Electron propagation along the one dimensional lattice

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date: January 07, 2016)

1. Introduction ((Feynman))

We consider a simpler example to illustrate the generality of the notion: a particle in a periodic potential. $V(x)=1-\cos(Gx)$ with $G=\dfrac{2\pi}{a}$ (reciprocal lattice) for the one dimensional chain with a lattice constant a. The minima are at $x=ma$, where m is any integer. The symmetry of the problem is the discrete translation $x=na\to(n+1)a$. The approximate states, $|n\rangle$, which are Gaussians centered around the classical minima, break the symmetry and are converted to each other by $\hat{T}_x(a)$, the operator that translates $x=na\to(n+1)a$

$$\hat{T}_x(a)|n\rangle=|n+1\rangle .$$

However, adjacent classical minima are connected by a nonzero tunneling amplitude of the type we just calculated and the Hamiltonian $\hat{H}$ has off-diagonal amplitudes between $|n\rangle$ and. (There are also solutions describing tunneling to next-nearest-neighbor minima, but these have roughly double the action as the nearest-neighbor tunneling process and lead to an off-diagonal matrix element that is roughly the square of the one due to nearest-neighbor tunneling.) Suppose the one-dimensional world were finite and forms a closed ring of size *N*, so that there were *N* degenerate classical minima. These would evolve into *N* nondegenerate levels due to the mixing due to tunneling.

The content of this topics can be found in the Feynman's lecture on physics.

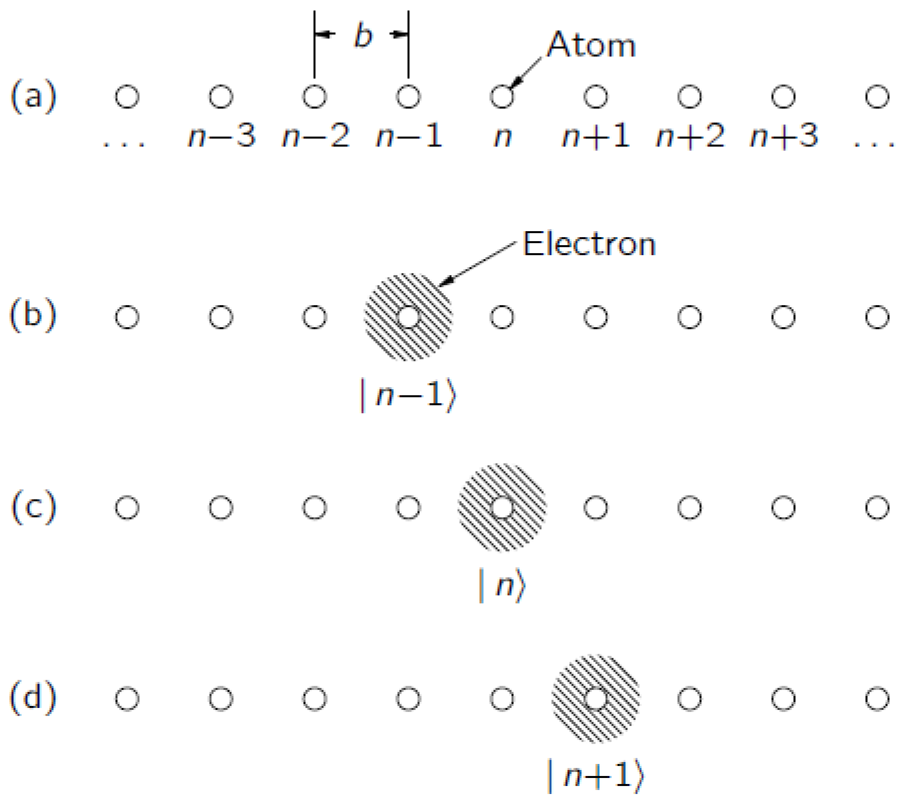


Fig. The base states of an electron in a one dimensional crystal.

