Energy splitting in a finite periodic multiple-well potential

Dae-Yup Song

Department of Physics Education, Sunchon National University, Jeonnam 57922, Korea

E-mail: dsong@sunchon.ac.kr

Received 17 April 2017, revised 4 June 2017
Accepted for publication 23 June 2017
Published 14 August 2017

Abstract
The low-lying states for a one-dimensional potential consisting of \( N \) identical wells are considered, assuming that the wells are parabolic around the minima. The \( N \) localized approximate eigenfunctions, each of which matches an eigenfunction of the simple harmonic oscillator in one of the wells, are constructed, relying on the WKB approximation. Diagonalizing the Hamiltonian in the subspace spanned by the approximate eigenfunctions, a formula for the energy eigenvalues is obtained. The present work will be useful for introducing Bloch wave functions in a periodic potential to undergraduate and graduate students. It is shown that the formula for the eigenvalues can reproduce a known rigorous expression on the Mathieu equation.

Keywords: 1D Schrödinger equation, quantum tunnelling, energy splitting, Bloch theorem

(Some figures may appear in colour only in the online journal)

1. Introduction
One of the fundamental aspects of quantum mechanics is that the wave functions should be considered in the entire space. For the system of a particle in a potential which has a parabolic well, while the classical particle released from rest in the well undergoes simple harmonic motion, an eigenfunction of the simple harmonic oscillator cannot, in general, be that of the system—even in the quadratic region of the potential. This global aspect can also be emphasized by considering the energy splitting and the resulting tunnelling dynamics in a symmetric double-well potential [1–5]; if an approximate energy eigenstate localized in one well is assumed in the limit of low probability for barrier penetration, the state localized in the other well can also be obtained, relying on the reflection symmetry of the system, so that the Hamiltonian is represented by a \( 2 \times 2 \) symmetric matrix in the subspace spanned by the two
localized states \([1, 2, 4]\). The eigenstates of the matrix Hamiltonian are then the symmetric and the antisymmetric combinations of the localized states which are not localized in a well any more, implying the tunnelling dynamics for the wave packet initially given as one of the approximate localized eigenfunctions \([2, 3]\). As an extension of the \(N = 2\) double-well potential, it may also be interesting to consider the finite periodic \(N\)-well potential \([1, 6, 7]\) which coincides in a finite domain with the fully periodic potential, consisting of the infinite repetition of the single-well potential. For this potential, we may also construct \(N\) localized states from an approximate eigenstate localized in a well, to find that the Hamiltonian is then represented by an \(N \times N\) matrix in the \(N\)-level approximation.

In this article, we will consider the finite periodic \(N\)-well potential by assuming that the wells are parabolic. Upon the assumption of parabolicity \([4]\), we approximate a localized eigenfunction by that of the simple harmonic oscillator in one of the wells, and by a WKB wave function which matches the eigenfunction of the oscillator in a barrier attached to the well. With the \(N\) approximate eigenfunctions, each of which is localized in a well and the two barriers attached to it, we proceed to evaluate the elements of the tridiagonal Hamiltonian matrix, and then to find the eigenvectors and a formula for the eigenvalues. The resulting eigenfunctions of the \(N\)-well system are largely the linear combinations of the eigenfunctions of the simple harmonic oscillators, which do not depend on the details of the Hamiltonian matrix. Since the WKB approximation is a typical topic in undergraduate quantum mechanics classes (chapter 8 of \([3]\) for example), this \(N\)-level approach will be accessible to undergraduates.

Another approach to this problem is to construct a single eigenfunction in the entire space through wave function matching, as is done for \(N = 2\) \([8]\). From that the eigenfunction, which is exactly described by the parabolic cylinder function in the parabolic wells, should match the WKB functions of the barriers in the overlapping regions, and we arrive at a consistency condition. The consistency condition then gives the same formula for the eigenvalues which the \(N\)-level approach gives. As the parabolic cylinder function and its asymptotic expansions are discussed, and applied to a double-well potential in \([2]\), this approach of constructing a single eigenfunction will be of interest to advanced undergraduate students who are acquainted with the leading order representations of the expansions.

In the following section, the exact wave functions in the wells and the WKB wave functions in the barriers are introduced. In section 3, matching the wave functions in the overlapping asymptotic regions, the linear relations between the coefficients introduced for the wave functions are given, and a formula for the energy eigenvalues is found from the consistency of the relations. In section 4, the formula for the eigenvalues is re-obtained through the \(N\)-level approach. In section 5, the energy eigenvalues of the Bloch wave functions in the low-lying energy bands of the fully periodic system are evaluated by utilizing the localized approximate eigenstates \([1]\), and the widths of the narrow energy bands of the Mathieu equation are calculated.

### 2. Exact solutions and WKB wave functions

We assume the finite periodic \(N\)-well potential \(V(x)\) satisfying \(V(x + a) = V(x)\) with a positive constant \(a\) for \(x_1 \leq x \leq x_1 + (N - 2)a\), while the smooth \(V(x)\) monotonically decreases (increases) for \(x < x_1\) (for \(x > x_1 + (N - 1)a\)) (see figure 1) so that the low-lying energy spectrum is discrete with the square-integrable eigenfunctions. We also assume that \(V(x)\) has a quadratic minima at \(x = x_1 + ja\) \((j = 0, 1, ..., N - 1)\), and thus, in the quadratic region near \(x = x_1 + ja\), the potential is written as
with the particle mass $m$ and angular frequency $\omega$. For the eigenfunction $\psi(x)$ corresponding to the eigenvalues

$$E(\nu) = V_0 + \left(\nu + \frac{1}{2}\right)\hbar\omega,$$

the Schrödinger equation

$$H\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E(\nu)\psi(x)$$

is then written in the quadratic region near $x = x_1 + ja$ as

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{m\omega^2}{2}(x - x_1 - ja)^2\psi(x) = \hbar\omega\left(\nu + \frac{1}{2}\right)\psi(x).$$

