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Solving the Half-Infinite Potential Well Problem via the Application of Matrix Method

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Abstract— This paper adds up how the matrix method can be used for solving the one-dimensional time-independent Schrodinger's equation for some specific potential energy variation like half-infinite potential well. The matrix method is illustrated to obtain solution of the time-independent Schrodinger's equation for half-infinite potential well, which is generally done by ordinary algebraic and analytical methods. The transcendental equation determining the discrete eigenvalues for bound state and the corresponding eigenwave functions are obtained by the time-independent Schrodinger's equation for half-infinite potential well via the application of matrix method**.**

***Keywords** — Matrix Method; Schrodinger's Equation; Half-Infinite Potential Well.*

1. Introduction

Quantum mechanics has been perceived as an essential constituent in the modules of Physics, Chemistry and Electrical Engineering [1]. It deals with the quantization of various entities especially energy and needed to deal with the submicroscopic particles [2].The applications of time-independent Schrodinger's equation are generally analyzed by different algebraic and analytical methods [1], [2], [3]. The matrix method has been successfully implemented in science and engineering problems [4], [5], [6], [7], [8], [9], [10], [11], [12]. This paper puts forward the Matrix Method for analyzing one of the applications of Schrodinger's equation to half-infinite potential well problem. As we know for a square matrix B [5], [6], [7], [8] of order n with elements a_{ij}, we get a column matrix Z and a constant λ such that BZ = λZ or $|B - \lambda I|Z = 0$. This represents a matrix equation which results in n homogeneous linear equations [9], [10], [11], [12] having a non–trivial solution only if $|B - \lambda I| = 0$. On expand$|B - \lambda I|$, we will get n[th] degree equation in λ, known as the characteristic equation of B, whose roots i.e. λ_i $(where\ i = 1, 2, 3, \ldots\ldots n)$ are called Eigenvalues and corresponding to each Eigenvalue there is a non-zero solution $Z = \begin{bmatrix} z_1 \\ z_2 \\ \ldots \\ z_n \end{bmatrix}$ known as Eigenvector [4-12]. This paper discusses the application of matrix method for solving half-infinite potential well problem to find the transcendental equation determining the discrete eigenvalues for bound state and the corresponding eigenwave functions, which is generally done by ordinary algebraic and analytical methods [1-3]. To define half-infinite potential, considering a potential energy variation [1] as follows,

$$V(y) = \begin{bmatrix} \infty \text{ in the region } y < 0 \\ 0\ in\ the\ region\ y = 0\ to\ y = L \\ \boldsymbol{V_0\ in\ the\ region\ y} > L \end{bmatrix}$$

Such potential energy variation is known as half-infinite potential well.

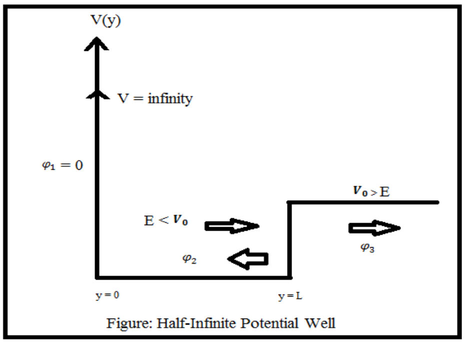

Fig.1: Half-infinite potential well

2. Material and Method

The one-dimensional time-independent Schrodinger's equation [3] is written as

$$\varphi''(y) + \frac{8\pi^2 m}{h^2}\{E - V\}\varphi(y) = 0 \ldots (1)$$

Let $\varphi_1(y)$, $\varphi_2(y)$ and $\varphi_3(y)$are the wave functions in the regions y < 0, 0 < y < L and **y > L respectively.**

Since the potential energy function V is infinite for y < 0, therefore from (1),

$$\varphi_1(y) = 0, \text{for } y < 0.$$

Since the wave function is continuous at the boundaries [4], therefore, we can write

$\varphi_1(0) = \varphi_2(0) = 0$

$\varphi_3(0) = a$ (say)

$\varphi_2{}'(0) = \varphi_3{}'(0) = b$ (say)

$\varphi_{2'}(L) = \varphi_{3'}(L)$

$\varphi_2(L) = \varphi_3(L)$

where a and b are constants.