2. Electron dispersion

We consider a periodic lattice with a lattice constant a. The translation operator commutes with the Hamiltonian

$$[T_x(a), \hat{H}] = 0.$$

The operator $\hat{T}_x(a)$ is unitary (a; lattice constant) and hence its eigenvalues need not be real. Let us suppose that the potential barrier between the lattice points is infinitely high. Let $|n\rangle$ be the state localized in the lattice cell n, i.e.

$$\langle x|n\rangle \neq 0 \qquad \text{only if } x \approx na.$$

Obviously $|n\rangle$ is a stationary state. Because all lattice cells are exactly alike we must have

$$\hat{H}|n\rangle = E_0|n\rangle, \qquad \text{for any } n.$$

Thus the system has countably infinite number of ground states $||n\rangle$, $n = -1, \ldots, \infty$.
Now

$$\hat{T}_x(a)|n\rangle = |n+1\rangle$$

so the state $|n\rangle$ is not an eigenstate of the translation (a). Let's try

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle,$$

where θ is a real parameter and

$$-\pi \le \theta \le \pi.$$

Obviously we have

$$\hat{H}|\theta\rangle = E_0|\theta\rangle$$

Furthermore we get

$$\begin{aligned}\hat{T}_x(a)|\theta\rangle &= \sum_{n=-\infty}^{\infty} e^{in\theta}\hat{T}_x(a)|n\rangle \\ &= \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle \\ &= \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}|n\rangle \\ &= e^{-i\theta}|\theta\rangle\end{aligned}$$

Thus every state corresponding to a value of the continuous parameter θ has the same energy, i.e. the ground state of the system infinitely degenerate.

Let us suppose further that $|n\rangle$ is a state localized at the point n so that

$$\hat{T}_x(a)|n\rangle = |n+1\rangle,$$

with

$$\langle x|n\rangle \neq 0 \text{ (but small)}, \qquad \text{when } |x-na| > a.$$

Due to the translational symmetry the diagonal elements of the Hamiltonian $\hat{H}$ in the basis $\{|n\rangle\}$ are all equal to each other:

$$\langle n|\hat{H}|n\rangle = E_0.$$

Let us suppose now that

$$\langle n'|\hat{H}|n\rangle \neq 0, \qquad \text{only if } n' = n, \text{ or } n' = n+1$$

We are dealing with the so called tight binding approximation. When we define

$$\langle n \pm 1|\hat{H}|n\rangle = -\Delta,$$

we can write

$$\hat{H}|n\rangle = E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle,$$

where we have exploited the orthonormality of the basis $\{|n\rangle\}$. Thus the state $|n\rangle$ is not an energy eigen state. Let us look again at the trial

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle$$

Like before we have

$$\hat{T}_x(a)|\theta\rangle = e^{-i\theta}|\theta\rangle$$

Furthermore

$$
\begin{aligned}
\hat{H}|\theta\rangle &= \sum_{n=-\infty}^{\infty} e^{in\theta}\hat{H}|n\rangle \\
&= \sum_{n=-\infty}^{\infty} e^{in\theta}(E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle) \\
&= \sum_{n=-\infty}^{\infty} e^{in\theta}E_0|n\rangle - \Delta e^{i(n+1)\theta}e^{-i\theta}|n+1\rangle - \Delta e^{i(n-1)\theta}e^{i\theta}|n-1\rangle) \\
&= (E_0 - \Delta e^{-i\theta} - \Delta e^{i\theta})|\theta\rangle \\
&= (E_0 - 2\Delta\cos\theta)|\theta\rangle
\end{aligned}
$$

The earlier degeneracy will be lifted if $\Delta \neq 0$ and

$$E = E_0 - 2\Delta\cos\theta$$

with

$$E_0 - 2\Delta \leq E \leq E_0 + 2\Delta$$

3. Feynman's approach

Eigenvalue problem:

$$\hat{H}|\theta\rangle = E|\theta\rangle$$

The translation operator

$$[T_x(a), \hat{H}] = 0$$

Then $|\theta\rangle$ should be a simultaneous eigenket of $T_x(a)$ and $\hat{H}$.

