfrac{101}{8}p_2p_1^2 - \tfrac{19}{4}p_1^4)] + \ldots. \tag{2.7}$$

When $\lambda = \tilde{\lambda}_n$, besides the eigenfunction $\tilde{u}_n(x)$ we introduce the second solution $\tilde{u}_n^{(2)}(x)$ exponentially increasing as $x \to \pm\infty$, so that the Wronskian $W(\tilde{u}_n(x), \tilde{u}_n^{(2)}(x)) = 2h$. When λ has arbitrary values we introduce the solution $\tilde{u}_1(\lambda, x)$ with the property: $\tilde{u}_1(\lambda, x) \to \tilde{u}_n(x)$ when $\lambda \to \tilde{\lambda}_n$. The function $\tilde{u}_1(\lambda, x)$ is a solution of the integral equation

$$\tilde{u}_1(\lambda, x) = \tilde{u}_n(x) + \frac{\delta}{2h} \int_{-\infty}^{x} (\tilde{u}_n(x)\tilde{u}_n^{(2)}(\xi) - \tilde{u}_n(\xi)\tilde{u}_n^{(2)}(x))\tilde{u}_1(\lambda, \xi)\, \mathrm{d}\xi$$

where $\delta = \lambda - \tilde{\lambda}_n$. Assume $\delta \ll 1$, then the first iteration of the above integral equation gives

$$\tilde{u}_1(\lambda, x) = \tilde{u}_n(x) + \frac{\delta}{2h} \int_{-\infty}^{x} (\tilde{u}_n(x)\tilde{u}_n^{(2)}(\xi) - \tilde{u}_n(\xi)u_n^{(2)}(x))\tilde{u}_n(\xi)\, \mathrm{d}\xi + \mathrm{O}(\delta^2).$$

When x is large $(x \gg 1, x \sim -\ln \delta)$, we find

$$\tilde{u}_1(\lambda, x) = \tilde{u}_n(x)(1 + \mathrm{O}(\delta)) - \frac{\delta N}{2h} \tilde{u}_n^{(2)}(x)(1 + \mathrm{O}(\delta^2)) \tag{2.8}$$

where N is the normalisation integral

$$N = \int_{-\infty}^{+\infty} \tilde{u}_n^2(x)\, \mathrm{d}x.$$

Equations (2.1) and (2.6) are identical on $[-e, e]$, consequently we choose the solution $u_1(\lambda, x)$ identical to $\tilde{u}_1(\lambda, x)$ on that interval. For the symmetrical potential we can assume that $\tilde{u}_n(-x) = (-1)^n \tilde{u}_n(x)$. Then the dispersion equation (2.5) becomes

$$\left(\tilde{u}_n(e)[\pm 1 + (-1)^n] \mp \frac{\delta N}{2h} \tilde{u}_n^{(2)}(e)\right) = 0$$

$$\left(\tilde{u}'_n(e)[\pm 1 + (-1)^n] \mp \frac{\delta N}{2h} \tilde{u}_n^{(2)\prime}(e)\right) = 0$$

where δ is $\lambda_n^p - \tilde{\lambda}_n$ or $\lambda_n^a - \tilde{\lambda}_n$. It is easy to show that at least in the first approximation with respect to h we have: $\tilde{u}_n(e)/\tilde{u}_n^{(2)} = \tilde{u}'_n(e)/\tilde{u}_n^{(2)\prime}(e)$. Then from the above dispersion equations we find for $\delta_n^{p,a} \equiv \lambda_n^{p,a} - \tilde{\lambda}_n$

$$\delta_n^{p,a} = \pm \frac{4h}{N} \frac{\tilde{u}_n(e)}{\tilde{u}_n^{(2)}(e)} \tag{2.9}$$

where the negative sign corresponds to the lower and the positive sign to the upper end of the allowed bands. Since the function $\tilde{u}_n(x)$ decreases exponentially and the function $\tilde{u}_n^{(2)}(x)$ increases exponentially in the underbarrier region, the deviations $\delta_n^{p,a}$ are exponentially small quantities with respect to the parameter h.

The band position, defined with the power accuracy with respect to h, is given by expression (2.7), and we assume that $\tilde{\lambda}_n = (\lambda_n^a + \lambda_n^p)/2$.

