ON THE EIGENVALUES OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION WITH PERIODIC POTENTIAL OF SAW-TOOTHED OR ROOF-SHAPED FORM

YOSHIYUKI SUGIYAMA

Department of Aeronautical Engineering

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Synopsis

The one-dimensional Schrödinger equation with a potential of saw-toothed or roof-shaped form is solved in the finite space. After the method presented by Oshida,[1] the matrix representation of the wave function and the method analogous to the circuit theory of the four terminal network are employed.

The low eigenvalues of energy are tabulated with the number of repetition of the individual potentials. Their comparison with the eigenvalues for the periodic square-well potential is also given.

§ I. Introduction

In case of the one-dimensional Schrödinger equation with a square-well potential varying periodically, Oshida[1] has presented a method to obtain its solution by making use of the transformation matrix of order 2 and obtained the equation which determines the eigenvalues of energy under some boundary conditions. Recently, Takizawa[2] has extended the method to solve the three-dimensional wave equation under some restricted conditions. Further, he has tried to generalize Oshida's method to the solution of the equations of higher order and to that in many dimensions.

Following to Oshida's method, in this paper the author presents eigenvalues of energy associated with the saw-toothed or with the roof-shaped potential, respectively. The calculation of the eigenvalues is carried out graphically, and their comparison with eigenvalues for the square-well potential is made in some detail.

The results obtained may find some applications to the energy state of free electrons in metals and in organic compounds.

§ II. The Saw-Toothed Potential with Infinitely High Barrier at the Both Ends

We shall consider the one-dimensional periodic potential field of the saw-toothed form as shown in Fig. 1. U denotes the height of the saw-toothed potential, and a its period. The one-dimensional Schrödinger equation in x-coordinate is expressed by

$$\frac{d^2\psi}{dx^2}+\beta^2(E-V)\psi=0, \tag{1}$$

with the potential:

$$V = \frac{2U}{a}x - U \quad \text{for} \quad 0 < x < a, \tag{2}$$

where $\beta^2 = \dfrac{8\pi^2 m}{h^2}$, and E the eigenvalue of energy. m shows the mass of the particle (electron) and h the Planck constant. Writing

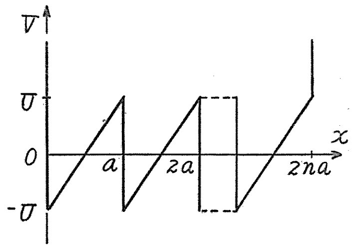

FIG. 1. The saw-toothed potential.

$$Z = E + U - \frac{2U}{a}x, \quad \text{and} \quad \xi = \frac{a\beta}{3U}Z^{3/2},$$

we obtain the solution of Eq. (1) with (2), if we know the (initial) values of the wave function $\psi(x)$ and its derivative $\zeta(x)$ at $x = 0$. In matrix form, we have

$$\begin{bmatrix} \psi(x) \\ \zeta(x) \end{bmatrix} = \begin{bmatrix} \dfrac{Z^{1/2}}{E_+^{1/2}\Delta_+}\{J_{2/3}(+)J_{1/3}(\xi) + J_{-2/3}(+)J_{-1/3}(\xi)\}, & \dfrac{Z^{1/2}}{\beta E_+\Delta_+}\{J_{1/3}(+)J_{-1/3}(\xi) - J_{-1/3}(+)J_{1/3}(\xi)\} \\ \dfrac{Z\beta}{E_+^{1/2}\Delta_+}\{J_{-2/3}(+)J_{2/3}(\xi) - J_{2/3}(+)J_{-2/3}(\xi)\}, & \dfrac{Z}{E_+\Delta_+}\{J_{-1/3}(+)J_{-2/3}(\xi) + J_{1/3}(+)J_{2/3}(\xi)\} \end{bmatrix} \begin{bmatrix} \psi_0 \\ \zeta_0 \end{bmatrix}$$

$$\equiv \mathbf{P}(\xi) \cdot \begin{bmatrix} \psi_0 \\ \zeta_0 \end{bmatrix}, \tag{3}$$