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In the regions, 0 < y < L and **y > L,**(1) can be written as

$\varphi_2''(y) + k_1^2\varphi_2(y) = 0$ …… (2)

$\varphi_3''(y) - k_2^2\varphi_3(y) = 0$ …… (3)

where $k_1 = \sqrt{\frac{8\pi^2 mE}{h^2}}$ and $k_2 = \sqrt{\frac{2\pi^2 m(V_0 - E)}{h^2}}$

To solve (2) by Matrix method [5-7],

Let $\varphi_2(y) = \varphi_{21}(y)$

And

$\varphi_{21}'(y) = \varphi_{22}(y)$... (4)

We can rewrite (2) as

$\varphi_{22}'(y) + k_1^2\varphi_{21}(y) = 0$

Or

$\varphi_{22}'(y) = -k_1^2\varphi_{21}(y)$ … ….(5)

Equations (4) and (5) can be written in matrix form as

$$\begin{bmatrix}\varphi_{21}'(y)\\ \varphi_{22}'(y)\end{bmatrix} = \begin{bmatrix}0 & 1\\ -k_1^2 & 0\end{bmatrix}\begin{bmatrix}\varphi_{21}(y)\\ \varphi_{22}(y)\end{bmatrix}$$

The characteristic equation is

$\begin{vmatrix}0-\lambda & 1\\ -k_1^2 & 0-\lambda\end{vmatrix} = 0$, where λ *is a scalar.*

Solving, we get

$\lambda^2 + k_1^2 = 0$

Or

$\lambda = \pm ik_1$… (6)

Now the characteristic vector for $\lambda = ik_1$ is given by

$$\begin{bmatrix}0 - ik_1 & 1\\ -k_1^2 & 0 - ik_1\end{bmatrix}\begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}0\\ 0\end{bmatrix}$$

Applying $R_2 \to R_2 + ik_1 R_1$, we can write

$$\begin{bmatrix}-ik_1 & 1\\ 0 & 0\end{bmatrix}\begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}0\\ 0\end{bmatrix}$$

This results

$-ik_1 y_1 + y_2 = 0$

Or

$\begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}1\\ ik_1\end{bmatrix}$….. (7)

The characteristic vector for $\lambda = -ik_1$ is given by

$$\begin{bmatrix}0 + ik_1 & 1\\ -k_1^2 & 0 + ik_1\end{bmatrix}\begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}0\\ 0\end{bmatrix}$$

Applying $R_2 \to R_2 - ik_1 R_1$, we can write

$$\begin{bmatrix}ik_1 & 1\\ 0 & 0\end{bmatrix}\begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}0\\ 0\end{bmatrix}$$

This results

$ik_1 y_1 + y_2 = 0$

Or

$\begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}1\\ -ik_1\end{bmatrix}$… (8)

The modal matrix of characteristic vectors is $\begin{bmatrix}1 & 1\\ ik_1 & -ik_1\end{bmatrix}$.

Let P = $\begin{bmatrix}1 & 1\\ ik_1 & -ik_1\end{bmatrix}$, then the inverse of modal matrix P is given by

$P^{-1} = \begin{bmatrix}\frac{1}{2} & \frac{1}{2ik_1}\\ \frac{1}{2} & \frac{-1}{2ik_1}\end{bmatrix}$…… (9)

To find $Pe^{\lambda y}P^{-1}$,

$$Pe^{\lambda y}P^{-1} = \begin{bmatrix}1 & 1\\ ik_1 & -ik_1\end{bmatrix}\begin{bmatrix}e^{ik_1 y} & 0\\ 0 & e^{-ik_1 y}\end{bmatrix}\begin{bmatrix}\frac{1}{2} & \frac{1}{2ik_1}\\ \frac{1}{2} & \frac{-1}{2ik_1}\end{bmatrix}$$

$$= \begin{bmatrix}e^{ik_1 y} & e^{-ik_1 y}\\ ik_1 e^{ik_1 y} & -ik_1 e^{-ik_1 y}\end{bmatrix}\begin{bmatrix}\frac{1}{2} & \frac{1}{2ik_1}\\ \frac{1}{2} & \frac{-1}{2ik_1}\end{bmatrix}$$

$$= \begin{bmatrix}\frac{1}{2}(e^{ik_1 y} + e^{-ik_1 y}) & \frac{1}{2ik_1}(e^{ik_1 y} - e^{-ik_1 y})\\ \frac{ik_1}{2}(e^{ik_1 y} - e^{-ik_1 y}) & \frac{1}{2}(e^{ik_1 y} + e^{-ik_1 y})\end{bmatrix}$$

$$= \begin{bmatrix}\cos k_1 y & \frac{1}{k_1}\sin k_1 y\\ -k_1 \sin k_1 y & \cos k_1 y\end{bmatrix} \text{…… (10)}$$