3. The symmetrical potential and the Mathieu equation

For the construction of the asymptotic expansions of the solutions of equation (2.1) and (2.6) we use the comparison equation method (see e.g. Slavyanov 1969, Cherry 1950). As a comparison equation we choose the Weber equation

$$W''(z) + (h\mu - h^2 z^2) W(z) = 0.$$

The general solution of the above equation can be expressed in terms of parabolic-cylinder functions

$$D_{(\mu-1)/2}(\pm\sqrt{2h}z)$$

(Bateman and Erdelyi 1953). When $\mu = \mu_n = 2n+1$ they transform into the harmonic oscillator eigenfunctions. We try to find the solutions of equation (2.1) and (2.6) in the form

$$u_1(\lambda, x) = (z')^{-1/2} D_{(\mu-1)/2}(-\sqrt{2h}z), \qquad \tilde{u}_n(\lambda, x) = (z')^{-1/2} D_n(-\sqrt{2h}z). \tag{3.1}$$

The function $z(x, h)$, the transformation of the independent variable and the spectral parameter λ, are expanded into the asymptotic series:

$$z(x, h) = \sum_{k=0}^{\infty} z_k(x) h^{-k}, \qquad \lambda = \sum_{k=0}^{\infty} \lambda_k h^{-k}.$$

For the purposes of practical calculations it is convenient to introduce the function

$$y(x, h) = z^2(x, h), \qquad y(x, h) = \sum_{k=0}^{\infty} y_k(x) h^{-k}.$$

Substituting (3.1) into (2.1) we find that $y(x, h)$ satisfies the nonlinear equation

$$\left(\frac{y'^2}{4} - p^2(x)\right) - \frac{1}{h}\left(\frac{\mu y'^2}{4y} - \lambda\right) - \frac{1}{2h^2}\left\{\frac{3}{8}\frac{y'^2}{y^2} + \frac{1}{2}\left[\frac{y''}{y'} - \frac{3}{2}\left(\frac{y''}{y'}\right)^2\right]\right\} = 0$$

which can be solved by an iterative procedure to find the functions $y_k(x)$. The conditions for the existence of smooth solutions yield expansion (2.7). Calculations give

$$y(x) = 2\int_0^x p(x)\,\mathrm{d}x + \frac{\mu}{h}\int_0^x \left(\frac{p(x)}{2\int_0^x p(x)\,\mathrm{d}x} - \frac{1}{p(x)}\right)\mathrm{d}x + \mathrm{O}(h^{-2}). \tag{3.2}$$

Using the asymptotic expansions for large values of the arguments of the parabolic-cylinder functions, from equation (2.5) (or using formula (2.9)) we obtain

$$\delta_n^{p,a} = \mp(-1)^n \frac{2^{n+2}}{\sqrt{\pi}n!} \exp(-hy_0(e))[y_0(e)]^{n+1/2} h^{n+1} \exp(-y_1(e))$$
$$\times\left[1+\frac{1}{h}\left((n+\tfrac{1}{2})\frac{y_1(e)}{y_0(e)} - y_2(e) - \frac{n^2+n\mp(-1)^n}{2y_0(e)}\right.\right.$$
$$\left.\left.+\frac{2y_0(e)y_0''(e)-y_0'(e)}{2y_0(e)[y_0'(e)]^2}\right)+\mathrm{O}(h^{-2})\right]\frac{\partial\tilde{\lambda}_n}{\partial\mu_n}. \tag{3.3}$$

Finally, from equations (2.7) and (3.3) and using the definitions $\Delta_{2k} = \lambda_{2k}^a - \lambda_{2k}^p$, $\Delta_{2k+1} = \lambda_{2k+1}^p - \lambda_{2k+1}^a$, we find the width of the nth band

$$\Delta_n = \frac{2^{n+3}}{\sqrt{\pi}n!}[y_0(e)]^{n+1/2} \exp(-y_1(e)) h^{n+1/2} \exp(-hy_0(e))$$
$$\times\left\{1+\frac{1}{h}\left[(2n+1)\left(\frac{y_1(e)}{2y_0(e)}+\frac{3}{2}p_2-3p_1^2\right)\right.\right.$$
$$\left.\left.-y_2(e)-\frac{n^2+n}{2y_0(e)}+\frac{2y_0(e)y''(e)-y_0'(e)}{2y_0(e)[y_0'(e)]^2}\right]+\mathrm{O}(h^{-2})\right\}. \tag{3.4}$$

