applied sciences

MDPI

Supplementary Materials

Towards the Analytical Generalization of the Transcendental Energy Equation, Group Velocity, and Effective Mass in One-Dimensional Periodic Potential Wells with a Computational Application to Common Coupled Potentials

F. Mendoza-Villa[1], E. V. Manrique Castillo[1*], Edson C. Passamani[2], and Juan A. Ramos-Guivar[1]

[1] Grupo de Investigación de Nanotecnología Aplicada para Biorremediación Ambiental, Energía, Biomedicina y Agricultura (NANOTECH), Facultad de Ciencias Físicas, Universidad Nacional Mayor de San Marcos, Av. Venezuela Cdra 34 S/N, Ciudad Universitaria, Lima 15081, Perú.

[2] Departamento de Física, Universidade Federal do Espírito Santo -UFES, Vitória 29075-910, ES, Brazil.

Correspondence: emanriquec@unmsm.edu.pe

Section S1 Periodic Potential of one potential $V = V(x)$ and a rectangular-like potential

Bloch functions must satisfy the following boundary and continuity conditions.

$$\begin{aligned}
\Psi_I(b) &= \Psi_{II}(b)\\
\Psi_I(-b) &= e^{ikT}\Psi_{II}(b+a)\\
\Psi_I^{'}(b) &= \Psi_{II}^{'}(b)\\
\Psi_I^{'}(-b) &= e^{ikT}\Psi_{II}^{'}(b+a)
\end{aligned}$$

We get the following matrix equation.

$$\begin{bmatrix} y_1(b) & z_1(b) & -e^{\beta b} & -e^{-\beta b} \\ y_1(-b) & z_1(-b) & -e^{ikT}e^{\beta(b+a)} & -e^{ikT}e^{-\beta(b+a)} \\ y_1^{'}(b) & z_1^{'}(b) & -\beta e^{\beta b} & \beta e^{-\beta b} \\ y_1^{'}(-b) & z_1^{'}(-b) & -\beta e^{ikT}e^{\beta(b+a)} & \beta e^{ikT}e^{-\beta(b+a)} \end{bmatrix} \cdot \begin{bmatrix} C_1 \\ D_1 \\ C_2 \\ D_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

As it is very tedious to solve the secular determinant, we transform the elements of the matrix into ones that are easier to handle.

$$\begin{aligned}
0 &= \begin{vmatrix} \mathrm{A} & \mathrm{B} & \mathrm{C} & \mathrm{D} \\ \mathrm{E} & \mathrm{F} & \mathrm{G} & \mathrm{H} \\ \mathrm{I} & \mathrm{J} & \mathrm{K} & \mathrm{L} \\ \mathrm{M} & \mathrm{N} & \mathrm{P} & \mathrm{Q} \end{vmatrix}\\
0 &= \mathrm{A}\cdot\begin{vmatrix} \mathrm{F} & \mathrm{G} & \mathrm{H} \\ \mathrm{J} & \mathrm{K} & \mathrm{L} \\ \mathrm{N} & \mathrm{P} & \mathrm{Q} \end{vmatrix} - \mathrm{B}\cdot\begin{vmatrix} \mathrm{E} & \mathrm{G} & \mathrm{H} \\ \mathrm{I} & \mathrm{K} & \mathrm{L} \\ \mathrm{M} & \mathrm{P} & \mathrm{Q} \end{vmatrix} + \mathrm{C}\cdot\begin{vmatrix} \mathrm{E} & \mathrm{F} & \mathrm{H} \\ \mathrm{I} & \mathrm{J} & \mathrm{L} \\ \mathrm{M} & \mathrm{N} & \mathrm{Q} \end{vmatrix} - \mathrm{D}\cdot\begin{vmatrix} \mathrm{E} & \mathrm{F} & \mathrm{G} \\ \mathrm{I} & \mathrm{J} & \mathrm{K} \\ \mathrm{M} & \mathrm{N} & \mathrm{P} \end{vmatrix}\\
0 &= \begin{vmatrix} \mathrm{AF - BE} & \mathrm{G} & \mathrm{H} \\ \mathrm{AJ - BI} & \mathrm{K} & \mathrm{L} \\ \mathrm{AN - BM} & \mathrm{P} & \mathrm{Q} \end{vmatrix} + \begin{vmatrix} \mathrm{E} & \mathrm{F} & \mathrm{CH - DG} \\ \mathrm{I} & \mathrm{J} & \mathrm{CL - DK} \\ \mathrm{M} & \mathrm{N} & \mathrm{CQ - DP} \end{vmatrix}\\
0 &= (\mathrm{AF - BE})(\mathrm{KQ - PL}) - (\mathrm{AJ - BI})(\mathrm{GQ - PH})\\
&\quad + (\mathrm{AN - BM})(\mathrm{GL - KH}) + (\mathrm{CH - DG})(\mathrm{IN - MJ})\\
&\quad - (\mathrm{CL - DK})(\mathrm{EN - MF}) + (\mathrm{CQ - DP})(\mathrm{EJ - IF})
\end{aligned}$$

where

$$
\begin{aligned}
\text{KQ - PL} &= 2\beta^2 e^{ikT} \sinh(\beta a) \\
\text{GL - KH} &= -2\beta e^{ikT} \cosh(\beta a) \\
\text{CL - DK} &= -2\beta \\
\text{GQ - PH} &= -2\beta e^{2ikT} \\
\text{CH - DG} &= -2e^{ikT} \sinh(\beta a) \\
\text{CQ - DP} &= -2\beta e^{ikT} \cosh(\beta a) \\
\text{AJ - BI} &= W\{y_1(x), z_1(x)\} \\
\text{EN - MF} &= W\{y_1(x), z_1(x)\} \\
2\cos(kT) &= e^{ikT} + e^{-ikT}
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
0 = {} & \beta \sinh(\beta a)(\text{AF - BE}) + e^{ikT} W\{y_1(x), z_1(x)\} \\
& - \cosh(\beta a)(\text{AN - BM}) - \sinh(\beta a)(\text{IN - MJ})/\beta \\
& + e^{-ikT} W\{y_1(x), z_1(x)\} - \cosh(\beta a)(\text{EJ - IF})
\end{aligned}
$$

The transcendental energy equation for the one potentials $V = V(x)$ and a rectangular-like potential is the following:

$$
\begin{aligned}
2\cos(kT) W\{y_1(x), z_1(x)\} &= \sinh(\beta a)\left[\frac{(\text{IN - MJ}) - \beta^2(\text{AF - BE})}{\beta}\right] + \cosh(\beta a)\left[(\text{AN - BM}) + (\text{EJ - IF})\right] \\
\cos(k(2b+a)) &= \frac{\sinh(\beta a)}{\beta}\left[\frac{M_1(E) - \beta^2 M_2(E)}{M_4(E)}\right] + \cosh(\beta a)\left[\frac{M_3(E)}{M_4(E)}\right]
\end{aligned}
$$

where

$$
\begin{aligned}
M_1(E) &= y_1'(b) z_1'(-b) - y_1'(-b) z_1'(b) \\
M_2(E) &= z_1(-b) y_1(b) - z_1(b) y_1(-b) \\
M_3(E) &= y_1(b) z_1'(-b) - y_1'(-b) z_1(b) + y_1(-b) z_1'(b) - y_1'(b) z_1(-b) \\
M_4(E) &= 2W\{y_1(x), z_1(x)\}
\end{aligned}
$$

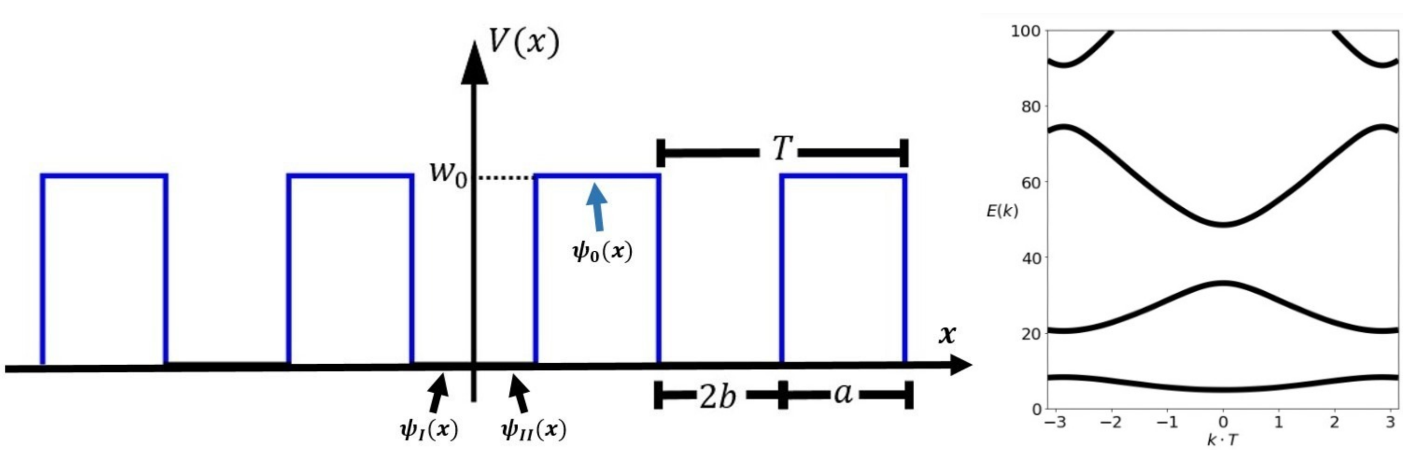

Figure S1: Left: Graphical scheme of the quantum potential representing the Kronig-Penney model and its corresponding parameters. Right: Energy curve graph for a rectangular-like potential..

Section S2 Periodic Potential of two potentials $V = V(x)$ and a rectangular-like potential

Bloch functions must satisfy the following boundary and continuity conditions.

$$\begin{aligned}
\Psi_I(0) &= \Psi_{II}(0)\\
\Psi'_I(0) &= \Psi'_{II}(0)\\
\Psi_{II}(b) &= \Psi_{III}(b)\\
\Psi'_{II}(b) &= \Psi'_{III}(b)\\
\Psi_I(-b) &= e^{ik(2b+a)}\Psi_{III}(b+a)\\
\Psi'_I(-b) &= e^{ik(2b+a)}\Psi'_{III}(b+a)
\end{aligned}$$

We get the following matrix equation.

$$\begin{bmatrix} y_1(0) & z_1(0) & -y_2(0) & -z_2(0) & 0 & 0\\ 0 & 0 & y_2(b) & z_2(b) & -e^{\beta b} & -e^{-\beta b}\\ y_1(-b) & z_1(-b) & 0 & 0 & -e^{ikT}e^{\beta(b+a)} & -e^{ikT}e^{-\beta(b+a)}\\ y_1'(0) & z_1'(0) & -y_2'(0) & -z_2'(0) & 0 & 0\\ 0 & 0 & y_2'(b) & z_2'(b) & -\beta e^{\beta b} & \beta e^{-\beta b}\\ y_1'(-b) & z_1'(-b) & 0 & 0 & -\beta e^{ikT}e^{\beta(b+a)} & \beta e^{ikT}e^{-\beta(b+a)} \end{bmatrix} \cdot \begin{bmatrix} C_1\\ D_1\\ C_2\\ D_2\\ C_3\\ D_3 \end{bmatrix} = \begin{bmatrix} 0\\0\\0\\0\\0\\0 \end{bmatrix}$$