Applying $\varphi_{2_1}(0) = 0$ and $D_y\varphi_2(0) = b$, we can write

$$\begin{bmatrix}\varphi_{2_1}(y)\\ \varphi_{2_2}(y)\end{bmatrix} = \begin{bmatrix}\cos k_1 y & \frac{1}{k_1}\sin k_1 y\\ -k_1 \sin k_1 y & \cos k_1 y\end{bmatrix}\begin{bmatrix}0\\ b\end{bmatrix}$$

Or

$$\begin{bmatrix}\varphi_{2_1}(y)\\ \varphi_{2_2}(y)\end{bmatrix} = \begin{bmatrix}\frac{b}{k_1}\sin k_1 y\\ b\cos k_1 y\end{bmatrix}\text{… (11)}$$

This gives

$\varphi_2(y) = \varphi_{2_1}(y) = \frac{b}{k_1}\sin(k_1 y)$ ….. (12)

To solve (3) by Matrix method [5-7],

Let $\varphi_3(y) = \varphi_{3_1}(y)$ …. (13)

And

$\varphi_{31}'(y) = \varphi_{3_2}(y)$... (14)

We can rewrite (3) as

$\varphi_{32}'(y) - k_2^2\varphi_{3_1}(y) = 0$

Or

$\varphi_{32}'(y) = k_2^2\varphi_{3_1}(y)$ ….(15)

Equations (18) and (19) can be written in matrix form as

$$\begin{bmatrix}\varphi_{3_1}'(y)\\ \varphi_{32}'(y)\end{bmatrix} = \begin{bmatrix}0 & 1\\ k_2^2 & 0\end{bmatrix}\begin{bmatrix}\varphi_{3_1}(y)\\ \varphi_{3_2}(y)\end{bmatrix}$$

The characteristic equation is

$\begin{vmatrix}0-\lambda & 1\\ k_2^2 & 0-\lambda\end{vmatrix} = 0$….. (16)

Solving, we get

$\lambda^2 - k_2^2 = 0$

Or

$\lambda = \pm k_2$….. (17)

Now the characteristic vector for $\lambda = ik_2$ is given by

$\begin{bmatrix}0 - k_2 & 1\\ k_2^2 & 0 - k_2\end{bmatrix}\begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}0\\ 0\end{bmatrix}$….. (18)

Applying $R_2 \to R_2 + k_2 R_1$, we can write

$\begin{bmatrix}-k_2 & 1\\ 0 & 0\end{bmatrix}\begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}0\\ 0\end{bmatrix}$….. (19)

This results

$-k_2 y_1 + y_2 = 0$

Or

$\begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}1\\ k_2\end{bmatrix}$…… (20)

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The characteristic vector for $\lambda = -ik_2$ is given by

$$\begin{bmatrix} 0+k_2 & 1 \\ {k_2}^2 & 0+k_2 \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \text{..... (21)}$$

Applying $R_2 \to R_2 - k_2 R_1$, we can write

$$\begin{bmatrix} k_2 & 1 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

This results

$$k_2 y_1 + y_2 = 0$$

Or

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -k_2 \end{bmatrix} \text{... (22)}$$

The modal matrix of characteristic vectors is $\begin{bmatrix} 1 & 1 \\ k_2 & -k_2 \end{bmatrix}$.

Let P $= \begin{bmatrix} 1 & 1 \\ k_2 & -k_2 \end{bmatrix}$, then the inverse modal matrix P is given by

$$P^{-1} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2k_2} \\ \frac{1}{2} & \frac{-1}{2k_2} \end{bmatrix} \text{..... (23)}$$

To find $Pe^{\lambda y}P^{-1}$,

$$Pe^{\lambda y}P^{-1} = \begin{bmatrix} 1 & 1 \\ k_2 & -k_2 \end{bmatrix}\begin{bmatrix} e^{k_2 y} & 0 \\ 0 & e^{-k_2 y} \end{bmatrix}\begin{bmatrix} \frac{1}{2} & \frac{1}{2k_2} \\ \frac{1}{2} & \frac{-1}{2k_2} \end{bmatrix}$$

$$= \begin{bmatrix} e^{k_2 y} & e^{-k_2 y} \\ k_2 e^{k_2 y} & -k_2 e^{-k_2 y} \end{bmatrix}\begin{bmatrix} \frac{1}{2} & \frac{1}{2k_2} \\ \frac{1}{2} & \frac{-1}{2k_2} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{2}(e^{k_2 y} + e^{-k_2 y}) & \frac{1}{2k_2}(e^{k_2 y} - e^{-k_2 y}) \\ \frac{k_2}{2}(e^{k_2 y} - e^{-k_2 y}) & \frac{1}{2}(e^{k_2 y} + e^{-k_2 y}) \end{bmatrix}$$

$$= \begin{bmatrix} coshk_2 y & \frac{1}{k_2} sinhk_2 y \\ k_2 sinhk_2 y & coshk_2 y \end{bmatrix} \text{... (24)}$$