By introducing

$$z_j = \sqrt{\frac{2}{l}}(x - x_1 - ja), \quad j = 0, 1, \ldots, N - 1$$

with

$$l = \sqrt{\frac{\hbar}{m\omega}},$$

we rewrite (4) as

$$\frac{d^2\psi}{dz_j^2} + \left(\nu + \frac{1}{2} - \frac{z_j^2}{4}\right)\psi = 0.$$ 

The solutions of (7) are parabolic cylinder functions [2], and we write the wave function $\psi(x)$, near $x = x_1 + ja$ with $j = 1, 2, \ldots, N - 2$, as

Figure 1. A finite periodic $N$-well potential $V(x)$. We assume that $V(x)$ is quadratic around its minima at $x = x_1 + ja$ ($j = 0, 1, \ldots, N - 1$) with angular frequency $\omega$. 

$$V(x) = V_0 + \frac{m\omega^2}{2}(x - x_1 - ja)^2,$$

(1)
\[ \psi_j(x) = C_j^+ D_\nu(\sqrt{2}(x - x_j - ja)/l) + C_j^- D_\nu(-\sqrt{2}(x - x_j - ja)/l) \]
\[ = C_j^+ D_\nu(z_j) + C_j^- D_\nu(-z_j), \tag{8} \]
with constant \(C_j^+\) and \(C_j^-\). On the other hand, with constant \(C_0\) and \(C_{N-1}\), near \(x = x_1\) and near \(x = x_1 + (N - 1)a\), we write the wave function \(\psi(x)\) as
\[ \psi_0(x) = C_0 D_\nu(-z_0) \quad \text{and} \quad \psi_{N-1}(x) = C_{N-1} D_\nu(z_{N-1}), \tag{9} \]
respectively, as is done for the double-well potentials in [2, 8].

2.1. Asymptotic expansions of the exact solutions

For real and positive \(z\) satisfying \(z \gg |\nu|\), we have the asymptotic expansion [2]:
\[ D_\nu(z) \sim z^\nu \exp \left( -\frac{z^2}{4} \right) [1 + O(z^{-2})], \tag{10} \]
while for real and negative \(z\) satisfying \(|z| \gg |\nu|\), the asymptotic representation, which is explicitly real, is given as (appendix of [9] for example)
\[ D_\nu(z) \sim \cos(\nu \pi)|z|^\nu \exp \left( -\frac{z^2}{4} \right) [1 + O(z^{-2})] \]
\[ - \frac{\sin(\nu \pi)\nu!}{|z|^{\nu+1}} \frac{\sqrt{2}}{\pi} \exp \left( -\frac{z^2}{4} \right) [1 + O(z^{-2})]. \tag{11} \]
In the quadratic region near \(x = x_1\), if \(z_0 \gg |\nu|\), we thus have
\[ \psi_0(x) \simeq C_0 \left[ \cos(\nu \pi)z_0^\nu \exp \left( -\frac{z_0^2}{4} \right) - \frac{\sin(\nu \pi)\nu!}{z_0^{\nu+1}} \frac{\sqrt{2}}{\pi} \exp \left( -\frac{z_0^2}{4} \right) \right]. \tag{12} \]

For \(j = 1, 2, \ldots, N-2\), in the quadratic region near \(x = x_j + ja\), using (8), (10) and (11) we find for \(z_j \gg |\nu|\)
\[ \psi_j(x) \simeq \left[ C_j^+ + C_j^- \cos(\nu \pi) \right] z_j^\nu \exp \left( -\frac{z_j^2}{4} \right) - \frac{\sin(\nu \pi)\nu!}{z_j^{\nu+1}} \frac{\sqrt{2}}{\pi} \exp \left( -\frac{z_j^2}{4} \right), \tag{13} \]
and for \(-z_j \gg |\nu|\)
\[ \psi_j(x) \simeq \left[ C_j^+ + C_j^- \cos(\nu \pi) \right] |z_j|^\nu \exp \left( -\frac{z_j^2}{4} \right) - \frac{\sin(\nu \pi)\nu!}{|z_j|^{\nu+1}} \frac{\sqrt{2}}{\pi} \exp \left( -\frac{z_j^2}{4} \right). \tag{14} \]
In the quadratic region near \(x = x_1 + (N - 1)a\), if \(-z_{N-1} \gg |\nu|\), we have
\[ \psi_{N-1}(x) \simeq C_{N-1} \cos(\nu \pi)|z_{N-1}|^\nu \exp \left( -\frac{z_{N-1}^2}{4} \right) \]
\[ - \frac{\sin(\nu \pi)\nu!}{|z_{N-1}|^{\nu+1}} \frac{\sqrt{2}}{\pi} \exp \left( -\frac{z_{N-1}^2}{4} \right). \tag{15} \]
2.2. WKB wave functions and the asymptotic expansions

We assume $a \gg l$ and $x = x_1 + \left( j - \frac{1}{2} \right) a$ to be in the classically forbidden region, with the classical turning points at $x = x_1 + (j - 1)a + l\sqrt{2\nu + 1}$, $x_1 + ja - l\sqrt{2\nu + 1}$ satisfying (see figure 2)

$$V(x_1 + (j - 1)a + l\sqrt{2\nu + 1}) = V(x_1 + ja - l\sqrt{2\nu + 1}) = E. \quad (16)$$

In the forbidden region near $x = x_1 + \left( j - \frac{1}{2} \right) a$, the WKB approximation to an eigenfunction is written as

$$\psi_j^{WKB}(x) = B_j^+ \sqrt{\frac{\hbar}{p(x)}} \exp \left( \int_{x_1 + (j - \frac{1}{2})a}^x \frac{p(y)}{\hbar} \, dy \right)$$

$$+ B_j^- \sqrt{\frac{\hbar}{p(x)}} \exp \left( - \int_{x_1 + (j - \frac{1}{2})a}^x \frac{p(y)}{\hbar} \, dy \right), \quad (17)$$

where $p(x)$ is defined as

$$p(x) = \sqrt{2m[V(x) - E]}, \quad (18)$$

with constant $B_j^+$ and $B_j^-$. In the forbidden region of the quadratic potential near $x = x_1 + (j - 1)a + l\sqrt{2\nu + 1}$, we have
\[ \int_{x_1+(j-\frac{1}{2})a}^{x \atop h} \frac{p(y) \, dy}{h} = -\int_{x_1+(j-1)a+\sqrt{2\nu+1}}^{x \atop h} \frac{p(y) \, dy}{h} + \frac{1}{7} \int_{x_1+(j-1)a+\sqrt{2\nu+1}}^{x \atop h} \sqrt{(y-x_1-(j-1)a)^2 \over \ell^2} - 2\nu - 1 \, dy. \]