Again, we transform the elements of the matrix into ones that are easier to handle, following the matrix properties as:

$$0 = \begin{vmatrix} \mathrm{A} & \mathrm{B} & \mathrm{C} & \mathrm{D} & 0 & 0\\ 0 & 0 & \mathrm{E} & \mathrm{F} & \mathrm{G} & \mathrm{H}\\ \mathrm{I} & \mathrm{J} & 0 & 0 & \mathrm{K} & \mathrm{L}\\ \mathrm{M} & \mathrm{N} & \mathrm{P} & \mathrm{Q} & 0 & 0\\ 0 & 0 & \mathrm{R} & \mathrm{S} & \mathrm{T} & \mathrm{U}\\ \mathrm{V} & \mathrm{W} & 0 & 0 & \mathrm{X} & \mathrm{Y} \end{vmatrix}$$

$$0 = \mathrm{A}\cdot\begin{vmatrix} 0 & \mathrm{E} & \mathrm{F} & \mathrm{G} & \mathrm{H}\\ \mathrm{J} & 0 & 0 & \mathrm{K} & \mathrm{L}\\ \mathrm{N} & \mathrm{P} & \mathrm{Q} & 0 & 0\\ 0 & \mathrm{R} & \mathrm{S} & \mathrm{T} & \mathrm{U}\\ \mathrm{W} & 0 & 0 & \mathrm{X} & \mathrm{Y} \end{vmatrix} - \mathrm{B}\cdot\begin{vmatrix} 0 & \mathrm{E} & \mathrm{F} & \mathrm{G} & \mathrm{H}\\ \mathrm{I} & 0 & 0 & \mathrm{K} & \mathrm{L}\\ \mathrm{M} & \mathrm{P} & \mathrm{Q} & 0 & 0\\ 0 & \mathrm{R} & \mathrm{S} & \mathrm{T} & \mathrm{U}\\ \mathrm{V} & 0 & 0 & \mathrm{X} & \mathrm{Y} \end{vmatrix} + \mathrm{C}\cdot\begin{vmatrix} 0 & 0 & \mathrm{F} & \mathrm{G} & \mathrm{H}\\ \mathrm{I} & \mathrm{J} & 0 & \mathrm{K} & \mathrm{L}\\ \mathrm{M} & \mathrm{N} & \mathrm{Q} & 0 & 0\\ 0 & 0 & \mathrm{S} & \mathrm{T} & \mathrm{U}\\ \mathrm{V} & \mathrm{W} & 0 & \mathrm{X} & \mathrm{Y} \end{vmatrix} - \mathrm{D}\cdot\begin{vmatrix} 0 & 0 & \mathrm{E} & \mathrm{G} & \mathrm{H}\\ \mathrm{I} & \mathrm{J} & 0 & \mathrm{K} & \mathrm{L}\\ \mathrm{M} & \mathrm{N} & \mathrm{P} & 0 & 0\\ 0 & 0 & \mathrm{R} & \mathrm{T} & \mathrm{U}\\ \mathrm{V} & \mathrm{W} & 0 & \mathrm{X} & \mathrm{Y} \end{vmatrix}$$

$$0 = \begin{vmatrix} 0 & \mathrm{E} & \mathrm{F} & \mathrm{G} & \mathrm{H}\\ \mathrm{AJ - BI} & 0 & 0 & \mathrm{K} & \mathrm{L}\\ \mathrm{AN - BM} & \mathrm{P} & \mathrm{Q} & 0 & 0\\ 0 & \mathrm{R} & \mathrm{S} & \mathrm{T} & \mathrm{U}\\ \mathrm{AW - BV} & 0 & 0 & \mathrm{X} & \mathrm{Y} \end{vmatrix} + \begin{vmatrix} \mathrm{CF - DE} & 0 & 0 & \mathrm{G} & \mathrm{H}\\ 0 & \mathrm{I} & \mathrm{J} & \mathrm{K} & \mathrm{L}\\ \mathrm{CQ - DP} & \mathrm{M} & \mathrm{N} & 0 & 0\\ \mathrm{CS - DR} & 0 & 0 & \mathrm{T} & \mathrm{U}\\ 0 & \mathrm{V} & \mathrm{W} & \mathrm{X} & \mathrm{Y} \end{vmatrix}$$

Solving the resulting determinants, we have:

$$\begin{aligned}
0 = &-(\mathrm{AJ - BI})(\mathrm{EQ - PF})(\mathrm{TY - XU}) - (\mathrm{AJ - BI})(\mathrm{PS - RQ})(\mathrm{GY - XH})\\
&+ (\mathrm{AW - BV})(\mathrm{PF - EQ})(\mathrm{KU - TL}) + (\mathrm{AW - BV})(\mathrm{PS - RQ})(\mathrm{GL - KH})\\
&- (\mathrm{CF - DE})(\mathrm{JM - NI})(\mathrm{TY - XU}) - (\mathrm{CF - DE})(\mathrm{WM - NV})(\mathrm{KU - TL})\\
&+ (\mathrm{CS - DR})(\mathrm{JM - NI})(\mathrm{GY - XH}) + (\mathrm{CS - DR})(\mathrm{NV - WM})(\mathrm{GL - KH})\\
&+ (\mathrm{AN - BM})(\mathrm{RF - ES})(\mathrm{KY - XL}) - (\mathrm{CQ - DP})(\mathrm{WI - JV})(\mathrm{GU - TH})
\end{aligned}$$

Grouping the result of the determinant in terms of complex exponentials we can rewrite as:

$$\begin{aligned}0 &= (\text{XU - TY})[(\text{AJ - BI})(\text{EQ - PF}) + (\text{CF - DE})(\text{JM - NI})]\\ &+ (\text{GY - XH})[(\text{CS - DR})(\text{JM - NI}) + (\text{BI - AJ})(\text{PS - RQ})]\\ &+ (\text{KU - TL})[(\text{AW - BV})(\text{PF - EQ}) + (\text{DE - CF})(\text{WM - NV})]\\ &+ (\text{GL - KH})[(\text{AW - BV})(\text{PS - RQ}) + (\text{CS - DR})(\text{NV - WM})]\\ &+ (\text{KY - XL})[(\text{AN - BM})(\text{ RF - ES})] - (\text{GU - TH})[(\text{CQ - DP})(\text{WI - JV})]\end{aligned}$$

Where

$$\begin{aligned}\gamma &= e^{ikT}\\ \text{GY - XH} &= -2\beta\gamma\cosh(\beta a)\\ \text{KU - TL} &= -2\beta\gamma\cosh(\beta a)\\ \text{GL - KH} &= -2\gamma\sinh(\beta a)\\ \text{XU - TY} &= -2\beta^2\gamma\sinh(\beta a)\\ \text{KY - XL} &= -2\beta\gamma^2\\ \text{GU - TH} &= -2\beta\\ \text{AN - BM} &= W\{y_1(x), z_1(x)\}\\ \text{WI - JV} &= W\{y_1(x), z_1(x)\}\\ \text{CQ - DP} &= W\{y_2(x), z_2(x)\}\\ \text{ES - RF} &= W\{y_2(x), z_2(x)\}\\ \gamma + \gamma^{-1} &= 2\cos(kT)\end{aligned}$$

Therefore, we can summary as:

$$\begin{aligned}0 &= -\beta\sinh(\beta a)[(\text{BI - AJ})(\text{EQ - PF}) + (\text{DE - CF })(\text{JM - NI})]\\ &+ \cosh(\beta a)[(\text{CS - DR})(\text{JM - NI}) + (\text{BI - AJ})(\text{PS - RQ})]\\ &+ \cosh(\beta a)[(\text{AW - BV})(\text{PF - EQ}) + (\text{DE - CF})(\text{WM - NV})]\\ &+ \frac{\sinh(\beta a)}{\beta}[(\text{AW - BV})(\text{PS - RQ}) + (\text{CS - DR})(\text{NV - WM})]\\ &- 2\cos(kT)W\{y_1(x), z_1(x)\}W\{y_2(x), z_2(x)\}\end{aligned}$$

The transcendental energy equation for the two potentials $V = V(x)$ and a rectangular-like potential is the following:

$$\begin{aligned}2\cos(kT) &= -\beta\sinh(\beta a)\frac{[(\text{BI -AJ})(\text{EQ - PF}) + (\text{DE - CF})(\text{JM - NI})]}{2W\{y_1(x), z_1(x)\}W\{y_2(x), z_2(x)\}}\\ &+ \cosh(\beta a)\frac{[(\text{CS - DR})(\text{JM - NI}) + (\text{BI - AJ})(\text{PS - RQ})]}{2W\{y_1(x), z_1(x)\}W\{y_2(x), z_2(x)\}}\\ &+ \cosh(\beta a)\frac{[(\text{AW - BV})(\text{PF - EQ}) + (\text{DE - CF})(\text{WM - NV})]}{2W\{y_1(x), z_1(x)\}W\{y_2(x), z_2(x)\}}\\ &+ \frac{\sinh(\beta a)}{\beta}\frac{[(\text{AW - BV})(\text{PS - RQ}) + (\text{CS - DR})(\text{NV - WM})]}{2W\{y_1(x), z_1(x)\}W\{y_2(x), z_2(x)\}}\\ \cos(k(2b+a)) &= \frac{\sinh(\beta a)}{\beta}\left[\frac{N_1(E) - \beta^2 N_2(E)}{N_4(E)}\right] + \cosh(\beta a)\left[\frac{N_3(E)}{N_4(E)}\right]\end{aligned}$$

Where,

$$\begin{aligned}
N_1(E) &= [y_1(0)z_1^{'}(-b) - z_1(0)y_1^{'}(-b)] \cdot [z_2^{'}(0)y_2^{'}(b) - y_2^{'}(0)z_2^{'}(b)] \\
&\quad + [z_2(0)y_2^{'}(b) - y_2(0)z_2^{'}(b)] \cdot [y_1^{'}(-b)z_1^{'}(0) - z_1^{'}(-b)y_1^{'}(0)] \\
N_2(E) &= [z_1(0)y_1(-b) - y_1(0)z_1(-b)] \cdot [z_2(b)y_2^{'}(0) - y_2(b)z_2^{'}(0)] \\
&\quad + [y_2(0)z_2(b) - z_2(0)y_2(b)] \cdot [z_1(-b)y_1^{'}(0) - y_1(-b)z_1^{'}(0)] \\
N_3(E) &= [z_1(0)y_1(-b) - y_1(0)z_1(-b)] \cdot [z_2^{'}(0)y_2^{'}(b) - y_2^{'}(0)z_2^{'}(b)] \\
&\quad + [z_2(0)y_2^{'}(b) - y_2(0)z_2^{'}(b)] \cdot [z_1(-b)y_1^{'}(0) - y_1(-b)z_1^{'}(0)] \\
&\quad + [y_1(0)z_1^{'}(-b) - z_1(0)y_1^{'}(-b)] \cdot [y_2(b)z_2^{'}(0) - z_2(b)y_2^{'}(0)] \\
&\quad + [y_2(0)z_2(b) - z_2(0)y_2(b)] \cdot [z_1^{'}(-b)y_1^{'}(0) - y_1^{'}(-b)z_1^{'}(0)] \\
N_4(E) &= 2W\{y_1(x), z_1(x)\} \cdot W\{y_2(x), z_2(x)\}
\end{aligned}$$

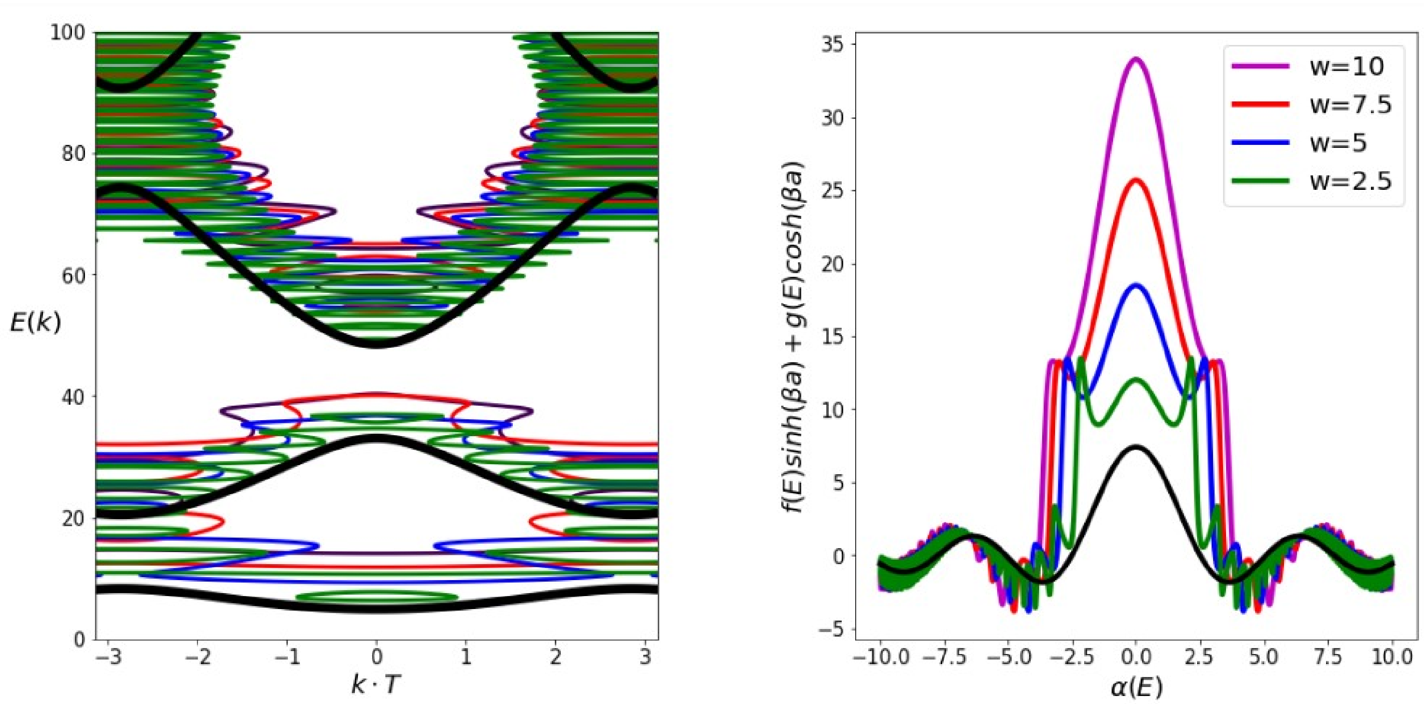

Figure S2: Numerical simulation of the transcendental energy equation for the periodic triangular-like potential ▲ together with the rectangular-like potential at different values of w. The height of the rectangle is $w_0 = 100$. The black solid lines correspond to the rectangular-like potential that simulates the Kroning-Penney model.