$$T_x(a), \hat{H}] = 0$$

$$\langle k|\hat{H}|\theta\rangle = \langle k|E|\theta\rangle$$

$$|\theta\rangle = \sum_k a_k|k\rangle$$

with

$$a_k = \langle k|\theta\rangle$$

Eigenvalue problem:

$$\hat{H}|\theta\rangle = E|\theta\rangle$$

$$\begin{aligned}
\langle k|\hat{H}|\theta\rangle &= \sum_l \langle k|\hat{H}|l\rangle\langle l|\theta\rangle \\
&= \sum_l (E_0\delta_{k,q}l - \Delta\delta_{k,l-1} - \Delta\delta_{k,l+1})\langle l|\theta\rangle \\
&= E_0\langle k|\theta\rangle - \Delta\langle k+1|\theta\rangle - \Delta\langle k-1|\theta\rangle \\
&= E\langle k|\theta\rangle
\end{aligned}$$

or

$$\begin{pmatrix} E_0 & -\Delta & 0 & \cdot & 0 & 0 \\ -\Delta & E_0 & -\Delta & \cdot & 0 & 0 \\ 0 & -\Delta & E_0 & \cdot & 0 & 0 \\ 0 & 0 & -\Delta & \cdot & -\Delta & 0 \\ \cdot & \cdot & \cdot & \cdot & E_0 & -\Delta \\ 0 & 0 & 0 & 0 & -\Delta & E_0 \end{pmatrix} \begin{pmatrix} \langle 1|\theta\rangle \\ \langle 2|\theta\rangle \\ \langle 3|\theta\rangle \\ \langle 4|\theta\rangle \\ \cdot \\ \langle N|\theta\rangle \end{pmatrix} = E \begin{pmatrix} \langle 1|\theta\rangle \\ \langle 2|\theta\rangle \\ \langle 3|\theta\rangle \\ \langle 4|\theta\rangle \\ \cdot \\ \langle N|\theta\rangle \end{pmatrix} \tag{1}$$

We also note that

$$T_x(a)|\theta\rangle = \lambda|\theta\rangle$$

$$\begin{aligned}
T_x(a)|\theta\rangle &= T_x(a)\sum_k |k\rangle\langle k|\theta\rangle \\
&= \sum_k |k+1\rangle\langle k|\theta\rangle \\
&= \sum_k |k\rangle\langle k-1|\theta\rangle \\
&= \lambda\sum_k |k\rangle\langle k|\theta\rangle
\end{aligned}$$

or

$$\langle k-1|\theta\rangle = \lambda\langle k|\theta\rangle$$

or

$$\langle k|\theta\rangle = \frac{1}{\lambda}\langle k-1|\theta\rangle \qquad (2)$$

What is the value of λ? We use the periodic boundary condition such that

$$\hat{T}_x(a)|k-1\rangle = |k\rangle, \qquad |k-1\rangle = \hat{T}_x^{\,+}(a)|k\rangle$$

$$\langle k-1| = \langle k|\hat{T}_x(a)$$

Then we have

$$\langle k|\hat{T}_x(a)|\theta\rangle = \langle k-1|\theta\rangle = \lambda\langle k|\theta\rangle,$$

$$\langle k|\hat{T}_x(a)^N|\theta\rangle = \langle k-N|\theta\rangle = \lambda^N\langle k|\theta\rangle$$

We assume that

$$\langle k-N|\theta\rangle = \langle k|\theta\rangle \qquad \text{(periodic boundary condition)}$$

which leads to

$$\lambda^N = 1$$

$$\lambda = e^{ika}$$

with

$$k = \frac{2\pi}{Na}n = \frac{2\pi}{a}\frac{n}{N} \qquad (n = 0, 1, 2, \quad , N\text{-}1),$$

or

$$-\frac{\pi}{a} \le k \le \frac{\pi}{a}, \qquad \Delta k = \frac{2\pi}{Na}$$

The number of the freedom is given by N (the total number of atoms in the 1D chain).