under the conditions $\psi(0) = \psi_0$ and $\zeta(0) = \zeta_0$, where $\zeta(x) = \dfrac{d\psi}{dx}$, $\Delta_+ = \sqrt{3}\Big/\pi \dfrac{a\beta}{3U}(E+U)^{3/2}$, $E_+ = E + U$ and $J_\nu(+) = J_\nu\left(\dfrac{a\beta}{3U}[E+U]^{3/2}\right)$: Bessel function of order ν. If the potential is repeated n times, we obtain from (3)

$$\begin{bmatrix} \psi_{na} \\ \zeta_{na} \end{bmatrix} = \begin{bmatrix} \dfrac{E_-^{1/2}}{E_+^{1/2}\Delta_+}\{J_{2/3}(+)J_{1/3}(-) + J_{-2/3}(+)J_{-1/3}(-)\}, & \dfrac{E_-^{1/2}}{\beta E_+\Delta_+}\{J_{1/3}(+)J_{-1/3}(-) - J_{-1/3}(+)J_{1/3}(-)\} \\ \dfrac{E_-\beta}{E_+^{1/2}\Delta_+}\{J_{-2/3}(+)J_{2/3}(-) - J_{2/3}(+)J_{-2/3}(-)\}, & \dfrac{E_-}{E_+\Delta_+}\{J_{-1/3}(+)J_{-2/3}(-) + J_{1/3}(+)J_{2/3}(-)\} \end{bmatrix}^n \begin{bmatrix} \psi_0 \\ \zeta_0 \end{bmatrix}$$

$$\equiv \mathbf{P}^n \begin{bmatrix} \psi_0 \\ \zeta_0 \end{bmatrix}, \tag{4}$$

where $\psi_{na} = \psi(na)$, $\zeta_{na} = \zeta(na)$, $E_- = E - U$ and $J_\nu(-) = J_\nu\left(\dfrac{a\beta}{3U}[E-U]^{3/2}\right)$.

By applying Sylvester's theorem[3] in matrix theory, the calculation of the transformation matrix $\mathbf{P}^n$ can be simplified by making use of the substitution

$$\cos r \equiv \frac{P_{11} + P_{22}}{2}$$

$$= \frac{\sqrt{3}\pi}{6}\Big[(-)(+)^2]^{1/3}[J_{2/3}(+)J_{1/3}(-) + J_{-2/3}(+)J_{-1/3}(-) +$$

$$+\{J_{-1/3}(+)J_{-2/3}(-)+J_{1/3}(+)J_{2/3}(-)\}\left\{\frac{(-)}{(+)}\right\}^{1/3}\Bigg], \tag{5}$$

where P_{ij} $(i, j=1, 2)$ represents the elements of matrix $\mathbf{P}$, and $(\pm)$ is an abbreviation of the expression $a\beta(3U)^{-1}(E\pm U)^{3/2}$. Thus the matrix $\mathbf{P}^n$ in the above Eq. (4) reduces to

$$\mathbf{P}^n=\frac{1}{\sin r}\begin{bmatrix} P_{11}\cdot\sin nr-\sin(n-1)r & P_{12}\cdot\sin nr \\ P_{21}\cdot\sin nr & P_{22}\cdot\sin nr-\sin(n-1)r \end{bmatrix}. \tag{6}$$

Considering boundary conditions $\psi_0=0$ and $\psi_{na}=0$, *i.e.* the potential barrier is infinitely high at the both ends, eigenvalues of energy are determined by

$$[P^n]_{12}\equiv P_{12}\cdot\frac{\sin nr}{\sin r}=0.$$

For

$$P_{12}\equiv\frac{E_-^{1/2}}{\beta E_+\Delta_+}\{J_{1/3}(+)J_{-1/3}(-)-J_{-1/3}(+)J_{1/3}(-)\}\neq 0,$$

we obtain

$$\frac{\sin nr}{\sin r}=0,$$

i.e.

$$\begin{aligned}\cos\frac{k\pi}{n}&=\frac{\sqrt{3}\,\pi}{6}[(-)(+)^2]^{1/3}\Big[J_{2/3}(+)J_{1/3}(-)+J_{-2/3}(+)J_{-1/3}(-)\\&\qquad+\{J_{-1/3}(+)J_{-2/3}(-)+J_{1/3}(+)J_{2/3}(-)\}\left\{\frac{(-)}{(+)}\right\}^{1/3}\Big]\\&\equiv G(-),\end{aligned} \tag{7}$$

taking into account of (5), with k and n integers ($n>1$, k/n must not be an integer).