Applying $\varphi_{3_1}(0) = a$ and $D_y\varphi_3(0) = b$, we can write

$$\begin{bmatrix} \varphi_{R_1}(y) \\ \varphi_{R_2}(y) \end{bmatrix} = \begin{bmatrix} cosk_2 y & \frac{1}{k_2} sink_2 y \\ k_2 sink_2 y & cosk_2 y \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix}$$

Or

$$\begin{bmatrix} \varphi_{3_1}(y) \\ \varphi_{3_2}(y) \end{bmatrix} = \begin{bmatrix} acosk_2 y + \frac{b}{k_2} sink_2 y \\ ak_2 sink_2 y + b\, cosk_2 y \end{bmatrix}$$

$$\varphi_3(y) = \varphi_{3_1}(y) = a \cosh k_2 y + \frac{b}{k_2} \sinh k_2 y \text{...... (25)}$$

Or

$$\varphi_3(y) = a\,\frac{e^{k_2 y} + e^{-k_2 y}}{2} + \frac{b}{k_2}\frac{e^{k_2 y} - e^{-k_2 y}}{2}$$

Or

$$\varphi_3(y) = (\frac{a}{2} + \frac{b}{2k_2})e^{k_2 y} + (\frac{a}{2} - \frac{b}{2k_2})e^{-k_2 y} \text{... (26)}$$

Now $\varphi_3(y)$ *approaches to zero at* $y = infinity$ *only if*

$$\left(\frac{a}{2} + \frac{b}{2k_2}\right) = 0$$

Or

$$b = -k_2 a \text{..... (27)}$$

Using (27) in (26), we can write

$$\varphi_3(y) = ae^{-k_2 y} \text{.... (28)}$$

Applying $\varphi_2(L) = \varphi_3(L)$ and solving, we get

$$\frac{b}{k_1} \sin(k_1 L) = ae^{-k_2 L}$$

Or

$$a = \frac{b}{k_1} \sin(k_1 L)e^{k_2 L} \text{.... (29)}$$

Using (29) in (28). We get

$$\varphi_3(y) = \frac{b}{k_1} \sin(k_1 L)e^{k_2 L}e^{-k_2 y}$$

Or

$$\varphi_3(y) = \frac{b}{k_1} \sin(k_1 L)e^{-k_2(y-L)} \text{.... (30)}$$

According to the normalization condition [5, 9], we have

$$\int_{y=-\infty}^{y=\infty} \varphi(y)\, \varphi(y)^* dy = 1$$

Or

$$\int_{y=0}^{y=L} \varphi_2(y)\, \varphi_2(y)^* dy + \int_{y=L}^{y=\infty} \varphi_3(y)\, \varphi_3(y)^* dy = 1$$

Using (12) and (30) and simplifying, we get

$$b = \frac{k_1}{\sqrt{\frac{L}{2} + \frac{\sin(k_1 L)}{4k_1 L} + \frac{sin^2(k_2 L)}{2k_2 L}}} \text{....... (31)}$$

Again, applying $\varphi_2'(L) = \varphi_3'(L)$ and solving, we get

$$\tan(k_1 L) = -k_1 k_2 \text{..... (32)}$$

This is the required transcendental equation determining the discrete eigenvalues for bound state.

The corresponding eigenwave function is given by

$$\varphi(y) = \begin{cases} 0 \text{ for } y < 0 \\ \frac{1}{\sqrt{\frac{L}{2} + \frac{\sin(k_1 L)}{4k_1 L} + \frac{sin^2(k_2 L)}{2k_2 L}}} \sin(k_1 y) \; for\; 0 < y < L \\ \frac{1}{\sqrt{\frac{L}{2} + \frac{\sin(k_1 L)}{4k_1 L} + \frac{sin^2(k_2 L)}{2k_2 L}}} \sin(k_1 L)e^{-k_2(y-L)} for\; y > L \end{cases} \text{... (33)}$$

3. Conclusion

The time-independent Schrodinger's equation for half-infinite potential well has been solved successfully by matrix method to find the transcendental equation determining the discrete eigenvalues for bound state and

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the corresponding eigenwave function. The results obtained are the same as obtained with ordinary algebraic and analytical methods [1-3, 13, 14]. The matrix method has been proved to be a successful approach for solving the half-infinite potential well problem.

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