Numerical problems on Quantum

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Problem: 1 :→

The given Hamiltonian: $H = -\frac{\hbar^2}{2I}\cdot\frac{\partial^2}{\partial\phi^2} + Mga(1-\cos\phi)$

So T.I.S.E gives:

$$-\frac{\hbar^2}{2I}\frac{d^2\psi(\phi)}{d\phi^2} + Mga(1-\cos\phi)\cdot\psi(\phi) = E\psi(\phi) \cdots (1)$$

given: $M=1$; $a=1$; $g=1$; $I=300$.

I've assumed $\hbar = 1$. (in proper unit for all)

To solve eq (1); I've taken the methode of discretisation.

The limit of ϕ be given by $\phi \in [0, 2\pi]$.

I've broken the interval in N discrete spacial points of equal interval.

i.e $\{\phi_1, \phi_2, \ldots, \phi_N\}$; $\begin{cases} \phi_{i+1} - \phi_i = h \\ \phi_1 = 0;\ \phi_N = 2\pi;\ \phi_{N+1} = \phi_1 \end{cases}$

Let $\psi_i = \psi(\phi_i)$; $V_i = V(\phi_i)$

Now at small h; the derivative of ψ be given (approximated) by:

$$\frac{d^2\psi}{d\phi^2} \simeq \frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{h^2}\Bigg|_{h=\text{small}}$$

So: in discrete form; eq (1) can be written by:

$$-\frac{\hbar^2}{2mI}\cdot\frac{\psi_{i+1}+\psi_{i-1}-2\psi_i}{h^2}+V_i\psi_i=E\psi_i$$

$$\rightarrow \underbrace{\left(+\frac{\hbar^2\times 2}{2Ih^2}+V_i\right)}_{\beta_i}\psi_i+\underbrace{\left(-\frac{\hbar^2}{2Ih^2}\right)}_{\alpha}(\psi_{i+1}+\psi_{i-1})=E\psi_i$$

$$\rightarrow \alpha\psi_{i-1}+\beta_i\psi_i+\alpha\psi_{i+1}=E\psi_i$$

putting $i=1,2,3,\cdots,N$ we get; the set of eqn's; (using $\phi_{N+1}=\phi_1$)

$$\beta_1\psi_1+\alpha\psi_2+\alpha\psi_N=E\psi_1$$
$$\alpha\psi_1+\beta_2\psi_2+\alpha\psi_3=E\psi_2$$
$$\alpha\psi_2+\beta_3\psi_3+\alpha\psi_4=E\psi_3$$
$$\cdots\cdots\quad\cdots\cdots$$
$$\alpha\psi_{N-2}+\beta_{N-1}\psi_{N-1}+\alpha\psi_N=E\psi_{N-1}$$
$$\alpha\psi_{N-1}+\beta_N\psi_N=E\psi_N.$$

$\alpha\psi_1+$

So in matrix form we get:

$$\begin{pmatrix}\beta_1 & \alpha & 0 & 0 & 0 & \cdots & 0 & \alpha\\ \alpha & \beta_2 & \alpha & 0 & 0 & \cdots & 0 & 0\\ 0 & \alpha & \beta_3 & \alpha & 0 & \cdots & 0 & 0\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\ 0 & 0 & \cdots & \alpha & \beta_i & \alpha & \cdots & 0\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\ 0 & 0 & \cdots & 0 & \alpha & \beta_{N-1} & \alpha & 0\\ \alpha & 0 & \cdots & 0 & 0 & \alpha & \beta_N & \end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_N\end{pmatrix}=E\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_N\end{pmatrix}$$

i^{th} row

$\hat{H}$ matrix.

In maaiae; I've given $\hat{H}$ as input matrix and its eigenvalues will be possible energy values.

Obviously we must have to take at least $N \geq 300$ (i.e 300 space interval) to get a $(N \times N)$ matrix to get N eigenvalues. Here the required no of eig-vals is 300. Moreover larger N will give more & more precise eigenvalues.

With those 300 eig-vals; I've plotted the energy bands and the band gaps (not properly band gap but energy difference between states.)

(Spin interaction problem is a good checkpoint for this discretization method.)

As asked in question; first; 50th & 200th energy eigenvalues are given by:

$E_1 = 0.02876$ unit
$E_{50} = 2.17278$ unit.
$E_{200} = 17.061328$ unit.

Answer

To get a good precession; I have first broken the whole interval into 3000 small intervals. After that from ~~first~~ 3000 eigenvalues of H; I have collected first 300 & worked on them.

After $n = 43$ rd state the energy eigenvalue exceeds the maximum of potential.