We calculate the right-hand side of (7), say $G(-)$, as a function of $(-)$

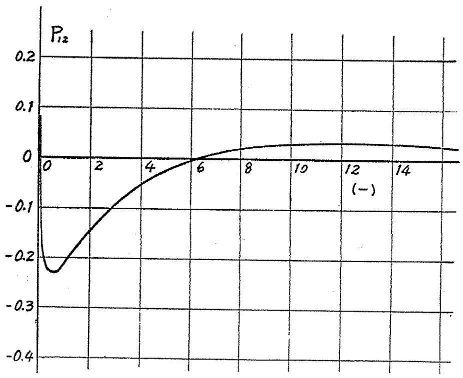

FIG. 2. P_{12} versus $(-)=\dfrac{a\beta}{3U}(E-U)^{3/2}$, $n=1$.

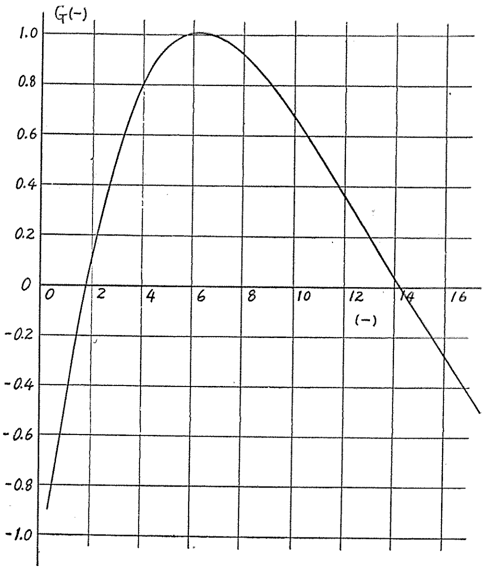

FIG. 3. $G(-)$ versus $(-)=\dfrac{a\beta}{3U}(E-U)^{3/2}$, $n\geq 2$.

(cf. Fig. 3), by making use of the numerical table[4] of Bessel functions of order $\pm 1/3$ and $\pm 2/3$.

Then, we draw straight lines $\cos\frac{k\pi}{n}$ =const. in Fig. 3 and find E from the points of intersection of the straight lines and the curve $G(-)$. The numerical values used here are m = mass of electron, $U = 8.58$ eV and $a = 2$ Å. The eigenvalues of energy are listed in Table 1.

TABLE 1. The Eigenvalues of Energy E in eV (Saw-toothed)

n	1	2	3	4	5
E	9.08 37.69	21.37 59.01	17.16 26.27 51.40 66.30	15.34 21.37 28.99 47.92 59.01	14.13 18.80 24.30 30.45 45.89 54.42 63.51

n: The number of potentials repeated.

§ III. The Roof-Shaped Potential with Infinitely High Barrier at the Both Ends

As another form of the finitely extended potential field varying periodically, we consider the case shown in Fig. 4. The potential is expressed by $V = \frac{2U}{a}x - U$ for $0 \leq x \leq a$ and $V = -\frac{2U}{a}x + 3U$ for $a \leq x \leq 2a$. The Schrödinger equations are written as

$$\frac{d^2\psi}{dx^2} + \beta^2\left\{E - \frac{2U}{a}x + U\right\}\psi = 0, \qquad (8)_1$$

and

$$\frac{d^2\psi}{dx^2} + \beta^2\left\{E + \frac{2U}{a}x - 3U\right\}\psi = 0, \qquad (8)_2$$

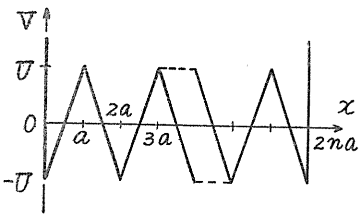

FIG. 4. The roof-shaped potential.

in the two regions, respectively.