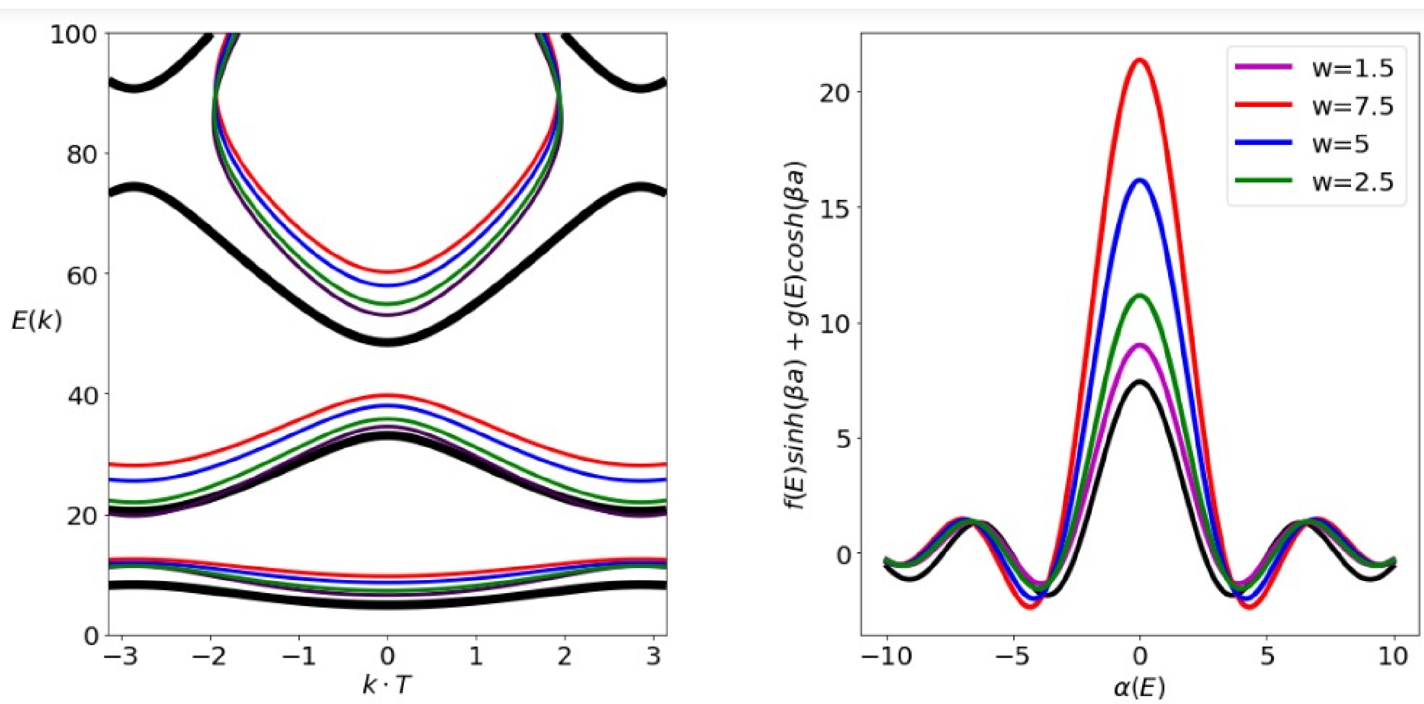

Figure S3: Numerical simulation of the transcendental energy equation for the periodic triangular-like potential ▼ together with the rectangular-like potential at different values of w. The height of the rectangle is $w_0 = 100$. The black solid lines correspond to the rectangular-like potential that simulates the Kroning-Penney model.

Section S3 The Transcendental Energy Equation

$$\cos(kT) = f(E)\sinh(\beta(E)a) + g(E)\cosh(\beta(E)a)$$

Where,

$$f(E) = \frac{M_1(E) - \beta^2 M_2(E)}{\beta M_4(E)} \qquad f(E) = \frac{N_1(E) - \beta^2 N_2(E)}{\beta N_4(E)}$$
$$g(E) = \frac{M_3(E)}{M_4(E)} \qquad g(E) = \frac{N_3(E)}{N_4(E)}$$

The variables $M_1(E), M_2(E), M_3(E)$, and $M_4(E)$ for a potential $V = V(x)$ and rectangular-like potential are given by:

$$\begin{aligned}
M_1(E) &= y_2'(-b)y_1'(b) - y_2'(b)y_1'(-b)\\
M_2(E) &= y_2(-b)y_1(b) - y_2(b)y_1(-b)\\
M_3(E) &= y_1(b)y_2'(-b) - y_1'(-b)y_2(b) + y_1(-b)y_2'(b) - y_1'(b)y_2(-b)\\
M_4(E) &= 2W\{y_1(x), y_2(x)\}
\end{aligned}$$

The variables $N_1(E), N_2(E), N_3(E)$, and $N_4(E)$ for a two potentials $V = V(x)$ plus rectangular-like potential are given by:

$$\begin{aligned}
N_1(E) &= [y_1(0)y_2'(-b) - y_2(0)y_1'(-b)] \cdot [z_2'(0)z_1'(b) - z_1'(0)z_2'(b)]\\
&\quad + [z_2(0)z_1'(b) - z_1(0)z_2'(b)] \cdot [y_1'(-b)y_2'(0) - y_2'(-b)y_1'(0)]\\
N_2(E) &= [y_2(0)y_1(-b) - y_1(0)y_2(-b)] \cdot [z_2(b)z_1'(0) - z_1(b)z_2'(0)]\\
&\quad + [z_1(0)z_2(b) - z_2(0)z_1(b)] \cdot [y_2(-b)y_1'(0) - y_1(-b)y_2'(0)]\\
N_3(E) &= [y_2(0)y_1(-b) - y_1(0)y_2(-b)] \cdot [z_2'(0)z_1'(b) - z_1'(0)z_2'(b)]\\
&\quad + [z_2(0)z_1'(b) - z_1(0)z_2'(b)] \cdot [y_2(-b)y_1'(0) - y_1(-b)y_2'(0)]\\
&\quad + [y_1(0)y_2'(-b) - y_2(0)y_1'(-b)] \cdot [z_1(b)z_2'(0) - z_2(b)z_1'(0)]\\
&\quad + [z_1(0)z_2(b) - z_2(0)z_1(b)] \cdot [y_2'(-b)y_1'(0) - y_1'(-b)y_2'(0)]\\
N_4(E) &= 2W\{y_1(x), y_2(x)\} \cdot W\{z_1(x), z_2(x)\}
\end{aligned}$$

The variable $\beta = \beta(E)$ is a function of energy and its energy derivatives are written as

$$\begin{aligned}
\beta(E) &= \frac{\sqrt{2m(w-E)}}{\hbar}\\
\frac{d\beta(E)}{dE} &= -\frac{m}{\hbar\sqrt{2m(w-E)}}\\
\frac{d^2\beta(E)}{dE^2} &= -\frac{m^2}{\hbar(2m(w-E)^{3/2}}
\end{aligned}$$

Section S4 The Group Velocity

$$
\begin{aligned}
\cos(kT) &= f(E)\sinh(\beta(E)a) + g(E)\cosh(\beta(E)a) \\
-T\sin(kT) &= \frac{df(E)}{dE}\frac{dE}{dk}\sinh(\beta(E)a) + af(E)\frac{d\beta(E)}{dE}\frac{dE}{dk}\cosh(\beta(E)a) \\
&+ \frac{dg(E)}{dE}\frac{dE}{dk}\cosh(\beta(E)a) + ag(E)\frac{d\beta(E)}{dE}\frac{dE}{dk}\sinh(\beta(E)a) \\
-T\sin(kT) &= \left(\frac{df(E)}{dE} + ag(E)\frac{d\beta(E)}{dE}\right)\frac{dE}{dk}\sinh(\beta(E)a) + \left(\frac{dg(E)}{dE} + af(E)\frac{d\beta(E)}{dE}\right)\frac{dE}{dk}\cosh(\beta(E)a) \\
-T\sin(kT) &= \left[\left(\frac{df(E)}{dE} + ag(E)\frac{d\beta(E)}{dE}\right)\sinh(\beta(E)a) + \left(\frac{dg(E)}{dE} + af(E)\frac{d\beta(E)}{dE}\right)\cosh(\beta(E)a)\right]\frac{dE}{dk} \\
\frac{dE}{dk} &= -T\sin(kT)\left[\left(\frac{df(E)}{dE} + ag(E)\frac{d\beta(E)}{dE}\right)\sinh(\beta(E)a) + \left(\frac{dg(E)}{dE} + af(E)\frac{d\beta(E)}{dE}\right)\cosh(\beta(E)a)\right]^{-1} \\
v_G &= -\frac{T\sin(kT)}{\hbar}\left[\left(\frac{df(E)}{dE} + ag(E)\frac{d\beta(E)}{dE}\right)\sinh(\beta(E)a) + \left(\frac{dg(E)}{dE} + af(E)\frac{d\beta(E)}{dE}\right)\cosh(\beta(E)a)\right]^{-1} \\
v_G &= -\frac{T\sin(kT)}{\hbar H_0(E)}
\end{aligned}
$$

Where,

$$
H_0(E) = \left(\frac{df(E)}{dE} + ag(E)\frac{d\beta(E)}{dE}\right)\sinh(\beta(E)a) + \left(\frac{dg(E)}{dE} + af(E)\frac{d\beta(E)}{dE}\right)\cosh(\beta(E)a)
$$

The energy $H_0(E)$ function can also be simulated numerically and explains to some extent the orientation for the rectangular-like potential of negative intensity.

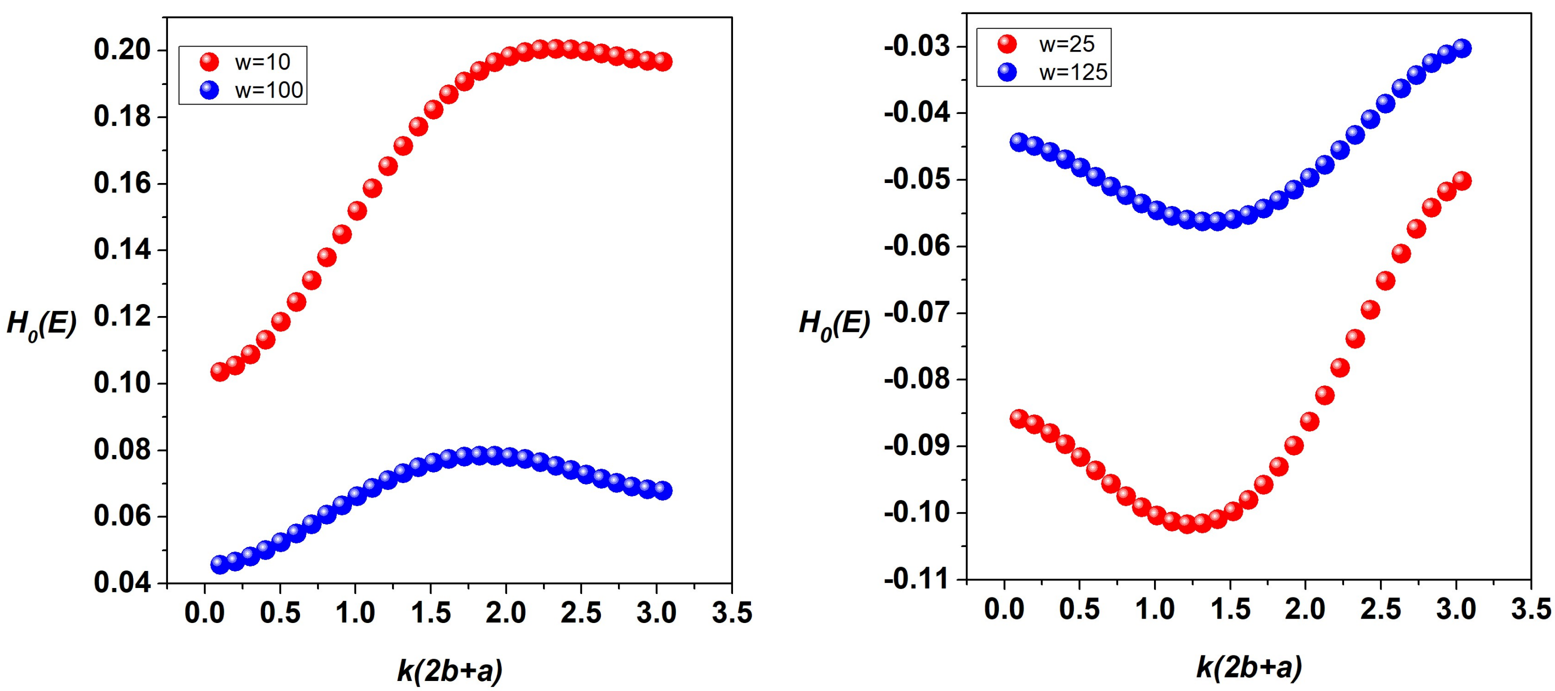

Figure S4: Numerical simulation of the energy $H_0(E)$ function for 30 energy values and for heights of 10, 25, 100, and 125 as indicated in the figure. The colors represent the simulated heights used in Figure 7.