For \( z_{j-1} \gg \sqrt{2\nu+1} \), we find that \[ \int_{\sqrt{2\nu+1}}^{z_{j-1}} \sqrt{u^2 - 2\nu - 1} \, du = \frac{z_{j-1}^2}{4} - \frac{1}{2} \left( \nu + \frac{1}{2} \right) - \left( \nu + \frac{1}{2} \right) \ln \frac{z_{j-1}}{\sqrt{\nu + 1/2}} + O \left( \frac{\nu + 1/2}{z_{j-1}^2} \right), \] and, using the finite periodicity of \( V(x) \), we arrive at

\[ \exp \left( \int_{x_1+(j-\frac{1}{2})a}^{x \atop h} \frac{p(y) \, dy}{h} \right) \approx \sqrt{2\pi} g_{\nu} e^{z_{j-1}^2/4} \exp \left( -\int_{x_1+\sqrt{2\nu+1}}^{x \atop h} \frac{p(y) \, dy}{h} \right), \] where

\[ g_{\nu} = \sqrt{2\pi} \left( \nu + \frac{1}{2} \right)^{\nu+1/2} e^{-\nu^2/2}. \]  

In the quadratic region near \( x = x_1 + (j-1)a + \sqrt{2\nu+1} \), for negative \( z_j \) with \( |z_j| \gg \sqrt{2\nu+1} \), we have

\[ \epsilon_L = \sqrt{\frac{\nu+1/2}{\nu}} \exp \left( -\int_{x_1+\sqrt{2\nu+1}}^{x \atop h} \frac{p(y) \, dy}{h} \right), \]

we rewrite (23) as

\[ \psi_j^{\text{WKB}}(x) = B_j^+ \epsilon_L^\nu \sqrt{\frac{e^{z_j^2/4}}{z_j+1}} + B_j^{-\nu} \sqrt{\frac{e^{-z_j^2/4}}{z_j+1}} \epsilon_L. \]
\[
\int_{x_i + (j - \frac{1}{2})a}^{x} \frac{p(y)}{h} \, dy = - \int_{x_i}^{x_i + ja - l\sqrt{2n+1}} \frac{p(y)}{h} \, dy + \int_{x_i + (j - \frac{1}{2})a}^{x_i + ja - l\sqrt{2n+1}} \frac{p(y)}{h} \, dy \\
\approx - \frac{\mu_j^2}{4} + \left( \nu + \frac{1}{2} \right) \ln \frac{\sqrt{E}}{|z_j|} + \int_{x_i + ja - l\sqrt{2n+1}}^{x_i + ja - l\sqrt{2n+1}} \frac{p(y)}{h} \, dy,
\]

(26)

and thus

\[
\psi_j^{WKB}(x) \approx B_j^+ \sqrt{\frac{\mu_j}{\sqrt{\pi}}} |z_j|^n e^{-\mu_j/4} \exp \left( \int_{x_i + ja - l\sqrt{2n+1}}^{x_i + ja - l\sqrt{2n+1}} \frac{p(y)}{h} \, dy \right) \\
+ B_j^- \sqrt{\frac{\mu_j}{\sqrt{\pi}}} \frac{e^{\mu_j/4}}{|z_j|^{n+1}} \exp \left( - \int_{x_i + ja - l\sqrt{2n+1}}^{x_i + ja - l\sqrt{2n+1}} \frac{p(y)}{h} \, dy \right),
\]

(27)

for \( j = 1, 2, \ldots, N - 1 \). Introducing

\[
\epsilon_R = \sqrt{\frac{|z_j|}{\sqrt{\pi}}} \exp \left( - \int_{x_i + a/2}^{x_i + ja - l\sqrt{2n+1}} \frac{p(y)}{h} \, dy \right),
\]

(28)

we rewrite (27) as

\[
\psi_j^{WKB}(x) \approx B_j^+ \sqrt{2l} |z_j|^n e^{-\mu_j/4} \frac{\epsilon_R^{\mu_j/4}}{\epsilon_R} + B_j^- \epsilon_R \sqrt{l} \frac{e^{\mu_j/4}}{|z_j|^{n+1}}.
\]

(29)

3. Relations for the coefficients: a quantization condition

As \( \psi(x) \) is described by \( \psi_j(x) \) or by \( \psi_j^{WKB}(x) \) depending on the regions, if \( \psi(x) \) is described by two different functions in an overlapping region (see figure 2), the functions should match onto each other for the continuity in the region, giving the relations between the coefficients introduced for the wave function. Since we are interested in the low-lying states with \( a \gg l \), we assume that

\[
\nu = n + \delta_n,
\]

(30)

where \( |\delta_n| \ll 1 \), and \( n \) is a small non-negative integer.

For \( j = 2, 3, \ldots, N - 1 \), due to the assumed parabolicity of the potential near \( x = x_i + (j - 1)a + l\sqrt{2n+1} \), \( \psi(x) \) is described by \( \psi_{j-1}(x) \) and also by \( \psi_j^{WKB}(x) \) in the overlapping region of \( z_{j-1} \gg \sqrt{2n+1} \) (figure 3(a)). With the linear approximations near \( \delta_n = 0 \), comparing the leading terms of \( \psi_{j-1}(x) \) given in (13) and that of \( \psi_j^{WKB}(x) \) given by (25), in the overlapping region, we have

\[
C_{j-1}^+ + (-1)^n C_{j-1}^- = \sqrt{\frac{2l}{\epsilon_R}} B_j^+,
\]

(31)

\[
(-1)^n l! \sqrt{2\pi} \delta_n C_{j-1}^- = \sqrt{l} \epsilon_R \frac{e^{\mu_j/4}}{|z_j|^{n+1}} B_j^-.
\]