Solving the above two equations in the matrix form under the conditions: $\psi(0) = \psi_0$ and $\zeta(0) = \zeta_0$; and connecting their solution at $x = a$, we obtain the following wave function at $x = 2a$:

$$\begin{bmatrix} \psi_{2a} \\ \zeta_{2a} \end{bmatrix} = \mathbf{Q}\begin{bmatrix} \psi_0 \\ \zeta_0 \end{bmatrix},$$

where

$$\mathbf{Q} = \mathbf{P}(+) \cdot \mathbf{P}(-),$$

and

$$\mathbf{P}(+)=\begin{bmatrix} \dfrac{E_+^{1/2}}{E_-^{1/2}\Delta_-}\{J_{2/3}(-)J_{1/3}(+)+J_{-2/3}(-)J_{-1/3}(+)\}, & \dfrac{E_+^{1/2}}{E_-\beta\Delta_-}\{J_{-1/3}(-)J_{1/3}(+)-J_{1/3}(-)J_{-1/3}(+)\} \\ \dfrac{\beta E_+}{E_-^{1/2}\Delta_-}\{J_{2/3}(-)J_{-2/3}(+)-J_{-2/3}(-)J_{2/3}(+)\}, & \dfrac{E_+}{E_-\Delta_-}\{J_{-1/3}(-)J_{-2/3}(+)+J_{1/3}(-)J_{2/3}(+)\} \end{bmatrix}$$

$$\mathbf{P}(-)=\begin{bmatrix} \dfrac{E_-^{1/2}}{E_+^{1/2}\Delta_+}\{J_{2/3}(+)J_{1/3}(-)+J_{-2/3}(+)J_{-1/3}(-)\}, & \dfrac{E_-^{1/2}}{\beta E_+\Delta_+}\{J_{1/3}(+)J_{-1/3}(-)-J_{-1/3}(+)J_{1/3}(-)\} \\ \dfrac{E_-\beta}{E_+^{1/2}\Delta_+}\{J_{-2/3}(+)J_{2/3}(-)-J_{2/3}(+)J_{-2/3}(-)\}, & \dfrac{E_-}{E_+\Delta_+}\{J_{-1/3}(+)J_{-2/3}(-)+J_{1/3}(+)J_{2/3}(-)\} \end{bmatrix}.$$

If the potential is repeated n times, we see that the wave function at $x=2na$ is expressed by

$$\begin{bmatrix}\psi_{2na}\\ \zeta_{2na}\end{bmatrix}=\mathbf{Q}^n\begin{bmatrix}\psi_0\\ \zeta_0\end{bmatrix}$$

$$=\frac{1}{\Delta_+\Delta_-}\begin{bmatrix} \begin{array}{l}(J_{-1/3}(+)J_{-2/3}(-)+J_{1/3}(+)J_{2/3}(-))\\ \quad\times(J_{2/3}(+)J_{1/3}(-)+J_{-2/3}(+)J_{-1/3}(-))\\ \quad+(J_{-2/3}(+)J_{2/3}(-)-J_{2/3}(+)J_{-2/3}(-))\\ \quad\times(J_{-1/3}(-)J_{1/3}(+)-J_{1/3}(-)J_{-1/3}(+)),\end{array} & \begin{array}{l}\dfrac{2}{\beta E_+^{1/2}}\cdot(J_{2/3}(-)J_{1/3}(+)+J_{-2/3}(-)J_{-1/3}(+))\\ \quad\times(J_{-1/3}(-)J_{1/3}(+)-J_{1/3}(-)J_{-1/3}(+)),\end{array} \\ \begin{array}{l}2\beta E_+^{1/2}\cdot(J_{2/3}(-)J_{-2/3}(+)-J_{-2/3}(-)J_{2/3}(+))\\ \quad\times(J_{2/3}(+)J_{1/3}(-)+J_{-2/3}(+)J_{-1/3}(-))\end{array} & \begin{array}{l}(J_{-2/3}(+)J_{2/3}(-)-J_{2/3}(+)J_{-2/3}(-))\\ \quad\times(J_{-1/3}(-)J_{1/3}(+)-J_{1/3}(-)J_{-1/3}(+))\\ \quad+(J_{2/3}(+)J_{1/3}(-)+J_{-2/3}(+)J_{-1/3}(-))\\ \quad\times(J_{2/3}(-)J_{1/3}(+)+J_{-2/3}(-)J_{-1/3}(+))\end{array} \end{bmatrix}^n\begin{bmatrix}\psi_0\\ \zeta_0\end{bmatrix} \quad (9)$$