As an example, we consider the Mathieu equation for which, in our notation, we have $e=\frac{1}{2}\pi$, $q(x)=\sin^2 x$. Formula (3.2) gives

$$y(x) = 4\sin^2\tfrac{1}{2}x + \frac{\mu}{h}\ln|\cos\tfrac{1}{2}x| + \frac{1}{h^2}\left[\frac{\mu^2}{8}\left(\frac{\ln|\cos\frac{1}{2}x|}{\sin^2\frac{1}{2}x}+1\right) - \frac{\mu^2+3}{32}\tan^2\tfrac{1}{2}x\right] + \mathrm{O}(h^{-3})$$

and from (3.4) we obtain

$$\Delta_n = \frac{2^{3n+4}}{\sqrt{\pi}n!} \mathrm{e}^{-2h} h^{n+1/2}\left(1-\frac{6n^2+14n+7}{8h}+\mathrm{O}(h^{-2})\right). \tag{3.5}$$

This asymptotic expression is in agreement with the result of Meixner and Schäfke (1954). The form of the correcting term in equation (3.5) shows that our approximation is valid under the assumption

$$n^2 \ll h. \tag{3.6}$$

4. The non-symmetrical potential, discussion

In the case of the non-symmetrical potential we introduce the following set of two linearly independent solutions of equation (2.1):

$$u_1(\lambda, x) = (z')^{-1/2} D_{(\mu-1)/2}(-\sqrt{2h}z), \qquad u_2(\lambda, x) = (z')^{-1/2} D_{(\mu-1)/2}(\sqrt{2h}z).$$

The asymptotic expansions of the function $z(x, h)$ and the auxiliary function $y(x, h) = z^2(x, h)$ can be constructed analogously to the preceding case, and formula (3.2) also holds here. Introducing the notations: $\nu = (\mu-1)/2$, $z_\pm^{(k)} = z^{(k)}(\pm e)$,

$\zeta_{\pm}=\sqrt{2h}z_{\pm}$ ($z_{-}<0$, $z_{+}>0$), the dispersion equation (2.4) becomes of the form

$$\begin{aligned}\tfrac{1}{2}(2hz'_{+}z'_{-})^{-1/2}\left(\frac{z''_{+}}{z'_{+}}-\frac{z''_{-}}{z'_{-}}\right)&(D_\nu(\zeta_+)D_\nu(-\zeta_-)-D_\nu(\zeta_-)D_\nu(-\zeta_+))\\ &-\sqrt{z'_{-}/z'_{+}}(D_\nu(-\zeta_+)D'_\nu(\zeta_-)+D_\nu(\zeta_+)D'_\nu(-\zeta_-))\\ &-\sqrt{z'_{+}/z'_{-}}(D_\nu(\zeta_-)D'_\nu(-\zeta_+)+D_\nu(\zeta_-)D'_\nu(\zeta_+))=\pm 2\frac{\sqrt{2\pi}}{\Gamma(-\nu)}.\end{aligned}$$

Using the asymptotic expressions of the parabolic-cylinder functions again and solving the above dispersion equation by iteration we find the leading term of the bandwidth asymptotic expansion:

$$\begin{aligned}\Delta_\lambda^n=\frac{4}{n!}\sqrt{\frac{2}{\pi}}(4h^2y_0(e)y_0(-e))^{(2n+1)/4}\exp[&-\tfrac{1}{2}h(y_0(e)+y_0(-e))\\ &-\tfrac{1}{2}(y_1(e)+y_1(-e))](1+\mathrm{O}(h^{-1})).\end{aligned}\tag{4.1}$$

The position of the band is given as before, by equation (2.7).

The validity criterion of formulae (2.7), (3.3) and (4.1) is given by condition (3.6). This restricts the applicability of the present results to the low-lying bands, where the overlapping of the wavefunctions corresponding to the neighbouring elementary cells is exponentially small. It could happen that the wavefunction has not the explicit asymptotic representation in the vicinity of the origin. In that case in order to use formula (2.9) it is necessary to know only the asymptotic expression of the wavefunction in the underbarrier region, and the normalisation constant N must be calculated numerically.

Within the present approach it is possible to calculate the asymptotic expansions of the more complicated quantities characterising the motion of the particle in a periodical field, for example, the effective mass. Also, the phenomena connected with the deviations due to aperiodical fields can be considered. An interesting effect of the degeneracy of the bands is investigated in the work of Kuni and Storonkin (1977).

The question arises whether the present results could be used for the calculation of the bandwidths of the three-dimensional potentials. This can be done for problems with almost separable variables, where the potential can be considered as spherically symmetric within each elementary cell. In this case, one can introduce the analogues of the functions $\tilde{u}_n$ and $\tilde{u}_n^{(2)}$ and obtain a formula similar to (2.4).

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