Energy eigenvalues:

$$
\begin{aligned}
E\langle k|\theta\rangle &= E_0\langle k|\theta\rangle - \Delta\langle k+1|\theta\rangle - \Delta\langle k-1|\theta\rangle \\
&= [E_0 - (\lambda + \frac{1}{\lambda})\Delta]\langle k|\theta\rangle
\end{aligned}
$$

since

$$\langle k-1|\theta\rangle = \lambda\langle k|\theta\rangle, \qquad \langle k+1|\theta\rangle = \frac{1}{\lambda}\langle k|\theta\rangle$$

Thus we have

$$E = E_0 - \Delta(e^{ika} + e^{-ika})\Delta = E_0 - 2\Delta\cos(ka)$$

where

$$-\frac{\pi}{a} \le k \le \frac{\pi}{a},$$

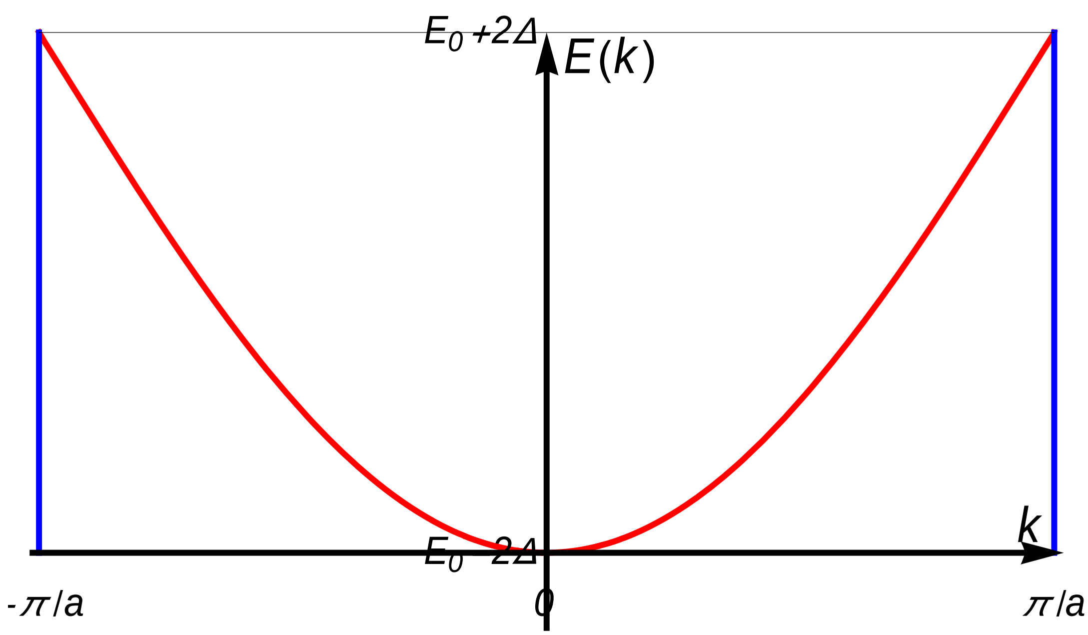


Fig. Energy dispersion for the phonon for the 1D system with a lattice constant *a*. The energy dispersion curve is expressed by $E(k) = E_0 - 2\Delta\cos(ka)$. We use E_0 = 1.0. $\Delta = 0.1$. a = 1.

4. Numerical calculation

((**Feynman**))

All we have to do is take the determinant, but wait! Determinants are fine when there are 2, 3, or 4 equations. But if there are a large number—or an infinite number—of equations, the determinants are not very convenient. We'd better just try to solve the equations directly.