(32)

For \( j = 1, 2, \ldots, N - 2 \), in the region of the quadratic potential near \( x = x_i + ja - l\sqrt{2n+1} \), satisfying \( -z_j \gg \sqrt{2n+1} \), the wave function is described by \( \psi_j(x) \) as well as \( \psi_j^{WKB}(x) \) (see figure 3(b)); then, the asymptotic relations in (14) and (29) imply that
Comparing the asymptotic expansion of $y(x)$ given by (12) and that of $y(x)$ WKB given in (25) for $j = 1$ in the overlapping region near $x = x_0 + l\sqrt{2n + 1}$, we have

$$(-1)^n C_j^+ + C_j^- = \frac{\sqrt{2l}}{\epsilon^R} B_j^+,$$

$$(-1)^{n+1} n! \sqrt{2\pi} \delta_n C_j^+ = \sqrt{l} \epsilon^R B_j^+.$$  \hfill (33)

Comparing the asymptotic expansion of $\psi_0(x)$ given by (12) and that of $\psi_{WKB}^{(N)}(x)$ given in (25) for $j = 1$ in the overlapping region near $x = x_1 + l\sqrt{2n + 1}$, we have

$$(-1)^n C_0 = \frac{\sqrt{2l}}{\epsilon^L} B_1^+,$$

$$(-1)^{n+1} n! \sqrt{2\pi} \delta_n C_0 = \sqrt{l} \epsilon^L B_1^+.$$  \hfill (35)

Using the asymptotic expansion of $\psi_N^{-1}(x)$ of (15) and that of $\psi_{N-1}^{WKB}(x)$ in the overlapping region near $x = x_1 + (N - 1)a - l\sqrt{2n + 1}$, we also find

$$(-1)^n C_{N-1} = \frac{\sqrt{2l}}{\epsilon^R} B_{N-1}^+,$$

$$(-1)^{n+1} n! \sqrt{2\pi} \delta_n C_{N-1} = \sqrt{l} \epsilon^R B_{N-1}^+.$$  \hfill (37)

While we have introduced $4(N - 1)$ coefficients: $C_{0j}$, $B_j^+$, $B_j^-$ ($j = 1, 2, \ldots, N - 1$), $C_{k}^+$, $C_{k}^-$ ($k = 1, 2, \ldots, N - 2$), $C_{N-1}$, (31)–(38) constitute $4(N - 1)$ linear homogeneous
equations for the coefficients. Instead of analyzing these equations directly, we wish to extract \( N \) equations for the \( N \) coefficients: \( C_0, C_j^+ + (-1)^n C_j^- \) \( (j = 1, 2, \ldots, N - 2), C_{N-1} \).

Substituting \( j + 1 \) for \( j \) in (31)–(33), we have

\[
C_j^+ + (-1)^n C_j^- = \frac{\sqrt{2l}}{\epsilon L} B_{j+1}^+,
\]

\[
(-1)^n + n!\sqrt{2\pi} \delta_n C_j^- = \sqrt{l} \epsilon L B_{j+1}^-,
\]

\[
(-1)^n C_{j+1}^+ + C_{j+1}^- = \frac{\sqrt{2l}}{\epsilon R} B_{j+1}^+.
\]

respectively. We rewrite (40) as

\[
-n!\sqrt{2\pi} \delta_n [C_j^+ + (-1)^n C_j^-] + n!\sqrt{2\pi} \delta_n C_j^+ = \sqrt{l} \epsilon L B_{j+1}^+.
\]

Using (31), (34) and (41), we then arrive at

\[
\delta_n (C_j^+ + (-1)^n C_j^-) + \frac{(-1)^n \epsilon L \epsilon R}{2\sqrt{\pi} n!} [(C_j^+ + (-1)^n C_{j-1}^-) + (C_{j+1}^+ + (-1)^n C_{j+1}^-)] = 0
\]

which is valid for \( j = 2, 3, \ldots, N - 3 \).

Equation (33) for \( j = 1 \) and (36) yields

\[
\delta_n C_0 + \frac{\epsilon L \epsilon R}{2\sqrt{\pi} n!} (C_1^+ + (-1)^n C_1^-) = 0.
\]

Using (34) for \( j = 1 \) and (35), we have

\[
-n!\sqrt{2\pi} \delta_n C_1^+ = -\frac{\epsilon L \epsilon R}{\sqrt{2}} C_0.
\]

Plugging the expression of \( C_1^+ \) in (45) into (42) for \( j = 1 \), and using (34), we find

\[
\delta_n (C_1^+ + (-1)^n C_1^-) + \frac{\epsilon L \epsilon R}{2\sqrt{\pi} n!} [C_0 + (-1)^n (C_2^+ + (-1)^n C^-_2)] = 0.
\]

Using (31) and (38) with \( j = N - 1 \), we have

\[
\delta_n C_{N-1} + (-1)^n \frac{\epsilon L \epsilon R}{2\sqrt{\pi} n!} (C_{N-2}^+ + (-1)^n C_{N-2}^-) = 0.
\]

By a similar procedure to the previous cases, (37) can be used to give

\[
\delta_n (C_{N-2}^+ + (-1)^n C_{N-2}^-) + \frac{(-1)^n \epsilon L \epsilon R}{2\sqrt{\pi} n!} [(C_{N-3}^+ + (-1)^n C_{N-3}^-) + C_{N-1}] = 0.
\]

Equations (43), (44), (46)–(48) constitute the \( N \) equations. By defining \( \tilde{C}_0 = (-1)^n C_0, \)

\( C_j = C_j^+ + (-1)^n C_j^- \) \( (j = 1, 2, \ldots, N - 2) \),

\[
\Delta_n = \frac{\hbar \omega \epsilon L \epsilon R}{\sqrt{\pi} n!} = \frac{\hbar \omega}{\pi} \exp \left( -\int_{\frac{\pi}{\hbar}}^{\frac{\pi n + 1}{\hbar}} p(y) \frac{dy}{\hbar} \right).
\]
and an $N \times N$ symmetric Toeplitz tridiagonal matrix

$$T = \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & \cdots & 0 \\
1 & 0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 1 & 0 & 1 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & 0 & 1 & 0 & 1 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 \\
0 & \cdots & 0 & 0 & 0 & 0 & 1
\end{pmatrix},$$

(50)

the $N$ equations can be written as

$$\left(\hbar \omega \delta_n + \frac{(-1)^n \Delta_n}{2} T \right) \begin{pmatrix} \hat{C}_0 \\ C_1 \\ C_2 \\ \vdots \\ C_{N-1} \end{pmatrix} = 0,$$

(51)

where $I$ denotes the unit matrix.