Section S5 The Effective Mass

$$
\begin{aligned}
-T\sin(kT) &= \left(\frac{df(E)}{dE} + ag(E)\frac{d\beta(E)}{dE}\right)\frac{dE}{dk}\sinh(\beta(E)a) + \left(\frac{dg(E)}{dE} + af(E)\frac{d\beta(E)}{dE}\right)\frac{dE}{dk}\cosh(\beta(E)a) \\
-T^2\cos(kT) &= \left[\frac{dE}{dk}\left(ag(E)\frac{d^2\beta(E)}{dE^2} + a\frac{dg(E)}{dE}\frac{d\beta(E)}{dE} + \frac{d^2f(E)}{dE^2}\right)\right]\frac{dE}{dk}\sinh(\beta(E)a) \\
&+ \left(ag(E)\frac{d\alpha(E)}{dE} + \frac{df(E)}{dE}\right)\left[a\frac{d\beta(E)}{dE}\left(\frac{dE}{dk}\right)^2\cosh(\beta(E)a) + \frac{d^2E}{dk^2}\sinh(\beta(E)a)\right] \\
&+ \left[\frac{dE}{dk}\left(af(E)\frac{d^2\beta(E)}{dE^2} + a\frac{df(E)}{dE}\frac{d\beta(E)}{dE} + \frac{d^2g(E)}{dE^2}\right)\right]\frac{dE}{dk}\cosh(\beta(E)a) \\
&+ \left(af(E)\frac{d\beta(E)}{dE} + \frac{dg(E)}{dE}\right)\left[a\frac{d\beta(E)}{dE}\left(\frac{dE}{dk}\right)^2\sinh(\beta(E)a) + \frac{d^2E}{dk^2}\cosh(\beta(E)a)\right] \\
-T^2\cos(kT) &= \left(\frac{dE}{dk}\right)^2\left(ag(E)\frac{d^2\beta(E)}{dE^2} + a\frac{dg(E)}{dE}\frac{d\beta(E)}{dE} + \frac{d^2f(E)}{dE^2}\right)\sinh(\beta(E)a) \\
&+ \left(ag(E)\frac{d\beta(E)}{dE} + \frac{df(E)}{dE}\right)\left[a\frac{d\beta(E)}{dE}\left(\frac{dE}{dk}\right)^2\cosh(\beta(E)a) + \frac{d^2E}{dk^2}\sinh(\beta(E)a)\right] \\
&+ \left(\frac{dE}{dk}\right)^2\left(af(E)\frac{d^2\beta(E)}{dE^2} + a\frac{df(E)}{dE}\frac{d\beta(E)}{dE} + \frac{d^2g(E)}{dE^2}\right)\cosh(\beta(E)a) \\
&+ \left(af(E)\frac{d\beta(E)}{dE} + \frac{dg(E)}{dE}\right)\left[a\frac{d\beta(E)}{dE}\left(\frac{dE}{dk}\right)^2\sinh(\beta(E)a) + \frac{d^2E}{dk^2}\cosh(\beta(E)a)\right] \\
-T^2\cos(kT) &= \left(\frac{dE}{dk}\right)^2\left[ag(E)\frac{d^2\beta(E)}{dE^2} + a\frac{dg(E)}{dE}\frac{d\beta(E)}{dE} + \frac{d^2f(E)}{dE^2}\right]\sinh(\beta(E)a) \\
&+ \left(\frac{dE}{dk}\right)^2\left[af(E)\frac{d^2\beta(E)}{dE^2} + a\frac{df(E)}{dE}\frac{d\beta(E)}{dE} + \frac{d^2g(E)}{dE^2}\right]\cosh(\beta(E)a) \\
&+ a\frac{d\beta(E)}{dE}\left(\frac{dE}{dk}\right)^2\left[\left(ag(E)\frac{d\beta(E)}{dE} + \frac{df(E)}{dE}\right)\cosh(\beta(E)a) + \left(af(E)\frac{d\beta(E)}{dE} + \frac{dg(E)}{dE}\right)\sinh(\beta(E)a)\right] \\
&+ \frac{d^2E}{dk^2}\left[\left(ag(E)\frac{d\beta(E)}{dE} + \frac{df(E)}{dE}\right)\sinh(\beta(E)a) + \left(af(E)\frac{d\beta(E)}{dE} + \frac{dg(E)}{dE}\right)\cosh(\beta(E)a)\right] \\
-T^2\cos(kT) &= \left(\frac{dE}{dk}\right)^2\left[ag(E)\frac{d^2\beta(E)}{dE^2} + 2a\frac{dg(E)}{dE}\frac{d\beta(E)}{dE} + \frac{d^2f(E)}{dE^2} + a^2f(E)\left(\frac{d\beta(E)}{dE}\right)^2\right]\sinh(\beta(E)a) \\
&+ \left(\frac{dE}{dk}\right)^2\left[af(E)\frac{d^2\beta(E)}{dE^2} + 2a\frac{df(E)}{dE}\frac{d\beta(E)}{dE} + \frac{d^2g(E)}{dE^2} + a^2g(E)\left(\frac{d\beta(E)}{dE}\right)^2\right]\cosh(\beta(E)a) \\
&+ \frac{d^2E}{dk^2}\left[\left(ag(E)\frac{d\beta(E)}{dE} + \frac{df(E)}{dE}\right)\sinh(\beta(E)a) + \left(af(E)\frac{d\beta(E)}{dE} + \frac{dg(E)}{dE}\right)\cosh(\beta(E)a)\right] \\
\frac{d^2E}{dk^2} &= -\left(\frac{T^2\cos(kT) + \hbar^2 v_G^2 H_1(E)}{H_2(E)}\right)
\end{aligned}
$$

The effective mass is given by the following equation.

$$
\begin{aligned}
m^* &= \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1} \\
m^* &= \hbar^2\left(\frac{-T^2\cos(kT) - \hbar^2 v_G^2 H_1(E)}{H_2(E)}\right)^{-1} \\
m^* &= \frac{-\hbar^2 H_2(E)}{T^2\cos(kT) + \hbar^2 v_G^2 H_1(E)}
\end{aligned}
$$

Where,

$$
\begin{aligned}
H_1(E) = {} & \left[ag(E)\frac{d^2\beta(E)}{dE^2} + 2a\frac{dg(E)}{dE}\frac{d\beta(E)}{dE} + \frac{d^2 f(E)}{dE^2} + a^2 f(E)\left(\frac{d\beta(E)}{dE}\right)^2\right]\sinh\left(\beta(E)a\right) \\
& + \left[af(E)\frac{d^2\beta(E)}{dE^2} + 2a\frac{df(E)}{dE}\frac{d\beta(E)}{dE} + \frac{d^2 g(E)}{dE^2} + a^2 g(E)\left(\frac{d\beta(E)}{dE}\right)^2\right]\cosh\left(\beta(E)a\right) \\
H_2(E) = {} & \left(ag(E)\frac{d\beta(E)}{dE} + \frac{df(E)}{dE}\right)\sinh\left(\beta(E)a\right) + \left(af(E)\frac{d\beta(E)}{dE} + \frac{dg(E)}{dE}\right)\cosh\left(\beta(E)a\right)
\end{aligned}
$$

Section S6 Generalization for N-potentials coupled to a known potential

Using Bloch's theorem for N coupled potentials of the form $V = \{V_1, V_2, V_3, \cdots, V_N\}$ and a known potential, the following conditions must be satisfied:

$$
\begin{aligned}
\Psi_1(b_2) &= \Psi_2(b_2)\\
\Psi_2(b_3) &= \Psi_3(b_3)\\
\Psi_3(b_4) &= \Psi_4(b_4)\\
\Psi_4(b_5) &= \Psi_5(b_5)\\
\vdots &= \vdots\\
\Psi_1(b_1) &= e^{ikT}\Psi_{n+1}(b_m)\\
\Psi_1^{'}(b_2) &= \Psi_2^{'}(b_2)\\
\Psi_2^{'}(b_3) &= \Psi_3^{'}(b_3)\\
\Psi_3^{'}(b_4) &= \Psi_4^{'}(b_4)\\
\Psi_4^{'}(b_5) &= \Psi_5^{'}(b_5)\\
\vdots &= \vdots\\
\Psi_1^{'}(b_1) &= e^{ikT}\Psi_{n+1}^{'}(b_m)
\end{aligned}
$$

The transcendental energy equation is obtained by calculating the secular determinant of the transcendental energy equation for N potentials coupled to a known potential.

$$
0 = \begin{vmatrix}
y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) & -y_{n+1}(b_{n+1}) & -z_{n+1}(b_{n+1})\\
y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & -e^{ikT}y_{n+1}(b_m) & -e^{ikT}z_{n+1}(b_m)\\
y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n^{'}(b_{n+1}) & z_n^{'}(b_{n+1}) & -y_{n+1}^{'}(b_{n+1}) & -z_{n+1}^{'}(b_{n+1})\\
y_1^{'}(b_1) & z_1^{'}(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & -e^{ikT}y_{n+1}^{'}(b_m) & -e^{ikT}z_{n+1}^{'}(b_m)
\end{vmatrix}
$$

By rearranging some rows of the secular determinant, we obtain this new determinant.

$$
0 = \begin{vmatrix}
y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) & 0 & 0\\
y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) & -y_{n+1}(b_{n+1}) & -z_{n+1}(b_{n+1})\\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n^{'}(b_{n+1}) & z_n^{'}(b_{n+1}) & -y_{n+1}^{'}(b_{n+1}) & -z_{n+1}^{'}(b_{n+1})\\
y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & -e^{ikT}y_{n+1}(b_m) & -e^{ikT}z_{n+1}(b_m)\\
y_1^{'}(b_1) & z_1^{'}(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & -e^{ikT}y_{n+1}^{'}(b_m) & -e^{ikT}z_{n+1}^{'}(b_m)
\end{vmatrix}
$$

To solve the secular determinant of the coefficient matrix, we will divide the determinant into four subdeterminants to make the calculation of the transcendental energy equation easier to be handle and the expected result is:

$$0 = D_1 + D_2 + D_3 + D_4$$

Therefore,

applied sciences MDPI

Section S6.1 Determinant D1

$$D1 = z_{n+1}(b_{n+1}) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) & 0 \\ y_1'(b_2) & z_1'(b_2) & -y_2'(b_2) & -z_2'(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2'(b_3) & z_2'(b_3) & -y_3'(b_3) & -z_3'(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}'(b_n) & z_{n-1}'(b_n) & -y_n'(b_n) & -z_n'(b_n) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n'(b_{n+1}) & z_n'(b_{n+1}) & -y_{n+1}'(b_{n+1}) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & -e^{ikT}y_{n+1}(b_m) \\ y_1'(b_1) & z_1'(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & -e^{ikT}y_{n+1}'(b_m) \end{vmatrix}$$

The subdeterminants of the determinant D1 are the following three:

Section S6.1.1 $DH_1^1(E)$

$$DH_1^1(E) = -y_{n+1}'(b_{n+1}) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1'(b_2) & z_1'(b_2) & -y_2'(b_2) & -z_2'(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2'(b_3) & z_2'(b_3) & -y_3'(b_3) & -z_3'(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}'(b_n) & z_{n-1}'(b_n) & -y_n'(b_n) & -z_n'(b_n) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ y_1'(b_1) & z_1'(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Section S6.1.2 $DH_1^2(E)$

$$DH_1^2(E) = e^{ikT}y_{n+1}(b_m) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1'(b_2) & z_1'(b_2) & -y_2'(b_2) & -z_2'(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2'(b_3) & z_2'(b_3) & -y_3'(b_3) & -z_3'(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}'(b_n) & z_{n-1}'(b_n) & -y_n'(b_n) & -z_n'(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n'(b_{n+1}) & z_n'(b_{n+1}) \\ y_1'(b_1) & z_1'(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Section S6.1.3 $DH_1^3(E)$

$$DH_1^3(E) = -e^{ikT}y_{n+1}'(b_m) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1'(b_2) & z_1'(b_2) & -y_2'(b_2) & -z_2'(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2'(b_3) & z_2'(b_3) & -y_3'(b_3) & -z_3'(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}'(b_n) & z_{n-1}'(b_n) & -y_n'(b_n) & -z_n'(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n'(b_{n+1}) & z_n'(b_{n+1}) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Section S6.2 Determinant D2

$$D2 = -z'_{n+1}(b_{n+1}) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) & 0 \\ y'_1(b_2) & z'_1(b_2) & -y'_2(b_2) & -z'_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & y'_2(b_3) & z'_2(b_3) & -y'_3(b_3) & -z'_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y'_{n-1}(b_n) & z'_{n-1}(b_n) & -y'_n(b_n) & -z'_n(b_n) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) & -y_{n+1}(b_{n+1}) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & -e^{ikT}y_{n+1}(b_m) \\ y'_1(b_1) & z'_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & -e^{ikT}y'_{n+1}(b_m) \end{vmatrix}$$

The subdeterminants of the determinant D2 are the following three:

Section S6.2.1 $DH_2^1(E)$

$$DH_2^1(E) = -y_{n+1}(b_{n+1}) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y'_1(b_2) & z'_1(b_2) & -y'_2(b_2) & -z'_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y'_2(b_3) & z'_2(b_3) & -y'_3(b_3) & -z'_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y'_{n-1}(b_n) & z'_{n-1}(b_n) & -y'_n(b_n) & -z'_n(b_n) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ y'_1(b_1) & z'_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Section S6.2.2 $DH_2^2(E)$

$$DH_2^2(E) = e^{ikT}y_{n+1}(b_m) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y'_1(b_2) & z'_1(b_2) & -y'_2(b_2) & -z'_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y'_2(b_3) & z'_2(b_3) & -y'_3(b_3) & -z'_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y'_{n-1}(b_n) & z'_{n-1}(b_n) & -y'_n(b_n) & -z'_n(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) \\ y'_1(b_1) & z'_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Section S6.2.3 $DH_2^3(E)$

$$DH_2^3(E) = -e^{ikT}y'_{n+1}(b_m) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y'_1(b_2) & z'_1(b_2) & -y'_2(b_2) & -z'_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y'_2(b_3) & z'_2(b_3) & -y'_3(b_3) & -z'_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y'_{n-1}(b_n) & z'_{n-1}(b_n) & -y'_n(b_n) & -z'_n(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Section S6.3 Determinant D3

$$D3 = e^{ikT} z_{n+1}(b_m) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) & 0 \\ y_1'(b_2) & z_1'(b_2) & -y_2'(b_2) & -z_2'(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2'(b_3) & z_2'(b_3) & -y_3'(b_3) & -z_3'(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}'(b_n) & z_{n-1}'(b_n) & -y_n'(b_n) & -z_n'(b_n) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) & -y_{n+1}(b_{n+1}) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n'(b_{n+1}) & z_n'(b_{n+1}) & -y_{n+1}'(b_{n+1}) \\ y_1'(b_1) & z_1'(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & -e^{ikT} y_{n+1}'(b_m) \end{vmatrix}$$

The subdeterminants of the determinant D3 are the following three:

Section S6.3.1 $DH_3^1(E)$

$$DH_3^1(E) = -y_{n+1}(b_{n+1}) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1'(b_2) & z_1'(b_2) & -y_2'(b_2) & -z_2'(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2'(b_3) & z_2'(b_3) & -y_3'(b_3) & -z_3'(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}'(b_n) & z_{n-1}'(b_n) & -y_n'(b_n) & -z_n'(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n'(b_{n+1}) & z_n'(b_{n+1}) \\ y_1'(b_1) & z_1'(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Section S6.3.2 $DH_3^2(E)$

$$DH_3^2(E) = y_{n+1}'(b_{n+1}) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1'(b_2) & z_1'(b_2) & -y_2'(b_2) & -z_2'(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2'(b_3) & z_2'(b_3) & -y_3'(b_3) & -z_3'(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}'(b_n) & z_{n-1}'(b_n) & -y_n'(b_n) & -z_n'(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) \\ y_1'(b_1) & z_1'(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Section S6.3.3 $DH_3^3(E)$

$$DH_3^3(E) = -e^{ikT} y_{n+1}'(b_m) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1'(b_2) & z_1'(b_2) & -y_2'(b_2) & -z_2'(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2'(b_3) & z_2'(b_3) & -y_3'(b_3) & -z_3'(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}'(b_n) & z_{n-1}'(b_n) & -y_n'(b_n) & -z_n'(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n'(b_{n+1}) & z_n'(b_{n+1}) \end{vmatrix}$$

Section S6.4 Determinant D4

$$D4 = -e^{ikT} z_{n+1}^{'}(b_m) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) & 0 \\ y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) & -y_{n+1}(b_{n+1}) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n^{'}(b_{n+1}) & z_n^{'}(b_{n+1}) & -y_{n+1}^{'}(b_{n+1}) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 & -e^{ikT} y_{n+1}(b_m) \end{vmatrix}$$

The subdeterminants of the determinant D4 are the following three:

Section S6.4.1 $DH_4^1(E)$

$$DH_4^1(E) = -y_{n+1}(b_{n+1}) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n^{'}(b_{n+1}) & z_n^{'}(b_{n+1}) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Section S6.4.2 $DH_4^2(E)$

$$DH_4^2(E) = y_{n+1}^{'}(b_{n+1}) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Section S6.4.3 $DH_4^3(E)$

$$DH_4^3(E) = -e^{ikT} y_{n+1}(b_m) \cdot \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n^{'}(b_{n+1}) & z_n^{'}(b_{n+1}) \end{vmatrix}$$

Section S6.5 Transcendental Energy Equation

The resulting transcendental energy equation is given by the following respective equation.

$$
\begin{aligned}
&0 = D1 + D2 + D3 + D4\\
&0 = z_{n+1}(b_{n+1}) \cdot \left[-y^{'}_{n+1}(b_{n+1}) \cdot H^1_1(E) + e^{ikT} y_{n+1}(b_m) \cdot H^2_1(E) - e^{ikT} y^{'}_{n+1}(b_m) \cdot H^3_1(E)\right]\\
&- z^{'}_{n+1}(b_{n+1}) \cdot \left[-y_{n+1}(b_{n+1}) \cdot H^1_2(E) + e^{ikT} y_{n+1}(b_m) \cdot H^2_2(E) - e^{ikT} y^{'}_{n+1}(b_m) \cdot H^3_2(E)\right]\\
&+ e^{ikT} z_{n+1}(b_m) \cdot \left[-y_{n+1}(b_{n+1}) \cdot H^1_3(E) + y^{'}_{n+1}(b_{n+1}) \cdot H^2_3(E) - e^{ikT} y^{'}_{n+1}(b_m) \cdot H^3_3(E)\right]\\
&- e^{ikT} z^{'}_{n+1}(b_m) \cdot \left[-y_{n+1}(b_{n+1}) \cdot H^1_4(E) + y^{'}_{n+1}(b_{n+1}) \cdot H^2_4(E) - e^{ikT} y_{n+1}(b_m) \cdot H^3_4(E)\right]
\end{aligned}
$$

Simplifying e^{ikT} of the transcendental energy equation and collecting like terms.

$$
\begin{aligned}
&0 = z_{n+1}(b_{n+1}) \cdot \left[-e^{-ikT} y^{'}_{n+1}(b_{n+1}) \cdot H^1_1(E) + y_{n+1}(b_m) \cdot H^2_1(E) - y^{'}_{n+1}(b_m) \cdot H^3_1(E)\right]\\
&- z^{'}_{n+1}(b_{n+1}) \cdot \left[-e^{-ikT} y_{n+1}(b_{n+1}) \cdot H^1_2(E) + y_{n+1}(b_m) \cdot H^2_2(E) - y^{'}_{n+1}(b_m) \cdot H^3_2(E)\right]\\
&+ z_{n+1}(b_m) \cdot \left[-y_{n+1}(b_{n+1}) \cdot H^1_3(E) + y^{'}_{n+1}(b_{n+1}) \cdot H^2_3(E) - e^{ikT} y^{'}_{n+1}(b_m) \cdot H^3_3(E)\right]\\
&- z^{'}_{n+1}(b_m) \cdot \left[-y_{n+1}(b_{n+1}) \cdot H^1_4(E) + y^{'}_{n+1}(b_{n+1}) \cdot H^2_4(E) - e^{ikT} y_{n+1}(b_m) \cdot H^3_4(E)\right]
\end{aligned}
$$

Grouping the terms, we can have the following condition:

$$
\begin{aligned}
&0 = z_{n+1}(b_{n+1}) \cdot \left[+y_{n+1}(b_m) \cdot H^2_1(E) - y^{'}_{n+1}(b_m) \cdot H^3_1(E)\right]\\
&- z^{'}_{n+1}(b_{n+1}) \cdot \left[+y_{n+1}(b_m) \cdot H^2_2(E) - y^{'}_{n+1}(b_m) \cdot H^3_2(E)\right]\\
&+ z_{n+1}(b_m) \cdot \left[-y_{n+1}(b_{n+1}) \cdot H^1_3(E) + y^{'}_{n+1}(b_{n+1}) \cdot H^2_3(E)\right]\\
&- z^{'}_{n+1}(b_m) \cdot \left[-y_{n+1}(b_{n+1}) \cdot H^1_4(E) + y^{'}_{n+1}(b_{n+1}) \cdot H^2_4(E)\right]\\
&+ e^{-ikT} \left[-z_{n+1}(b_{n+1}) y^{'}_{n+1}(b_{n+1}) \cdot H^1_1(E) + z^{'}_{n+1}(b_{n+1}) y_{n+1}(b_{n+1}) \cdot H^1_2(E)\right]\\
&+ e^{ikT} \left[-z_{n+1}(b_m) y^{'}_{n+1}(b_m) \cdot H^3_3(E) + z^{'}_{n+1}(b_m) y_{n+1}(b_m) \cdot H^3_4(E)\right]
\end{aligned}
$$

where

$$
\begin{aligned}
H^2_4(E) &= H^3_2(E)\\
H^2_1(E) &= H^1_3(E)\\
H^1_1(E) &= H^1_2(E)\\
H^2_2(E) &= H^2_3(E)\\
H^3_3(E) &= H^3_4(E)\\
H^1_4(E) &= H^3_1(E)
\end{aligned}
$$

Substituting the previous equalities in the transcendental energy equation, we have the following:

$$
\begin{aligned}
&0 = z_{n+1}(b_{n+1}) \cdot \left[y_{n+1}(b_m) \cdot H^2_1(E) - y^{'}_{n+1}(b_m) \cdot H^1_4(E)\right]\\
&- z^{'}_{n+1}(b_{n+1}) \cdot \left[y_{n+1}(b_m) \cdot H^2_2(E) - y^{'}_{n+1}(b_m) \cdot H^2_4(E)\right]\\
&+ z_{n+1}(b_m) \cdot \left[-y_{n+1}(b_{n+1}) \cdot H^2_1(E) + y^{'}_{n+1}(b_{n+1}) \cdot H^2_2(E)\right]\\
&- z^{'}_{n+1}(b_m) \cdot \left[-y_{n+1}(b_{n+1}) \cdot H^1_4(E) + y^{'}_{n+1}(b_{n+1}) \cdot H^2_4(E)\right]\\
&+ e^{-ikT} \cdot H^1_1(E) \left[-z_{n+1}(b_{n+1}) y^{'}_{n+1}(b_{n+1}) + z^{'}_{n+1}(b_{n+1}) y_{n+1}(b_{n+1})\right]\\
&+ e^{ikT} \cdot H^3_3(E) \left[-z_{n+1}(b_m) y^{'}_{n+1}(b_m) + z^{'}_{n+1}(b_m) y_{n+1}(b_m)\right]
\end{aligned}
$$

Grouping again the terms, we can rewrite as

$$
\begin{aligned}
0 = {} & H_4^2(E)\left[z_{n+1}^{'}(b_{n+1})y_{n+1}^{'}(b_m) - z_{n+1}^{'}(b_m)y_{n+1}^{'}(b_{n+1})\right] \\
& + H_1^2(E)\left[z_{n+1}(b_{n+1})y_{n+1}(b_m) - z_{n+1}(b_m)y_{n+1}(b_{n+1})\right] \\
& + H_2^2(E)\left[-z_{n+1}^{'}(b_{n+1})y_{n+1}(b_m) + z_{n+1}(b_m)y_{n+1}^{'}(b_{n+1})\right] \\
& + H_4^1(E)\left[-z_{n+1}(b_{n+1})y_{n+1}^{'}(b_m) + z_{n+1}^{'}(b_m)y_{n+1}(b_{n+1})\right] \\
& + e^{-ikT}\cdot H_1^1(E)\left[-z_{n+1}(b_{n+1})y_{n+1}^{'}(b_{n+1}) + z_{n+1}^{'}(b_{n+1})y_{n+1}(b_{n+1})\right] \\
& + e^{ikT}\cdot H_3^3(E)\left[-z_{n+1}(b_m)y_{n+1}^{'}(b_m) + z_{n+1}^{'}(b_m)y_{n+1}(b_m)\right]
\end{aligned}
$$

If we apply Abel's identity to the transcendental energy equation, the transcendental energy equation is written by:

$$
\begin{aligned}
0 = {} & H_4^2(E)\left[z_{n+1}^{'}(b_{n+1})y_{n+1}^{'}(b_m) - z_{n+1}^{'}(b_m)y_{n+1}^{'}(b_{n+1})\right] \\
& + H_1^2(E)\left[z_{n+1}(b_{n+1})y_{n+1}(b_m) - z_{n+1}(b_m)y_{n+1}(b_{n+1})\right] \\
& + H_2^2(E)\left[-z_{n+1}^{'}(b_{n+1})y_{n+1}(b_m) + z_{n+1}(b_m)y_{n+1}^{'}(b_{n+1})\right] \\
& + H_4^1(E)\left[-z_{n+1}(b_{n+1})y_{n+1}^{'}(b_m) + z_{n+1}^{'}(b_m)y_{n+1}(b_{n+1})\right] \\
& + e^{-ikT}\cdot H_1^1(E)W\left\{y_{n+1}, z_{n+1}\right\} \\
& + e^{ikT}\cdot H_3^3(E)W\left\{y_{n+1}, z_{n+1}\right\}
\end{aligned}
$$