where $E_\pm=E\pm U$, $\Delta_\pm=\sqrt{3}\Big/\pi\dfrac{a\beta}{3U}E_\pm^{3/2}$ and $J_\nu(\pm)=J_\nu\left(\dfrac{a\beta}{3U}[E\pm U]^{3/2}\right)$.

After calculating nth power of the matrix $\mathbf{Q}$ under the conditions $\psi_0=0$ and $\psi_{2na}=0$, we obtain the eigenvalues of energy by the equation:

$$0=Q_{12}=\frac{2}{\beta E_+^{1/2}\Delta_+\Delta_-}[J_{1/3}(+)J_{2/3}(-)+J_{-2/3}(-)J_{-1/3}(+)]\times$$
$$\times[J_{-1/3}(-)J_{1/3}(+)-J_{1/3}(-)J_{-1/3}(+)] \qquad \text{for} \quad n=1, \qquad (10)$$

and

$$\frac{\sin nr}{\sin r}=0 \qquad \text{for} \quad n>1,$$

where

$$\cos r \equiv \frac{Q_{11}+Q_{22}}{2}$$

$$=1+\frac{2\pi^2}{3}(+)(-)\{J_{1/3}(+)J_{-1/3}(-)-J_{-1/3}(+)J_{1/3}(-)\}$$
$$\times\{J_{-2/3}(+)J_{2/3}(-)-J_{2/3}(+)J_{-2/3}(-)\},$$

i.e.

$$\cos\frac{k\pi}{n}=1+\frac{2\pi^2}{3}(+)(-)\{J_{1/3}(+)J_{-1/3}(-)-J_{-1/3}(+)J_{1/3}(-)\}$$
$$\times\{J_{-2/3}(+)J_{2/3}(-)-J_{2/3}(+)J_{-2/3}(-)\}$$
$$\equiv G(-). \tag{11}$$

Fig. 5 shows a plot of Q_{12} vs. $(-)$ for $n=1$.

The graphical calculation is carried out in the similar manner as cited in §II (cf. Figs. 2 and 3), with numerical values $U=8.58$ eV and $a=1$ Å.

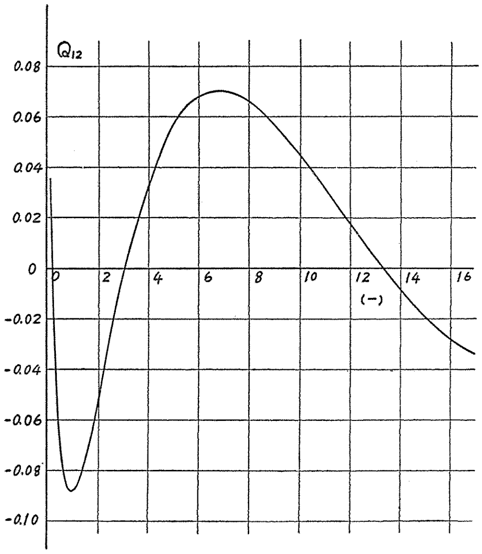

FIG. 5. Q_{12} versus $(-)$, $n=1$.