If $(C_0, C_1, \ldots, C_{N-1}) = (0, 0, \ldots, 0)$, for $\delta_n = 0$, (31)–(38) show that all the $4(N - 1)$ coefficients are zero, implying the wave function $\psi(x)$ vanishes everywhere. Hence, for an acceptable wave function, $\delta_n$ should satisfy the quantization condition:

$$\det \left(\hbar \omega \delta_n I + \frac{(-1)^n \Delta_n}{2} T \right) = 0.$$  

(52)

As is well known [11], the $N$ eigenvalues of $T$ are $2 \cos \frac{s \pi}{N + 1}$ ($s = 1, 2, \ldots, N$). Thus the quantization condition is satisfied when $\hbar \omega \delta_n = (-1)^{n+1} \Delta_n \cos \frac{s \pi}{N + 1}$, which, with (2) and (30), implies that the energy eigenvalue of the multiple-well system are given as

$$E_n(s) = E_n^{(0)} + (-1)^{n+1} \Delta_n \cos \frac{s \pi}{N + 1}; \quad s = 1, 2, \ldots, N,$$

(53)

when

$$(\hat{C}_0, C_1, \ldots, C_{N-1}) = \left(\sin \frac{s \pi}{N + 1}, \sin \frac{2s \pi}{N + 1}, \ldots, \sin \frac{Ns \pi}{N + 1}\right).$$

(54)

where $E_n^{(0)}$ denotes the energy eigenvalue of the corresponding harmonic oscillator: $E_n^{(0)} = V_0 + (n + \frac{1}{2}) \hbar \omega$.

The cases of $\delta_n = 0$ appear in (53) when $N$ is odd and $s = (N + 1)/2$; in these cases, (32), (34), (36) and (38) show $B_j^+ = B_j^- = 0$ ($j = 1, 2, \ldots, N - 1$), and then (31), (35) and (37) imply $(C_0, C_1, \ldots, C_{N-1}) = (0, 0, \ldots, 0)$ to denote that the wave function $\psi(x)$ vanishes everywhere. Indeed, it has been discussed for $N = 2$ that a two-level approximation would be appropriate in the limit of $\delta_n \to 0$ [12], and thus the $N$-level approximation will be explored in the next section.

### 4. $N$-level approximation

If barrier penetration could be ignored in the $N$-well potential, for the low-lying states, we may have $N$-fold degenerate states which are either the individual states localized in each
separate well or any combination of them. Barrier penetration lifts the degeneracy, to select specific linear combinations as the eigenstates [6].

In an extension of the two-level approximation for a double-well potential, for a non-negative integer \( n \), we hypothesize an approximate real solution \( \psi_n(j; x) \) (\( \langle x|\psi_n(j)\rangle \)) to the Schrödinger equation, which is primarily localized in the classically allowed region around a minimum at \( x = x_1 + ja \) with energy \( E_n^{(0)} \), and has a small probability distribution in the two classically forbidden regions attached to it, with a vanishing amplitude for \( x \geq x_1 + (j + 1)a - l\sqrt{2n + 1} \) and for \( x \leq x_1 + (j - 1)a + l\sqrt{2n + 1} \). Then, in the quadratic region containing \( x = x_1 + ja \), \( \psi_n(j; x) \) is naturally approximated by the wave function of the \( n \)th excited state of a simple harmonic oscillator centred at \( x = x_1 + ja \):

\[
\psi_n^\text{sho}(j; x) = \frac{1}{\pi^{\frac{1}{2}}\sqrt{2^n n!}} H_n\left(\frac{x - x_1 - aj}{l}\right)e^{-\left((x-x_1-aj)^2/2l^2\right)}
= \frac{1}{\pi^{\frac{1}{2}}\sqrt{2^n n!}} e^{aj}\left[1 - \frac{n(n-1)}{2z_j^2} + \cdots\right]e^{-z_j^2/2},
\]

(55)

where \( H_n \) denotes the \( n \)th order Hermite polynomial.

In the forbidden region attached to the left-hand side of the quadratic region containing \( x = x_1 + ja \), the pertinent WKB approximation to \( \psi_n(j; x) \) is

\[
\psi_n^L\text{WKB}(j; x) = N_L\sqrt{\frac{h}{p(x)}} e^{i\int_{x_1+ja}^x \frac{p(y)}{h} dy} ; \quad j = 1, 2, \ldots, N - 1
\]

(56)

the amplitude of which increases as \( x \) increases, where \( N_L \) is a constant. In the region of quadratic potential near \( x = x_1 + ja - l\sqrt{2n + 1} \) satisfying \( z_j \ll -\sqrt{2n + 1} \), using (26) and \( \frac{h}{p(x)} \simeq \frac{\sqrt{2l}}{|z_j|} \), we find

\[
\psi_n^L\text{WKB}(j; x) \simeq N_L\sqrt{\frac{2l}{n!g_n}} |z_j|^n e^{-z_j^2/4} e^{i\int_{x_1+ja}^{x_1+ja-l\sqrt{2n+1}} \frac{p(y)}{h} dy}.
\]

(57)

As \( \psi_n^L\text{WKB}(j; x) \) and \( \psi_n^\text{sho}(j; x) \) are approximations for the same wave function, \( \psi_n^L\text{WKB}(j; x) \) should match onto \( \psi_n^\text{sho}(j; x) \) in the overlapping region of \( z_j \ll -\sqrt{2n + 1} \). Comparing the leading terms in the region, we thus have

\[
N_L = (-1)^n \frac{2l}{\pi z_j^n} \exp\left(-\int_{x_1+ja}^{x_1+ja-l\sqrt{2n+1}} \frac{p(y)}{h} dy\right) = N_L,
\]

(58)

where the constant \( N_L \) is introduced since \( N_L \) does not depend on \( j \).