The above equation represents the generalization of the transcendental energy equation, which is derived for N potentials $V(x)$ coupled together with a null potential. Now, we will prove that the determinants $H_1^1(E)$ and $H_3^3(E)$ are equal. Let the determinants be $H_1^1(E)$ and $H_3^3(E)$

$$
H_1^1(E) = \begin{vmatrix}
y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\
y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) \\
y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\
y_1^{'}(b_1) & z_1^{'}(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0
\end{vmatrix}
$$

$$
H_3^3(E) = \begin{vmatrix}
y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\
y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n^{'}(b_{n+1}) & z_n^{'}(b_{n+1})
\end{vmatrix}
$$

If the determinants of the matrices $H_1^1(E)$ and $H_3^3(E)$ have the same value, their substractions them yields a value equal to zero. This would simplify the transcendental energy equation remarkably.

$$H_1^1(E) - H_3^3(E) = \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & -y_n(b_{n+1}) & -z_n(b_{n+1}) \\ y_1^{'}(b_1) & z_1^{'}(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & -y_n^{'}(b_{n+1}) & -z_n^{'}(b_{n+1}) \end{vmatrix}$$

$$0 = \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & -y_n(b_{n+1}) & -z_n(b_{n+1}) \\ y_1^{'}(b_1) & z_1^{'}(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & -y_n^{'}(b_{n+1}) & -z_n^{'}(b_{n+1}) \end{vmatrix}$$

However, the above equation represents the secular determinant of N coupled potentials. Therefore, its secular determinant must be equal to zero. This implies that the determinants $H_1^1(E)$ and $H_3^3(E)$ have the same value.

$$\begin{aligned} \Psi_1(b_2) &= \Psi_2(b_2) \\ \Psi_2(b_3) &= \Psi_3(b_3) \\ \Psi_3(b_4) &= \Psi_4(b_4) \\ \Psi_4(b_5) &= \Psi_5(b_5) \\ \vdots &= \vdots \\ \Psi_1(b_1) &= \Psi_n(b_{n+1}) \\ \Psi_1^{'}(b_2) &= \Psi_2^{'}(b_2) \\ \Psi_2^{'}(b_3) &= \Psi_3^{'}(b_3) \\ \Psi_3^{'}(b_4) &= \Psi_4^{'}(b_4) \\ \Psi_4^{'}(b_5) &= \Psi_5^{'}(b_5) \\ \vdots &= \vdots \\ \Psi_1^{'}(b_1) &= \Psi_n^{'}(b_{n+1}) \end{aligned}$$

Therefore,

$$\begin{aligned} 0 = & H_4^2(E)\left[z_{n+1}^{'}(b_{n+1})y_{n+1}^{'}(b_m) - z_{n+1}^{'}(b_m)y_{n+1}^{'}(b_{n+1})\right] \\ & + H_1^2(E)\left[z_{n+1}(b_{n+1})y_{n+1}(b_m) - z_{n+1}(b_m)y_{n+1}(b_{n+1})\right] \\ & + H_2^2(E)\left[-z_{n+1}^{'}(b_{n+1})y_{n+1}(b_m) + z_{n+1}(b_m)y_{n+1}^{'}(b_{n+1})\right] \\ & + H_4^1(E)\left[-z_{n+1}(b_{n+1})y_{n+1}^{'}(b_m) + z_{n+1}^{'}(b_m)y_{n+1}(b_{n+1})\right] \\ & + e^{-ikT}\cdot H_0^0(E)W\left\{y_{n+1}, z_{n+1}\right\} \\ & + e^{ikT}\cdot H_0^0(E)W\left\{y_{n+1}, z_{n+1}\right\} \end{aligned}$$

$$\cos(kT) = -\Lambda(E)$$

$$\cos(kT) = \Gamma(E)$$

Where $\Gamma(E)$ is the energy function of the system and it is given by the following equation:

$$\begin{aligned}\Gamma(E) = &\frac{H_4^2(E)}{2H_0^0(E)W\left\{y_{n+1},z_{n+1}\right\}}\left[z_{n+1}^{'}(b_{n+1})y_{n+1}^{'}(b_m)-z_{n+1}^{'}(b_m)y_{n+1}^{'}(b_{n+1})\right]\\ &+\frac{H_1^2(E)}{2H_0^0(E)W\left\{y_{n+1},z_{n+1}\right\}}\left[z_{n+1}(b_{n+1})y_{n+1}(b_m)-z_{n+1}(b_m)y_{n+1}(b_{n+1})\right]\\ &+\frac{H_2^2(E)}{2H_0^0(E)W\left\{y_{n+1},z_{n+1}\right\}}\left[-z_{n+1}^{'}(b_{n+1})y_{n+1}(b_m)+z_{n+1}(b_m)y_{n+1}^{'}(b_{n+1})\right]\\ &+\frac{H_4^1(E)}{2H_0^0(E)W\left\{y_{n+1},z_{n+1}\right\}}\left[-z_{n+1}(b_{n+1})y_{n+1}^{'}(b_m)+z_{n+1}^{'}(b_m)y_{n+1}(b_{n+1})\right]\end{aligned}$$

- **Group velocity:**
  The group velocity associated with the system is given by the following equation:

$$v_G = -\frac{T\sin(kT)}{\hbar}\left(\frac{d\Gamma(E)}{dE}\right)^{-1}$$

  The extreme value of the group velocity is given by the following equation:

$$\begin{aligned}\frac{dv_G}{dk} &= -\frac{T}{\hbar}\left(T\cos(kT)\frac{d\Gamma(E)}{dE}-\sin(kT)\frac{d^2\Gamma(E)}{dE^2}\frac{dE}{dk}\right)\left(\frac{d\Gamma(E)}{dE}\right)^{-2}\\ 0 &= T\cos(kT)\frac{d\Gamma(E)}{dE}-\sin(kT)\frac{d^2\Gamma(E)}{dE^2}\frac{dE}{dk}\\ 0 &= T\cos(kT)\frac{d\Gamma(E)}{dE}-\hbar v_G\sin(kT)\frac{d^2\Gamma(E)}{dE^2}\\ 0 &= T\cos(kT)\frac{d\Gamma(E)}{dE}-\left(-T\sin(kT)\left(\frac{d\Gamma(E)}{dE}\right)^{-1}\right)\sin(kT)\frac{d^2\Gamma(E)}{dE^2}\\ 0 &= \cos(kT)\left(\frac{d\Gamma(E)}{dE}\right)^{2}+\sin^2(kT)\frac{d^2\Gamma(E)}{dE^2}\\ 0 &= \left(\frac{d\Gamma(E)}{dE}\right)^{2}+\frac{d^2\Gamma(E)}{dE^2}\sin(kT)\tan(kT)\\ 0 &= \frac{d^2\Gamma(E)}{dE^2}+\frac{1}{\sin(kT)\tan(kT)}\left(\frac{d\Gamma(E)}{dE}\right)^{2}\end{aligned}$$

- **Effective mass:**
  The effective mass associated with the system is given by the following equation:

$$m^* = -\hbar^2\frac{d\Gamma(E)}{dE}\left(T^2\cos(kT)+\frac{d^2\Gamma(E)}{dE^2}\hbar^2v_G^2\right)^{-1}$$

  The value of the discontinuity of the effective mass is given by the following equation:

$$\begin{aligned}0 &= T^2\cos(kT)+\frac{d^2\Gamma(E)}{dE^2}\hbar^2v_G^2\\ 0 &= \frac{d^2\Gamma(E)}{dE^2}+\frac{T^2\cos(kT)}{\hbar^2v_G^2}\\ 0 &= \frac{d^2\Gamma(E)}{dE^2}+T^2\cos(kT)\left(\frac{d\Gamma(E)}{dE}\right)^{2}\frac{1}{T^2\sin^2(kT)}\\ 0 &= \frac{d^2\Gamma(E)}{dE^2}+\frac{1}{\sin(kT)\tan(kT)}\left(\frac{d\Gamma(E)}{dE}\right)^{2}\end{aligned}$$

Section S7 Generalization for N-coupled potentials together with another arbitrary potential

Section S7.1 Generalization of the coupled zero-potential and approximation to the Dirac-delta periodic potential

Starting from the general solution for a potential $V = V(x)$

$$\cos(kT) = \Gamma(E)$$

$$\begin{aligned}\cos(kT) = &-\frac{H_4^2(E)}{2H_0^0(E)W\{y_{n+1},z_{n+1}\}}\left[z'_{n+1}(b_{n+1})y'_{n+1}(b_m) - z'_{n+1}(b_m)y'_{n+1}(b_{n+1})\right]\\ &-\frac{H_1^2(E)}{2H_0^0(E)W\{y_{n+1},z_{n+1}\}}\left[z_{n+1}(b_{n+1})y_{n+1}(b_m) - z_{n+1}(b_m)y_{n+1}(b_{n+1})\right]\\ &-\frac{H_2^2(E)}{2H_0^0(E)W\{y_{n+1},z_{n+1}\}}\left[-z'_{n+1}(b_{n+1})y_{n+1}(b_m) + z_{n+1}(b_m)y'_{n+1}(b_{n+1})\right]\\ &-\frac{H_4^1(E)}{2H_0^0(E)W\{y_{n+1},z_{n+1}\}}\left[-z_{n+1}(b_{n+1})y'_{n+1}(b_m) + z'_{n+1}(b_m)y_{n+1}(b_{n+1})\right]\end{aligned}$$

Using $\{y_{n+1}(x), z_{n+1}(x)\} = \left\{e^{i\alpha x}, e^{-i\alpha x}\right\}$ and substituting into the transcendental energy equation.

$$\begin{aligned}\cos(kT) = &-\frac{H_4^2(E)}{2H_0^0(E)\left[-2i\alpha\right]}\left[2i\alpha^2\sin(\alpha a)\right] - \frac{H_1^2(E)}{2H_0^0(E)\left[-2i\alpha\right]}\left[2i\sin(\alpha a)\right]\\ &-\frac{H_2^2(E)}{2H_0^0(E)\left[-2i\alpha\right]}\left[2i\alpha\cos(\alpha a)\right] - \frac{H_4^1(E)}{2H_0^0(E)\left[-2i\alpha\right]}\left[-2i\alpha\cos(\alpha a)\right]\end{aligned}$$

Therefore, the transcendental energy equation is given by:

$$\cos(kT) = \sin(\alpha a)\left[\alpha H_4^2(E) + \frac{H_1^2(E)}{\alpha}\right] + \cos(\alpha a)\left[H_2^2(E) - H_4^1(E)\right]$$

$$\cos(kT) = \sin(\alpha a)\left[\frac{H_1^2(E) + \alpha^2 H_4^2(E)}{2\alpha H_0^0(E)}\right] + \cos(\alpha a)\left[\frac{H_2^2(E) - H_4^1(E)}{2H_0^0(E)}\right]$$

To find the group velocity and related effective mass, the energy $f_0(E)$ and $g_0(E)$ functions must first be defined as:

$$f_0(E) = \frac{H_1^2(E) + \alpha^2 H_4^2(E)}{2\alpha H_0^0(E)} \quad , \quad g_0(E) = \frac{H_2^2(E) - H_4^1(E)}{2H_0^0(E)}$$

Once $f_0(E)$ and $g_0(E)$ have been defined, we proceed to calculate the energy derivatives of $\Gamma(E)$ with in which, we can obtain the group velocity and related effective mass by:

$$\Gamma(E) = \sin(\alpha a)\left[\frac{H_1^2(E) + \alpha^2 H_4^2(E)}{2\alpha H_0^0(E)}\right] + \cos(\alpha a)\left[\frac{H_2^2(E) - H_4^1(E)}{2H_0^0(E)}\right]$$

$$\frac{d\Gamma(E)}{dE} = \left(\frac{df_0(E)}{dE} - ag_0(E)\frac{d\alpha(E)}{dE}\right)\sin(\alpha(E)a) + \left(af_0(E)\frac{d\alpha(E)}{dE} + \frac{dg_0(E)}{dE}\right)\cos(\alpha(E)a)$$

$$\begin{aligned}\frac{d^2\Gamma(E)}{dE^2} = &\left[\frac{d^2f_0(E)}{dE^2} - a^2 f_0(E)\left(\frac{d\alpha(E)}{dE}\right)^2\right]\sin(\alpha(E)a) - \left[ag_0(E)\frac{d^2\alpha(E)}{dE^2} + 2a\frac{dg_0(E)}{dE}\frac{d\alpha(E)}{dE}\right]\sin(\alpha(E)a)\\ &+\left[af_0(E)\frac{d^2\alpha(E)}{dE^2} + 2a\frac{df_0(E)}{dE}\frac{d\alpha(E)}{dE}\right]\cos(\alpha(E)a) + \left[\frac{d^2g_0(E)}{dE^2} + a^2 g_0(E)\left(\frac{d\alpha(E)}{dE}\right)^2\right]\cos(\alpha(E)a)\end{aligned}$$

To perform the Dirac-delta periodic potential approximation, the following limits must be satisfied:

$$\lim_{(b,w)\to(0,\infty)}\left(\alpha f_0(E)\right) = \lim_{(b,w)\to(0,\infty)}\left(\frac{H_1^2(E) + \alpha^2 H_4^2(E)}{2H_0^0(E)}\right) = F_d(b,w)$$

$$\lim_{(b,w)\to(0,\infty)}\left(g_0(E)\right) = \lim_{(b,w)\to(0,\infty)}\left(\frac{H_2^2(E) - H_4^1(E)}{2H_0^0(E)}\right) = 1$$