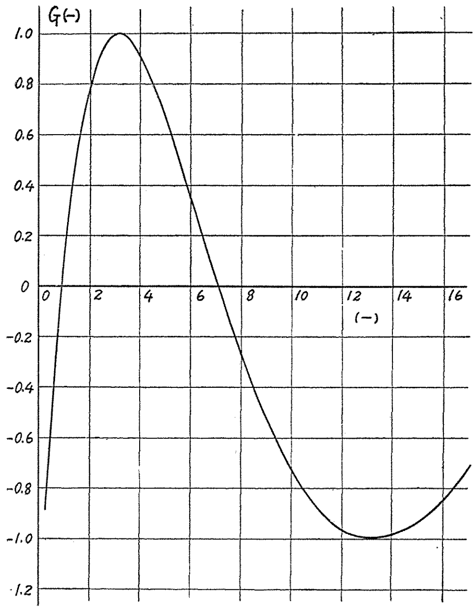

FIG. 6. $G(-)$ versus $(-)$, $n\geq 2$.

The eigenvalues of energy are listed in Table 2.

TABLE 2. The Eigenvalues of Energy E in eV (Roof-shaped)

n	1	2	3	4	5
E	12.73 37.34 85.10	21.37 58.89	17.83 26.19 51.37 67.16	15.97 21.46 29.18 47.82 58.89 71.38 98.80	15.08 19.32 24.13 30.91 45.70 54.30 63.69

By applying Oshida's method we obtain graphically the eigenvalues of energy associated with the square-well potential shown in Fig. 7. We make use of the same values of m, a and U as in § III.

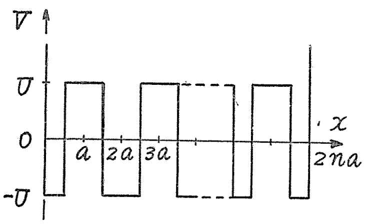

FIG. 7. The square-well potential.

Table 3 shows the eigenvalues associated with the square-well potential.

TABLE 3. The Eigenvalues of Energy E in eV (Square- well)

n	1	2	3	4	5
E	17.44 37.42 83.45 154.14 237.47 338.22	22.33 57.99 117.68 192.73 284.01 394.47	18.96 27.03 50.09 65.09 107.74 123.89	18.33 22.33 28.75 47.61 57.99 69.57	17.74 20.26 25.39 30.54 46.41 55.28

The eigenvalue equations of energy are

$$0 = \cos ap \cdot \sin aq + \sin ap \cdot \left\{ \frac{1}{2}\left(\frac{q}{p} - \frac{p}{q}\right) + \frac{1}{2}\left(\frac{p}{q} + \frac{q}{p}\right)\cos aq \right\}$$

$$\equiv R_{12} \qquad \text{for} \quad n = 1, \qquad (12)$$

$$\cos\frac{k\pi}{n} = \cos a(p+q) + \left\{1 - \frac{1}{2}\left(\frac{p}{q} + \frac{q}{p}\right)\right\}\sin ap \cdot \sin aq$$

$$\equiv G \qquad \text{for} \quad n \geq 2, \qquad (13)$$

where $p = \beta\sqrt{E-U}$ and $q = \beta\sqrt{E+U}$.

Figs. 8 and 9 show plots of the right-hand side of the above equations vs. p.

§ IV. Remarks

In Fig. 2 (saw-toothed, $n=1$), P_{12} tends to infinity, when $(E-U)$ approaches towards zero. The lowest energy-level 9.08 eV in Table 1 corresponds to the most left-sided intersection of this curve and the abscissa. The function $G(-)$ in Fig. 3 (saw-toothed, $n \geq 2$) tends to -1.11, when $(E-U)$ approaches towards zero. While, the function Q_{12} (roof-shaped, $n=1$) in Fig. 5 is found to tend to infinity, if $(E-U)$ vanishes. The smallest value 12.73 eV of eigenvalue of energy for $n=1$ (roof-shaped potential) in Table 2 is obtained from the most left-sided intersection of the curve Q_{12} and the abscissa in Fig. 5, and corresponds to the symmetric wave