In the forbidden region attached to the right-hand side of the well at \( x = x_1 + ja \), the pertinent WKB wave function, with the constant \( N_R \), is

\[
\psi_n^R\text{WKB}(j; x) = N_R\sqrt{\frac{h}{p(x)}} e^{i\int_{x_1+ja}^x \frac{p(y)}{h} dy} ; \quad j = 0, 1, \ldots, N - 2
\]

(59)

the amplitude of which decreases as \( x \) increases. Similarly, in the quadratic and forbidden region satisfying \( z_j \gg \sqrt{2n + 1} \), we have

\[
\psi_n^R\text{WKB}(j; x) \simeq N_R\sqrt{\frac{2l}{n!g_n}} |z_j|^n e^{-z_j^2/4} e^{i\int_{x_1+ja}^{x_1+ja+l\sqrt{2n+1}} \frac{p(y)}{h} dy}.
\]

(60)
Comparing the leading term of $\psi_{\text{WKB}}^R(j; x)$ and that of $\psi_{\text{WKB}}^{\text{sho}}(j; x)$, we find

$$N_R = \frac{\sqrt{2n_0}}{\sqrt{2\pi}} \frac{1}{l} \exp \left( -\int_{x_1 + l/2e+1}^{x_1 + \frac{l}{2} + \frac{d}{2}} \frac{p(y)}{\hbar} \, dy \right) \equiv N_R.$$  \hfill (61)

where, again, $N_R$ is a constant which does not depend on $j$. Indeed, the finite periodicity implies

$$\tilde{\psi}_n(j; x) = \tilde{\psi}_n(1; x - (j - 1)a)$$  \hfill (62)

for $j = 1, 2, \ldots, N - 2$, as can be seen through the explicit constructions.

As an approximation to include the tunnelling effect, we may restrict our attention to the $N$-dimensional subspace spanned by $\{ |\tilde{\psi}_n(j) >; j = 0, 1, \ldots, N - 1 \}$, as all the states have the approximate energy eigenvalue $E_{n0}^{(j)}$. Since for $|j - k| \geq 2$, $\tilde{\psi}_n(j; x)$ does not overlap with $\tilde{\psi}_n(k; x)$ by our construction, we have the matrix element of the Hamiltonian

$$\langle \tilde{\psi}_n(k) | H | \tilde{\psi}_n(j) \rangle = \int_{-\infty}^{\infty} \tilde{\psi}_n^*(k; x) H \tilde{\psi}_n(j; x) = 0 \quad (\text{for } |j - k| \geq 2).$$  \hfill (63)

As we are considering real $\tilde{\psi}_n(j; x)$, we also have

$$\langle \tilde{\psi}_n(j + 1) | H | \tilde{\psi}_n(j) \rangle = \langle \tilde{\psi}_n(j) | H | \tilde{\psi}_n(j + 1) \rangle.$$  

As a further approximation for estimating the matrix element of $\langle \tilde{\psi}_n(j + 1) | H | \tilde{\psi}_n(j) \rangle$, we restrict our attention to the two-dimensional subspace spanned by $|\tilde{\psi}_n(j) \rangle$ and $|\tilde{\psi}_n(j + 1) \rangle$, in which $\tilde{\psi}_n^\pm(j; x) = \frac{1}{\sqrt{2}}(|\tilde{\psi}_n(j; x) \mp (-1)^n \tilde{\psi}_n(j + 1; x)|)$ satisfy the Schrödinger equation:

$$H \tilde{\psi}_n^\pm(j; x) \approx E_n^\pm \tilde{\psi}_n^\pm(j; x)$$  \hfill (64)

with the eigenvalues $E_n^\pm = E_0(n) \pm \frac{\Delta_n(j)}{2}$, where

$$\Delta_n(j) = 2 \times (-1)^n \tilde{\psi}_n(j + 1) | H | \tilde{\psi}_n(j).$$  \hfill (65)

From the definitions of the localized wave functions, we have

$$\int_{x_1 + (j + \frac{1}{2})a}^{x_1 + (j + \frac{1}{2})a} \tilde{\psi}_n^2(j + 1; x) \approx 1, \quad \int_{x_1 + (j + \frac{1}{2})a}^{x_1 + (j + \frac{1}{2})a} \tilde{\psi}_n^2(j; x) \approx 0, \quad \int_{x_1 + (j + \frac{1}{2})a}^{x_1 + (j + \frac{1}{2})a} \tilde{\psi}_n(j; x) \approx 0.$$  \hfill (66)

We multiply the Schrödinger equation (64) for $\tilde{\psi}_n^\pm(j; x)$ by $\tilde{\psi}_n^\pm(j; x)$, and the equation for $\tilde{\psi}_n^\pm(j; x)$ by $\tilde{\psi}_n^\mp(j; x)$. Similarly as in [4], subtracting the two resulting expressions and integrating over $x \in [x_1 + (j + \frac{1}{2})a, \infty)$, we arrive at

$$\Delta_n(j) \approx (-1)^n \frac{\hbar^2}{m} \left( \frac{\tilde{\psi}_n(j; x)}{dx} \frac{\partial \tilde{\psi}_n(j + 1; x)}{dx} - \frac{\tilde{\psi}_n(j + 1; x)}{dx} \frac{\partial \tilde{\psi}_n(j; x)}{dx} \right) \bigg|_{x = x_1 + (j + \frac{1}{2})a}$$

$$= (-1)^n \frac{\hbar^2}{m} N_{j+1}N_R = (-1)^n \frac{\hbar^2}{m} N_LN_R$$

$$- \Delta_n.$$  \hfill (67)