Section S7.2 Generalization of the coupled rectangular-like potential and approximation the Kronig-Penney periodic potential

Starting from the general solution for a potential $V = V(x)$

$$\begin{aligned}
\cos(kT) &= \Gamma(E) \\
\cos(kT) &= -\frac{H_4^2(E)}{2H_0^0(E)W\{y_{n+1}, z_{n+1}\}}\left[z'_{n+1}(b_{n+1})y'_{n+1}(b_m) - z'_{n+1}(b_m)y'_{n+1}(b_{n+1})\right] \\
&\quad - \frac{H_1^2(E)}{2H_0^0(E)W\{y_{n+1}, z_{n+1}\}}\left[z_{n+1}(b_{n+1})y_{n+1}(b_m) - z_{n+1}(b_m)y_{n+1}(b_{n+1})\right] \\
&\quad - \frac{H_2^2(E)}{2H_0^0(E)W\{y_{n+1}, z_{n+1}\}}\left[-z'_{n+1}(b_{n+1})y_{n+1}(b_m) + z_{n+1}(b_m)y'_{n+1}(b_{n+1})\right] \\
&\quad - \frac{H_4^1(E)}{2H_0^0(E)W\{y_{n+1}, z_{n+1}\}}\left[-z_{n+1}(b_{n+1})y'_{n+1}(b_m) + z'_{n+1}(b_m)y_{n+1}(b_{n+1})\right]
\end{aligned}$$

Using the solution functions of the rectangular potential $\{y_{n+1}(x), z_{n+1}(x)\} = \left\{e^{\beta x}, e^{-\beta x}\right\}$ and substituting into the secular equation for a general potential $V = V(x)$, we have:

$$\begin{aligned}
\cos(kT) = &-\frac{H_4^2(E)}{2H_0^0(E)[-2\beta]}\left[-2\beta^2\sinh(\alpha a)\right] - \frac{H_1^2(E)}{2H_0^0(E)[-2\beta]}\left[2\sinh(\alpha a)\right] \\
&- \frac{H_2^2(E)}{2H_0^0(E)[-2\beta]}\left[2\beta\cosh(\alpha a)\right] - \frac{H_4^1(E)}{2H_0^0(E)[-2\beta]}\left[-2\beta\cosh(\alpha a)\right]
\end{aligned}$$

Therefore, the transcendental energy equation is rewriten as

$$\begin{aligned}
H_0^0(E)\left(e^{ikT} + e^{-ikT}\right) &= \sinh(\beta a)\left[-\beta H_4^2(E) + \frac{H_1^2(E)}{\beta}\right] + \cosh(\beta a)\left[H_2^2(E) - H_4^1(E)\right] \\
\cos(kT) &= \sinh(\beta a)\left[\frac{H_1^2(E) - \beta^2 H_4^2(E)}{2\beta H_0^0(E)}\right] + \cosh(\beta a)\left[\frac{H_2^2(E) - H_4^1(E)}{2H_0^0(E)}\right]
\end{aligned}$$

To find the group velocity and related effective mass, the energy $f_r(E)$ and $g_r(E)$ functions must first be defined as:

$$f_r(E) = \frac{H_1^2(E) - \beta^2 H_4^2(E)}{2\beta H_0^0(E)} \quad , \quad g_r(E) = \frac{H_2^2(E) - H_4^1(E)}{2H_0^0(E)}$$

Once $f_d(E)$ and $g_d(E)$ have been defined, we proceed to calculate the energy derivatives of $\Gamma(E)$ with in which, we can obtain the group velocity and related effective mass as:

$$\begin{aligned}
\Gamma(E) &= \sinh(\beta a)\left[\frac{H_1^2(E) - \beta^2 H_4^2(E)}{2\beta H_0^0(E)}\right] + \cosh(\beta a)\left[\frac{H_2^2(E) - H_4^1(E)}{2H_0^0(E)}\right] \\
\frac{d\Gamma(E)}{dE} &= \left(\frac{df_r(E)}{dE} + a g_r(E)\frac{d\beta(E)}{dE}\right)\sinh(\beta(E)a) + \left(\frac{dg_r(E)}{dE} + a f_r(E)\frac{d\beta(E)}{dE}\right)\cosh(\beta(E)a) \\
\frac{d^2\Gamma(E)}{dE^2} &= \left[a g_r(E)\frac{d^2\beta(E)}{dE^2} + 2a\frac{dg_r(E)}{dE}\frac{d\beta(E)}{dE}\right]\sinh(\beta(E)a) + \left[\frac{d^2 f_r(E)}{dE^2} + a^2 f_r(E)\left(\frac{d\beta(E)}{dE}\right)^2\right]\sinh(\beta(E)a) \\
&\quad + \left[a f_r(E)\frac{d^2\beta(E)}{dE^2} + 2a\frac{df_r(E)}{dE}\frac{d\beta(E)}{dE}\right]\cosh(\beta(E)a) + \left[\frac{d^2 g_r(E)}{dE^2} + a^2 g_r(E)\left(\frac{d\beta(E)}{dE}\right)^2\right]\cosh(\beta(E)a)
\end{aligned}$$

To perform the periodic potential approximation Kronig-Penney must satisfy the following limits:

$$\begin{aligned}
\lim_{w\to 0}(f_r) &= \lim_{w\to 0}\left(\frac{H_1^2(E) - \beta^2 H_4^2(E)}{2\beta H_0^0(E)}\right) = F_{kp}(b, w, E) \\
\lim_{w\to 0}(g_r) &= \lim_{w\to 0}\left(\frac{H_2^2(E) - H_4^1(E)}{2H_0^0(E)}\right) = G_{kp}(b, w, E)
\end{aligned}$$

Section S8 Proof of the value of the determinant $H_0^0(E)$

The determinant $H_0^0(E)$ is equal to $H_1^1(E)$ and $H_3^3(E)$. Therefore, it must first be shown that $H_1^1(E) = H_3^3(E)$.

Section S8.1 Determinant $H_1^1(E)$

$$H_1^1(E) = \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) \\ y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ y_1^{'}(b_1) & z_1^{'}(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{vmatrix}$$

Performing a row swap on the determinant of the matrix $H_1^1(E)$

$$H_1^1(E) = \begin{vmatrix} y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ y_1^{'}(b_1) & z_1^{'}(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y_1^{'}(b_2) & z_1^{'}(b_2) & -y_2^{'}(b_2) & -z_2^{'}(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2^{'}(b_3) & z_2^{'}(b_3) & -y_3^{'}(b_3) & -z_3^{'}(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}^{'}(b_n) & z_{n-1}^{'}(b_n) & -y_n^{'}(b_n) & -z_n^{'}(b_n) \end{vmatrix}$$

Now by means of mathematical induction we are going to prove the determinant $H_1^1(E)$ is equal to a product of wronskians of the Schrödinger wave functions.

Section S8.1.1 From k to $k+1$

The determinant D_{k+1} is given by the following equation:

$$D_{k+1} = \begin{vmatrix} y_k(b_k) & z_k(b_k) & 0 & 0 \\ y_k^{'}(b_k) & z_k^{'}(b_k) & 0 & 0 \\ y_k(b_{k+1}) & z_k(b_{k+1}) & -y_{k+1}(b_{k+1}) & -z_{k+1}(b_{k+1}) \\ y_k^{'}(b_{k+1}) & z_k^{'}(b_{k+1}) & -y_{k+1}^{'}(b_{k+1}) & -z_{k+1}^{'}(b_{k+1}) \end{vmatrix}$$

$$D_{k+1} = [y_k(b_k) \cdot z_k^{'}(b_k) - z_k(b_k) \cdot y_k^{'}(b_k)] \cdot \begin{vmatrix} -y_{k+1}(b_{k+1}) & -z_{k+1}(b_{k+1}) \\ -y_{k+1}^{'}(b_{k+1}) & -z_{k+1}^{'}(b_{k+1}) \end{vmatrix}$$

$$D_{k+1} = [y_k(b_k) \cdot z_k^{'}(b_k) - z_k(b_k) \cdot y_k^{'}(b_k)] \cdot [y_{k+1}(b_{k+1}) \cdot z_{k+1}^{'}(b_{k+1}) - z_{k+1}(b_{k+1}) \cdot y_{k+1}^{'}(b_{k+1})]$$

$$D_{k+1} = W\left\{y_k(b_k), z_k(b_k)\right\} \cdot W\left\{y_{k+1}(b_{k+1}), z_{k+1}(b_{k+1})\right\}$$

Section S8.1.2 From k to $k+1$ and from $k+1$ to $k+2$

The determinant D_{k+2} is given by the following equation:

$$D_{k+2} = \begin{vmatrix} y_k(b_k) & z_k(b_k) & 0 & 0 & 0 & 0 \\ y_k^{'}(b_k) & z_k^{'}(b_k) & 0 & 0 & 0 & 0 \\ y_k(b_{k+1}) & z_k(b_{k+1}) & -y_{k+1}(b_{k+1}) & -z_{k+1}(b_{k+1}) & 0 & 0 \\ 0 & 0 & y_{k+1}(b_{k+2}) & z_{k+1}(b_{k+2}) & -y_{k+2}(b_{k+2}) & -z_{k+2}(b_{k+2}) \\ y_k^{'}(b_{k+1}) & z_k^{'}(b_{k+1}) & -y_{k+1}^{'}(b_{k+1}) & -z_{k+1}^{'}(b_{k+1}) & 0 & 0 \\ 0 & 0 & y_{k+1}^{'}(b_{k+2}) & z_{k+1}^{'}(b_{k+2}) & -y_{k+2}^{'}(b_{k+2}) & -z_{k+2}^{'}(b_{k+2}) \end{vmatrix}$$

$$D_{k+2}=-\begin{vmatrix} y_k(b_k) & z_k(b_k) & 0 & 0 & 0 & 0\\ y_k'(b_k) & z_k'(b_k) & 0 & 0 & 0 & 0\\ y_k(b_{k+1}) & z_k(b_{k+1}) & -y_{k+1}(b_{k+1}) & -z_{k+1}(b_{k+1}) & 0 & 0\\ y_k'(b_{k+1}) & z_k'(b_{k+1}) & -y_{k+1}'(b_{k+1}) & -z_{k+1}'(b_{k+1}) & 0 & 0\\ 0 & 0 & y_{k+1}(b_{k+2}) & z_{k+1}(b_{k+2}) & -y_{k+2}(b_{k+2}) & -z_{k+2}(b_{k+2})\\ 0 & 0 & y_{k+1}'(b_{k+2}) & z_{k+1}'(b_{k+2}) & -y_{k+2}'(b_{k+2}) & -z_{k+2}'(b_{k+2}) \end{vmatrix}$$

$$D_{k+2}=-\left[y_k(b_k)\cdot z_k'(b_k)-z_k(b_k)\cdot y_k'(b_k)\right]\cdot\begin{vmatrix} -y_{k+1}(b_{k+1}) & -z_{k+1}(b_{k+1}) & 0 & 0\\ -y_{k+1}'(b_{k+1}) & -z_{k+1}'(b_{k+1}) & 0 & 0\\ y_{k+1}(b_{k+2}) & z_{k+1}(b_{k+2}) & -y_{k+2}(b_{k+2}) & -z_{k+2}(b_{k+2})\\ y_{k+1}'(b_{k+2}) & z_{k+1}'(b_{k+2}) & -y_{k+2}'(b_{k+2}) & -z_{k+2}'(b_{k+2}) \end{vmatrix}$$

$$D_{k+2}=-W\left\{y_k(b_k),z_k(b_k)\right\}\cdot\begin{vmatrix} -y_{k+1}(b_{k+1}) & -z_{k+1}(b_{k+1}) & 0 & 0\\ -y_{k+1}'(b_{k+1}) & -z_{k+1}'(b_{k+1}) & 0 & 0\\ y_{k+1}(b_{k+2}) & z_{k+1}(b_{k+2}) & -y_{k+2}(b_{k+2}) & -z_{k+2}(b_{k+2})\\ y_{k+1}'(b_{k+2}) & z_{k+1}'(b_{k+2}) & -y_{k+2}'(b_{k+2}) & -z_{k+2}'(b_{k+2}) \end{vmatrix}$$

$$D_{k+2}=-W\left\{y_k(b_k),z_k(b_k)\right\}\cdot\begin{vmatrix} y_{k+1}(b_{k+1}) & z_{k+1}(b_{k+1}) & 0 & 0\\ y_{k+1}'(b_{k+1}) & z_{k+1}'(b_{k+1}) & 0 & 0\\ y_{k+1}(b_{k+2}) & z_{k+1}(b_{k+2}) & -y_{k+2}(b_{k+2}) & -z_{k+2}(b_{k+2})\\ y_{k+1}'(b_{k+2}) & z_{k+1}'(b_{k+2}) & -y_{k+2}'(b_{k+2}) & -z_{k+2}'(b_{k+2}) \end{vmatrix}$$