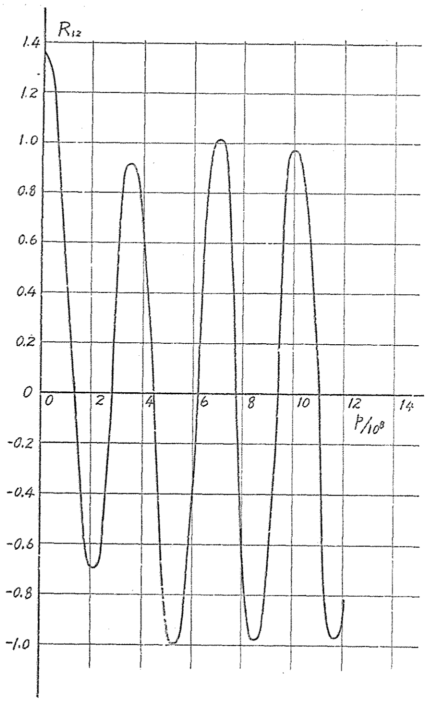

FIG. 8. R_{12} versus $p=\beta\sqrt{E-U}$, $n=1$.

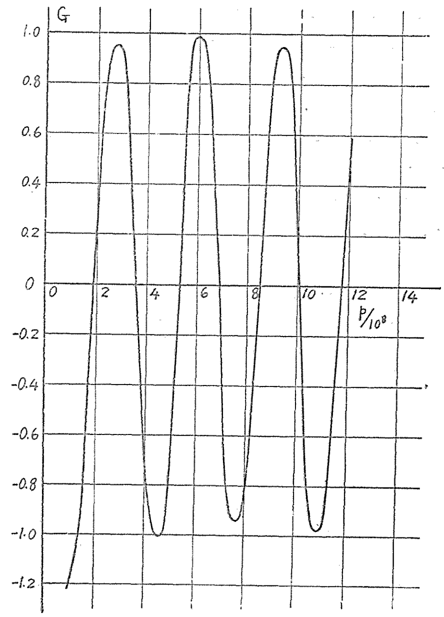

FIG. 9. G versus $p=\beta\sqrt{E-U}$, $n\geq 2$.

function as regard to $x=a$ (even wave function), while the other higher eigenvalues come from the antisymmetric functions. In Figs. 8 and 9, it should be also noted that $R_{12}\rightarrow 1.36$ for $p\rightarrow 0$, and $G\rightarrow -1.43$ for $p\rightarrow 0$.

The figures 9.08 eV (saw-toothed, $n=1$) and 12.73 eV (roof-shaped, $n=1$) seem to be quite reasonable, if one considers that the lowest energy level for square-

TABLE 4. Energy Difference Corresponding to Type of Potentials

n	Type of potential	Energy difference					
1	Saw-toothed	28.61					
	Roof-shaped	24.61	47.76				
	Square-well	19.98	46.08	70.69	83.33	100.75	
2	Saw-toothed	37.64					
	Roof-shaped	37.52					
	Square-well	35.66	59.69	75.05	91.28	110.46	
3	Saw-toothed	9.11	25.13	14.90			
	Roof-shaped	8.36	25.18	15.79			
	Square-well	8.07	23.06	15.00	42.65	16.15	
4	Saw-toothed	6.03	7.62	18.93	11.09		
	Root-shaped	5.49	7.72	18.64	11.07	12.49	27.42
	Square-well	4.00	6.42	18.86	10.38	11.58	
5	Saw-toothed	4.67	5.50	6.15	15.44	8.53	9.09
	Roof-shaped	4.24	4.81	6.78	14.79	8.60	9.39
	Square-well	2.52	5.13	5.15	15.87	8.87	

well potential ($n=1$) finds itself at 17.44 eV (cf. Table 3). As for the higher levels, the energy eigenvalues are not much different from each other with regard to the three types of potentials cited above. For reference, the energy differences are also listed in Table 4.

Hayashi and co-workers[5] have treated the Schrödinger wave equations with square-well or roof-shaped potential which has a defect and is extended *infinitely* in the one-dimensional space. They have also given the widths of forbidden band and eigenvalues of energy. The present author, however, treats the case of *finitely* extended potential in the one-dimensional space, and the detailed comparison with their results can not be given.

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