On the assumption that we can neglect the mutual overlap of the wave functions so that (complement $F_{X1}$ of [1])
\[ \langle \tilde{\psi}_n(j + 1) \tilde{\psi}_n(j) \rangle \approx 0, \quad (68) \]

the \( N \times N \) Hamiltonian matrix in the subspace spanned by \( |\tilde{\psi}_n(j)\rangle \) \((j = 0, 1, 2, \ldots, N - 1)\) is written as

\[ H = \left( E_n^{(0)} I + \frac{(-1)^{n+1}}{2} \Delta_n T \right), \quad (69) \]

whose eigenvalues \( E_n(x) \) are given by \((53)\). The wave function corresponding to the eigenvalue \( E_n(x) \) is given as (see \((54)\))

\[ \tilde{\psi}_{E_n(x)}(x) = \sqrt{\frac{2}{N + 1}} \sum_{j=0}^{N-1} \psi_n(j; x) \sin \frac{(j + 1)s\pi}{N + 1}, \quad (70) \]

where the normalization constant is determined by the fact that

\[ \sum_{j=0}^{N-1} \sin^2 \frac{(j + 1)s\pi}{N + 1} = \frac{N + 1}{2}. \]

Indeed, the fact

\[ D_n(z) = 2 \frac{n}{2\pi} e^{-\frac{z^2}{2}} H_n \left( \frac{z}{\sqrt{2}} \right) \]

implies \( \psi_0(x) \to \pi^{\frac{1}{4}} \sqrt{n!} \tilde{C}_0 \psi_{n}^{\text{sho}}(0; x) \) and \( \psi_j(x) \to \pi^{\frac{1}{4}} \sqrt{n!} \tilde{C}_j \psi_{n}^{\text{sho}}(j; x) \) \((j = 1, 2, \ldots, N - 1)\) in the limit as \( \nu \) goes to \( n \), to show that the wave function given in the \( N \)-level approach is equivalent to that found through the method of constructing a single eigenfunction in the entire space.

### 5. Comparison and applications

For the \((N = 2)\) double-well potential, \((53)\) shows that the energy eigenvalues associated with \( E_n^{(0)} \) are \( E_n^{(0)} = \frac{n}{2} \), with the level splitting \( \Delta_n \), which is in agreement with the expression in [4]. For large \( N \), the eigenvalues associated with \( E_n^{(0)} \) form a band, and the width of the energy band becomes \( 2\Delta_n \) as \( N \) goes to infinity (this fact has been discussed for \( n = 0 \) in [13]).

#### 5.1. Comparison with the strong bonding approximation

For a periodic potential \( V_p(x) \) which is equal to \( V(x) \) for \( x_3 \leq x \leq x_3 + (N - 1)a \), but with the full periodicity \( V_p(x + a) = V_p(x) \) for all \( x \), we construct the localized approximate eigenfunctions by considering that \((62)\) is true for all integer \( j \) in this case. The (unnormalized) wave function

\[ \varphi_{k,n}(x) = \sum_{j=-\infty}^{\infty} e^{ikj} \tilde{\psi}_n(j; x), \quad (71) \]

then satisfies the Bloch condition: \( \varphi_{k,n}(x + a) = e^{ika} \varphi_{k,n}(x) \), with the Bloch wavenumber \( k \) satisfying

\[ -\frac{\pi}{a} \leq k < \frac{\pi}{a}. \quad (72) \]

If we assume \((68)\) is valid for all integer \( j \), the wave function \( \varphi_{k,n}(x) \) can be shown to be an eigenfunction of the periodic system with the energy eigenvalue (complement F Xi of [1]).
Equation (73) suggests that the strong bonding approximation of [1] is, in fact, related to the rigorous tight-binding approach, and \( E_\nu(k) - E_\nu(0) \) may correspond to the wave-number-dependent corrections of the energy expectation value contributed by the nearest neighbours in the tight-binding approximation [14].

When the Bloch phase, \( \kappa a \), is equal to \( \pi/(N + 1) \), \( E_\nu(k) \) coincides with the eigenvalue \( E_\nu(s) \) of the finite periodic system given in (53) (see figure 4). For the system of a finite periodic potential which consists of \( N \) square wells, through the transfer matrix method, it has been shown that the low-lying states are described by the Bloch phases \( \pi/(N + 1) \) if the single square well is deep and wide [6], while the WKB approximation may not be useful for rectangular potential curves [10]. We also note that some other discrete Bloch phases have long been found for the unit transmission in the scattering by the finite periodic potentials [7, 15].

Comparing (70) and (71) at the discrete Bloch phase satisfying \( \kappa a = \pi/(N + 1) \), we find that \( \sqrt{(N + 1)/2} \tilde{\psi}_{E_\nu(0)}(x) = \text{Im} \left[ e^{ikx} \tilde{\varphi}_{E_\nu}(x) \right] \) for \( x \leq 1/2 + 1/n + 1 \). This relation between the wave functions in fact implies that although \( \tilde{\varphi}_{E_\nu}(x) \) satisfies the Bloch condition, the eigenfunctions of the finite system do not fulfill the periodicity property \( |\tilde{\psi}_{E_\nu(0)}(x + a)|^2 = |\tilde{\psi}_{E_\nu(0)}(x)|^2 \) in the domain of the periodicity of \( V(x) \) as detailed in [16]. Further, the relation may be consistent with the fact that the eigenvalues \( E_\nu(s) \) in the finite system are not degenerate while \( E_\nu(k) = E_\nu(-k) \).

5.2. The cosine potential

In order to compare the result with the rigorous expression for the widths of the low-lying energy bands of the Mathieu equation, we consider the 2\( N \)-well potential
with the positive constant \( q \) and \( l_e \), assuming that \( V_e(x) \) monotonically decreases (increases) for \( x \leq -N\pi l_e \) \((x \geq N\pi l_e)\). We find the approximate expression for \( \omega \) and \( l \) as:

\[
\omega = \left( \frac{1}{m} \frac{d^2 V_e(x)}{dx^2} \right)_{x=L_e/2}^{1/2} = \frac{1}{l_e} \sqrt{\frac{8q}{m}},
\]

\[
l = \frac{\hbar}{m\omega} = \frac{\sqrt{h l_e}}{(8mq)^{1/4}}.
\]

Introducing

\[
\varphi_M = \frac{\pi}{2} - l \frac{1}{l_e} \sqrt{2n + 1} = \frac{\pi}{2} - \sqrt{\frac{h^2}{2m l_e^2} q},
\]

for the energy \( E_n^{(0)} \left[ = -2q + \hbar \omega \left( n + \frac{1}{2} \right) \right] \), it may be appropriate to take \( x = \pm l \varphi_M \) as the turning points adjacent to \( x = 0 \), as we are interested in the limit of \( \varphi_M \to \frac{\pi}{2} \).