If $k+1=p$, then we may write as

$$D_{p+1}=-W\left\{y_{p-1}(b_{p-1}),z_{p-1}(b_{p-1})\right\}\cdot\begin{vmatrix} y_p(b_p) & z_p(b_p) & 0 & 0\\ y_p'(b_p) & z_p'(b_p) & 0 & 0\\ y_p(b_{p+1}) & z_{k+1}(b_{p+1}) & -y_{p+1}(b_{p+1}) & -z_{p+1}(b_{p+1})\\ y_p'(b_{p+1}) & z_p'(b_{p+1}) & -y_{p+1}'(b_{p+1}) & -z_{p+1}'(b_{p+1}) \end{vmatrix}$$

$$D_{p+1}=-W\left\{y_{p-1}(b_{p-1}),z_{p-1}(b_{p-1})\right\}\cdot W\left\{y_p(b_p),z_p(b_p)\right\}\cdot W\left\{y_{p+1}(b_{p+1}),z_{p+1}(b_{p+1})\right\}$$

$$D_{k+2}=-W\left\{y_k(b_k),z_k(b_k)\right\}\cdot W\left\{y_{k+1}(b_{k+1}),z_{k+1}(b_{k+1})\right\}\cdot W\left\{y_{k+2}(b_{k+2}),z_{k+2}(b_{k+2})\right\}$$

Therefore,

$$H_1^1(E)=\begin{vmatrix} y_1(b_1) & z_1(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0\\ y_1'(b_1) & z_1'(b_1) & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0\\ y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0\\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n)\\ y_1'(b_2) & z_1'(b_2) & -y_2'(b_2) & -z_2'(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0\\ 0 & 0 & y_2'(b_3) & z_2'(b_3) & -y_3'(b_3) & -z_3'(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}'(b_n) & z_{n-1}'(b_n) & -y_n'(b_n) & -z_n'(b_n) \end{vmatrix}$$

$$H_1^1(E)=W\left\{y_1(b_1),z_1(b_1)\right\}\cdot\prod_{k=2}^{n}\left[(-1)^n\cdot W\left\{y_k(b_k),z_k(b_k)\right\}\right]$$

$$H_1^1(E)=(-1)^n\cdot W\left\{y_1(b_1),z_1(b_1)\right\}\cdot W\left\{y_2(b_2),z_2(b_2)\right\}\cdot W\left\{y_3(b_3),z_3(b_3)\right\}\quad\cdots\quad W\left\{y_n(b_n),z_n(b_n)\right\}$$

Section S8.2 Determinant $H_3^3(E)$

$$H_3^3(E)=\begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0\\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n)\\ y_1'(b_2) & z_1'(b_2) & -y_2'(b_2) & -z_2'(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0\\ 0 & 0 & y_2'(b_3) & z_2'(b_3) & -y_3'(b_3) & -z_3'(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}'(b_n) & z_{n-1}'(b_n) & -y_n'(b_n) & -z_n'(b_n)\\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1})\\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n'(b_{n+1}) & z_n'(b_{n+1}) \end{vmatrix}$$

Now by means of mathematical induction we are going to prove the determinant $H_3^3(E)$ is equal to a product of wronskians of the Schrödinger wave functions respectively.

Section S8.2.1 From k to $k-1$

The determinant D_{k-1} is given by the following equation:

$$D_{k-1} = \begin{vmatrix} y_{k-1}(b_k) & z_{k-1}(b_k) & -y_k(b_k) & -z_k(b_k) \\ y'_{k-1}(b_k) & z'_{k-1}(b_k) & -y'_k(b_k) & -z'_k(b_k) \\ 0 & 0 & y_k(b_{k+1}) & z_k(b_{k+1}) \\ 0 & 0 & y'_k(b_{k+1}) & z'_k(b_{k+1}) \end{vmatrix}$$

$$D_{k-1} = [y_k(b_{k+1}) \cdot z'_k(b_{k+1}) - z_k(b_{k+1}) \cdot y'_k(b_{k+1})] \cdot \begin{vmatrix} y_{k-1}(b_k) & z_{k-1}(b_k) \\ y'_{k-1}(b_k) & z'_{k-1}(b_k) \end{vmatrix}$$

$$D_{k-1} = [y_k(b_{k+1}) \cdot z'_k(b_{k+1}) - z_k(b_{k+1}) \cdot y'_k(b_{k+1})] \cdot [y_{k-1}(b_k) \cdot z'_{k-1}(b_k) - z_{k-1}(b_k) \cdot y'_{k-1}(b_k)]$$

$$D_{k-1} = W\{y_k(b_{k+1}), z_k(b_{k+1})\} \cdot W\{y_{k-1}(b_k), z_{k-1}(b_k)\}$$

Section S8.2.2 From k to $k-1$ and from $k-1$ to $k-2$

The determinant D_{k-2} is given by the following equation:

$$D_{k-2} = \begin{vmatrix} y_{k-2}(b_{k-1}) & z_{k-2}(b_{k-1}) & -y_{k-1}(b_{k-1}) & -z_{k-1}(b_{k-1}) & 0 & 0 \\ 0 & 0 & y_{k-1}(b_k) & z_{k-1}(b_k) & -y_k(b_k) & -z_k(b_k) \\ y'_{k-2}(b_{k-1}) & z'_{k-2}(b_{k-1}) & -y'_{k-1}(b_{k-1}) & -z'_{k-1}(b_{k-1}) & 0 & 0 \\ 0 & 0 & y'_{k-1}(b_k) & z'_{k-1}(b_k) & -y'_k(b_k) & -z'_k(b_k) \\ 0 & 0 & 0 & 0 & y_k(b_{k+1}) & z_k(b_{k+1}) \\ 0 & 0 & 0 & 0 & y'_k(b_{k+1}) & z'_k(b_{k+1}) \end{vmatrix}$$

$$D_{k-2} = - \begin{vmatrix} y_{k-2}(b_{k-1}) & z_{k-2}(b_{k-1}) & -y_{k-1}(b_{k-1}) & -z_{k-1}(b_{k-1}) & 0 & 0 \\ y'_{k-2}(b_{k-1}) & z'_{k-2}(b_{k-1}) & -y'_{k-1}(b_{k-1}) & -z'_{k-1}(b_{k-1}) & 0 & 0 \\ 0 & 0 & y_{k-1}(b_k) & z_{k-1}(b_k) & -y_k(b_k) & -z_k(b_k) \\ 0 & 0 & y'_{k-1}(b_k) & z'_{k-1}(b_k) & -y'_k(b_k) & -z'_k(b_k) \\ 0 & 0 & 0 & 0 & y_k(b_{k+1}) & z_k(b_{k+1}) \\ 0 & 0 & 0 & 0 & y'_k(b_{k+1}) & z'_k(b_{k+1}) \end{vmatrix}$$

$$D_{k-2} = - \left[z'_k(b_{k+1}) \cdot y_k(b_{k+1}) - y'_k(b_{k+1}) \cdot z_k(b_{k+1})\right] \cdot \begin{vmatrix} y_{k-2}(b_{k-1}) & z_{k-2}(b_{k-1}) & -y_{k-1}(b_{k-1}) & -z_{k-1}(b_{k-1}) \\ y'_{k-2}(b_{k-1}) & z'_{k-2}(b_{k-1}) & -y'_{k-1}(b_{k-1}) & -z'_{k-1}(b_{k-1}) \\ 0 & 0 & y_{k-1}(b_k) & z_{k-1}(b_k) \\ 0 & 0 & y'_{k-1}(b_k) & z'_{k-1}(b_k) \end{vmatrix}$$

$$D_{k-2} = -W\{y_k(b_{k+1}), z_k(b_{k+1})\} \cdot \begin{vmatrix} y_{k-2}(b_{k-1}) & z_{k-2}(b_{k-1}) & -y_{k-1}(b_{k-1}) & -z_{k-1}(b_{k-1}) \\ y'_{k-2}(b_{k-1}) & z'_{k-2}(b_{k-1}) & -y'_{k-1}(b_{k-1}) & -z'_{k-1}(b_{k-1}) \\ 0 & 0 & y_{k-1}(b_k) & z_{k-1}(b_k) \\ 0 & 0 & y'_{k-1}(b_k) & z'_{k-1}(b_k) \end{vmatrix}$$

If $k-1=p$, once more, the expression can be write as:

$$D_{k-2} = -W\{y_{p+1}(b_{p+2}), z_{p+1}(b_{p+2})\} \cdot \begin{vmatrix} y_{p-1}(b_p) & z_{p-1}(b_p) & -y_p(b_p) & -z_p(b_p) \\ y'_{p-1}(b_p) & z'_{p-1}(b_p) & -y'_p(b_p) & -z'_p(b_p) \\ 0 & 0 & y_p(b_{p+1}) & z_p(b_{p+1}) \\ 0 & 0 & y'_p(b_{p+1}) & z'_p(b_{p+1}) \end{vmatrix}$$

$$D_{k-2} = -W\{y_{p+1}(b_{p+2}), z_{p+1}(b_{p+2})\} \cdot W\{y_{p-1}(b_p), z_{p-1}(b_p)\} \cdot W\{y_p(b_{p+1}), z_p(b_{p+1})\}$$

$$D_{k-2} = -W\{y_k(b_{k+1}), z_k(b_{k+1})\} \cdot W\{y_{k-1}(b_k), z_{k-1}(b_k)\} \cdot W\{y_{k-2}(b_{k-1}), z_{k-2}(b_{k-1})\}$$

Therefore,

$$H_3^3(E) = \begin{vmatrix} y_1(b_2) & z_1(b_2) & -y_2(b_2) & -z_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y_2(b_3) & z_2(b_3) & -y_3(b_3) & -z_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y_{n-1}(b_n) & z_{n-1}(b_n) & -y_n(b_n) & -z_n(b_n) \\ y'_1(b_2) & z'_1(b_2) & -y'_2(b_2) & -z'_2(b_2) & 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & y'_2(b_3) & z'_2(b_3) & -y'_3(b_3) & -z'_3(b_3) & \cdots & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & y'_{n-1}(b_n) & z'_{n-1}(b_n) & -y'_n(b_n) & -z'_n(b_n) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y_n(b_{n+1}) & z_n(b_{n+1}) \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 & y'_n(b_{n+1}) & z'_n(b_{n+1}) \end{vmatrix}$$

$$H_3^3(E) = W\left\{y_n(b_{n+1}), z_n(b_{n+1})\right\} \cdot \prod_{k=2}^{n} \left[(-1)^n \cdot W\left\{y_{n+1-k}(b_{n+2-k}), z_{n+1-k}(b_{n+2-k})\right\}\right]$$
$$H_3^3(E) = (-1)^n \cdot W\left\{y_n(b_{n+1}), z_n(b_{n+1})\right\} \cdot W\left\{y_{n-1}(b_n), z_{n-1}(b_n)\right\} \cdot W\left\{y_{n-2}(b_{n-1}), z_{n-2}(b_{n-1})\right\} \quad \cdots \quad W\left\{y_1(b_2), z_1(b_2)\right\}$$

Section S8.3 Determinant $H_0^0(E)$

The determinants found $H_1^1(E)$ and $H_3^3(E)$ have the following equations

$$H_1^1(E) = (-1)^n \cdot W\left\{y_1(b_1), z_1(b_1)\right\} \cdot W\left\{y_2(b_2), z_2(b_2)\right\} \cdot W\left\{y_3(b_3), z_3(b_3)\right\} \quad \cdots \quad W\left\{y_n(b_n), z_n(b_n)\right\}$$
$$H_3^3(E) = (-1)^n \cdot W\left\{y_n(b_{n+1}), z_n(b_{n+1})\right\} \cdot W\left\{y_{n-1}(b_n), z_{n-1}(b_n)\right\} \cdot W\left\{y_{n-2}(b_{n-1}), z_{n-2}(b_{n-1})\right\} \quad \cdots \quad W\left\{y_1(b_2), z_1(b_2)\right\}$$

However, because the Schrödinger equation has a constant wronskian, the following condition can be obtained from the Abel identity.

$$H_1^1(E) = (-1)^n \cdot W\left\{y_1(x), z_1(x)\right\} \cdot W\left\{y_2(x), z_2(x)\right\} \cdot W\left\{y_3(x), z_3(x)\right\} \quad \cdots \quad W\left\{y_n(x), z_n(x)\right\}$$
$$H_3^3(E) = (-1)^n \cdot W\left\{y_n(x), z_n(x)\right\} \cdot W\left\{y_{n-1}(x), z_{n-1}(x)\right\} \cdot W\left\{y_{n-2}(x), z_{n-2}(x)\right\} \quad \cdots \quad W\left\{y_1(x), z_1(x)\right\}$$

Therefore, the determinants $H_1^1(E)$ and $H_3^3(E)$ are of equal value.

$$H_0^0(E) = (-1)^n \cdot W\left\{y_1(x), z_1(x)\right\} \cdot W\left\{y_2(x), z_2(x)\right\} \cdot W\left\{y_3(x), z_3(x)\right\} \quad \cdots \quad W\left\{y_n(x), z_n(x)\right\}$$

The $(-1)^n$ term of $H_0^0(E)$ does not affect the sign of the transcendental energy equation, since the determinants $H_4^2(E), H_1^2(E), H_2^2(E)$ and $H_4^1(E)$ change sign in the same way as $H_0^0(E)$ does.