$E(43) \simeq 1.98$ unit } & $V_{max} = 2$ unit.
& $E(44) \simeq 2.001$ "

So after $n = 43$; the energy levels comes ~~doug~~ in pairs & the energy gap between them are very small (actually zero as they are degenerate levels.)
And we get (the difference is due to numerical error)

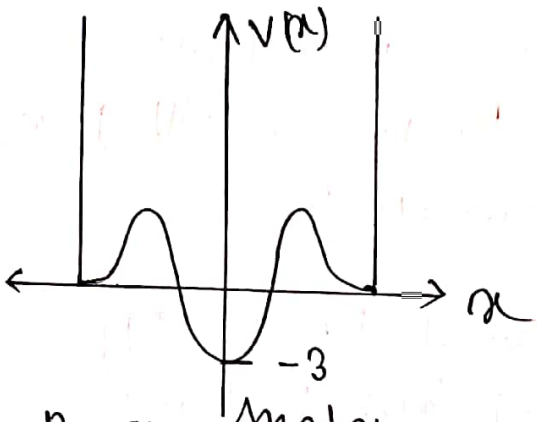
$E_{45} \simeq E_{46}$; $E_{47} \simeq E_{48}$; $E_{49} \simeq E_{50}$; ..... etc

Answer

Problem: 2 ⟶

Given potential $V(x) = (x^4 - 3)\, e^{-x^2/2}$

And it's in a box of length 10; $(x = -5 \text{ to } 5)$



Rough sketch of $V(x)$.

clearly from fig we get:

$E \geq -3$ (must)

As V is symmetric so we must get for all eig-state $\psi(x)$:

$\psi(-x) = \pm \psi(x)$.

due to infinity potential at edge: $\psi(\pm 5) = 0$.

Now here I've used the difference eq method to solve T.I.S.E.

where I've taken: $\frac{\hbar^2}{2m} = 1$.

i.e $-\frac{d^2\psi}{dx^2} + V\psi = E\psi$

discritizing space into small intervals like previous problem $x \to \{x_0, x_1, \ldots, x_N\}$

$x_0 \downarrow -5$, $x_N \downarrow 5$

the eq becomes:

$$-\frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{h^2} + V_i \psi_i = E\psi_i$$

$$\Rightarrow \psi_{i+1} = -\left(h^2(E - V_i) + 2\right)\psi_i + \psi_{i-1}$$

By running the loop for i with different values of E with the B.C

$\psi_0 = 0$ (obvious)

$\psi_1 =$ 0.1 or 0.01 or, ...

(any number upto normalization will give a similar curve with different amplitude.)

For proper choice of E; ψ will be close to zero at $x \to 5$

i.e $\psi_N \simeq 0$.

o/w for wrong choice ψ will blow up at edge.

Using proper error bound & shooting different E values in the loop; give collected the allowed energy values.

Lastly with proper ψ ($\psi_N \simeq 0$); the only task is to normalize it & going to higher energy value.

This method can give upto any arbitrary no of states ($E_1, E_2, \ldots$) as per we allow to vary E.

The checking was done by counting no of maxima, minima of ψ.

$\psi_{i\text{th}}^{eig}$ excited will have one more extrima than ψ_{i-1}^{eig} th state

And if ψ_i^{eig} is even/odd fn if ψ_{i-1}^{eig} is odd/even

(Infinite Sq well is a good checkpoint for this method; where it gives very good result.

Comments:-

I have done the same problem in python & mathematica. The mathematica code gives ~~more~~ better result. Here one important fact is as I've taken $m=\frac{1}{2}$; $\hbar=1$ I got one '-ve' energy where as my friends have taken $m=1$ & for them there are two states with '-ve' energy. Also the eig-values are different. However my mathematica & python file are producing same result I have checked my code for other potentials (infinite Sq well) as well as $m=1$ (other friends.)

One problem with the ~~the~~ python code is that, I was unable to find the ground state with the code. It can produce all states from 1st excited states and the probs are also consistant. I request the graders to kindly mention the possible change in my python code to give the complete result.

So the consecutive energy eigenvalues for the Schrodinger eq with $m = \frac{1}{2}$ & $\hbar = 1$ & $V(x) = (x^4 - 3)\, e^{-x^2/2}$ be given by:

1) From Python code:

0.676 unit.
1.298 "
1.464 "
2.738 "
3.772 "
4.879 "

→ ground state is missing in python code.

→ Answer

2) From mathematica :-

−1.7097 unit.
0.679 "
1.301 "
1.467 "
2.744 "

They are very close and the plots are also similar for different eigenstates.

(As sent both of them.)

2-2. Band gap near first Brillouin Zone = 2.046 unit.

I am greatly thankful to my friend Krishnendu Maji; who has helped me for doing problem 2-2. I have used the same algorithm developed by Krishnendu for that problem.