The integral in the exponential of (49) can thus be approximated as

\[
\int_{x_{l+1/2}}^{x_{l+1/4}} \frac{p(y)}{\hbar} dy \approx \int_{-l \varphi_M}^{l \varphi_M} \frac{p(y)}{\hbar} dy \approx \frac{2l_e \sqrt{mq}}{\hbar} \int_{-l \varphi_M}^{l \varphi_M} \sqrt{\cos(2\varphi) - \cos(2\varphi_M)} d\varphi
\]

\[
= \frac{4l_e \sqrt{2mq}}{\hbar} [E(\sin \varphi_M) - \cos^2 \varphi_M K(\sin \varphi_M)]
\]

\[
\approx \frac{4l_e \sqrt{2mq}}{\hbar} \left( n + \frac{1}{2} \right) \ln \left( \frac{16l_e \sqrt{2mq}}{\hbar(n + \frac{1}{2})} \right)
\]

in the limit of \( \varphi_M \to \frac{\pi}{2} \), where \( E \) and \( K \) denote the complete elliptic integrals. Substituting (22), (75) and (77) into (49), we find the widths of the narrow bands:

\[
2\Delta_n \approx \frac{\hbar^2}{2ml_e^2} \left( \frac{2^{2n+5}}{n!} \sqrt{\frac{2}{\pi}} \left( \frac{2ml_e^2}{\hbar^2} q \right)^{\frac{n+3}{4}} \exp \left( -4 \sqrt{\frac{2ml_e^2}{\hbar^2} q} \right) \right)
\]

which, if we take \( \frac{h^2}{2m l_e^2} = 1 \), reproduces the known result [17–19].

6. Conclusions

We have analyzed the low-lying states for the finite periodic \( N \)-well potential, assuming that the wells are parabolic around the minima. As originally suggested for \( N = 2 \) by Dekker [8], matching the exact wave functions around the minima and the WKB wave functions in the barriers, we find a formula for the energy eigenvalues of the low-lying bands, which can reproduce, in the large-\( N \) limit, the rigorous mathematical expression for the widths of the narrow energy bands of the Mathieu equation [17–19]. The same formula has also been derived through the \( N \)-level approximation in which, instead of the exact wave functions, the
eigenfunctions of a simple harmonic oscillator are used with other approximations of (63)–(65) and (68).

The energy eigenvalues for the fully periodic potential, which coincide with the finite periodic multiple-well potential on a finite domain, have also been explicitly written in terms of the potential, and it is found that the eigenvalues of the \(N\)-well potential are those that the eigenvalue formula of the fully periodic system give at some discrete Bloch wavenumbers (phases). The \(N\)-well system in the large-\(N\) limit is different from the fully periodic system, as the discrete Bloch wavenumbers of the \(N\)-well system densely fill the the interval \([0, \frac{\pi}{a(N+1)}]\) which is just half of the first Brillouin zone given in (72), and as the eigenvalues are not degenerate.

**Acknowledgments**

The author would like to thank Professors Jonathan Connor and Hans Dekker for their discussions and encouragement. This paper was supported by the Sunchon National University Research Fund in 2016.

**References**

[1] Cohen-Tannoudji C, Diu B and Laloë F 1977 *Quantum Mechanics* (Paris: Wiley)

[2] Merzbacher E 1998 *Quantum Mechanics* (New York: Wiley)

[3] Griffiths D J 2005 *Introduction to Quantum Mechanics* (Englewood Cliffs, NJ: Prentice-Hall)

[4] Dekker H 1986 Coherent tunnelling: on the level splitting of local ground states in a bistable potential *Phys. Lett.* **114A** 295

[5] Jelic V and Marsiglio F 2012 The double-well potential in quantum mechanics: a simple, numerically exact formulation *Eur. J. Phys.* **33** 1651

[6] Sprung D W L, Sigetich J D, Wu H and Martorell J 2000 Bound states of a finite periodic potential *Am. J. Phys.* **68** 715

[7] Grifths D J and Steinke C A 2001 Waves in locally periodic media *Am. J. Phys.* **69** 137

[8] Dekker H 1987 Quantum mechanical barrier problems: I. Coherence and tunneling in asymmetric potentials *Physica* **146A** 375

[9] Miller S C Jr and Good R H Jr 1953 A WKB-type approximation to the Schrödinger equation *Phys. Rev.* **91** 174

[10] Furry W H 1947 Two notes on phase-integral methods *Phys. Rev.* **71** 360

[11] Gray R M 2006 *Toeplitz and Circulant Matrices: A Review* (Boston: Now Publishers)

[12] Song D-Y 2015 Localization or tunneling in asymmetric double-well potentials *Ann. Phys.* **362** 609

[13] Coleman S 1985 *Aspects of Symmetry* (Cambridge: Cambridge University Press)

[14] Harrison W A 1979 *Solid State Theory* (New York: Dover)

[15] Sprung D W L, Wu H and Martorell J 1993 Scattering by a finite periodic potential *Am. J. Phys.* **61** 1118

[16] Pereyra P 2005 Eigenvalues, eigenfunctions, and surface states in finite periodic systems *Ann. Phys.* **320** 1

[17] Blanch G 1972 Mathieu functions *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical tables* ed M Abramowitz and I A Stegun (New York: Wiley)

[18] Connor J N L, Uzer T, Marcus R A and Smith A D 1984 Eigenvalues of the Schrödinger equation for a periodic potential with nonperiodic boundary conditions: a uniform semiclassical analysis *J. Chem. Phys.* **80** 5095

[19] Catelani G, Schoelkopf R J, Devoret M H and Glazman L I 2011 Relaxation and frequency shifts induced by quasiparticles in superconducting qubits *Phys. Rev. B* **84** 064517