We solve the eigenvalue problem for the Hamiltonian (12 x 12)

$$\begin{pmatrix} E_0 - E & -\Delta & 0 & \cdot & 0 & 0 \\ -\Delta & E_0 - E & -\Delta & \cdot & 0 & 0 \\ 0 & -\Delta & E_0 - E & \cdot & 0 & 0 \\ 0 & 0 & -\Delta & \cdot & -\Delta & 0 \\ \cdot & \cdot & \cdot & \cdot & E_0 - E & -\Delta \\ 0 & 0 & 0 & 0 & -\Delta & E_0 - E \end{pmatrix} \begin{pmatrix} \langle 1|\theta\rangle \\ \langle 2|\theta\rangle \\ \langle 3|\theta\rangle \\ \langle 4|\theta\rangle \\ \cdot \\ \langle N|\theta\rangle \end{pmatrix} = 0$$

by using the Mathematica. For simplicity we assume that

$$E_0 = 1, \qquad \Delta = 0.1, \qquad N = 12$$

$$\hat{H} \qquad (N \times N \text{ matrix})$$

$$\hat{H}|\theta\rangle = E|\theta\rangle$$

with $E_0 - 2\Delta \le E \prec E_0 + 2\Delta$

$$|\theta\rangle = \sum_{n=1}^{N} a_n |n\rangle$$

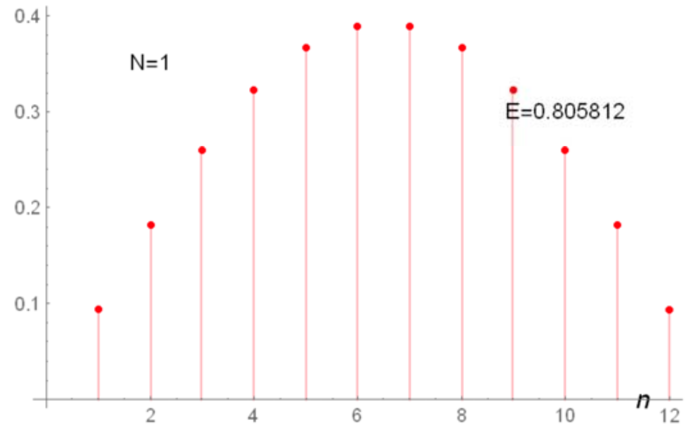
with a_n (real), $\qquad a_n = \langle n|\theta\rangle$

$$\sum_{n=1}^{N} a_n^{\ 2} = 1$$

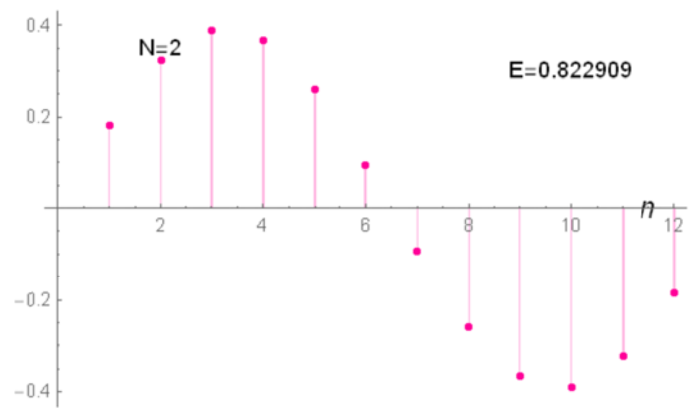
We determine the energy eigenvalues and the corresponding eigenkets. For each energy eigenvalue, we make a plot of the normalized amplitude a_n as a function of n

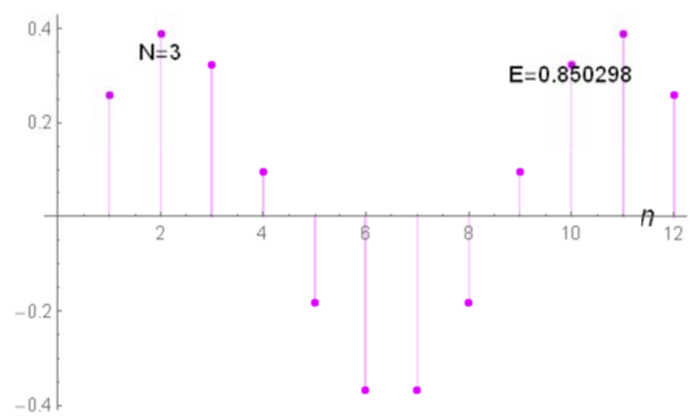
((**Mathematica**))

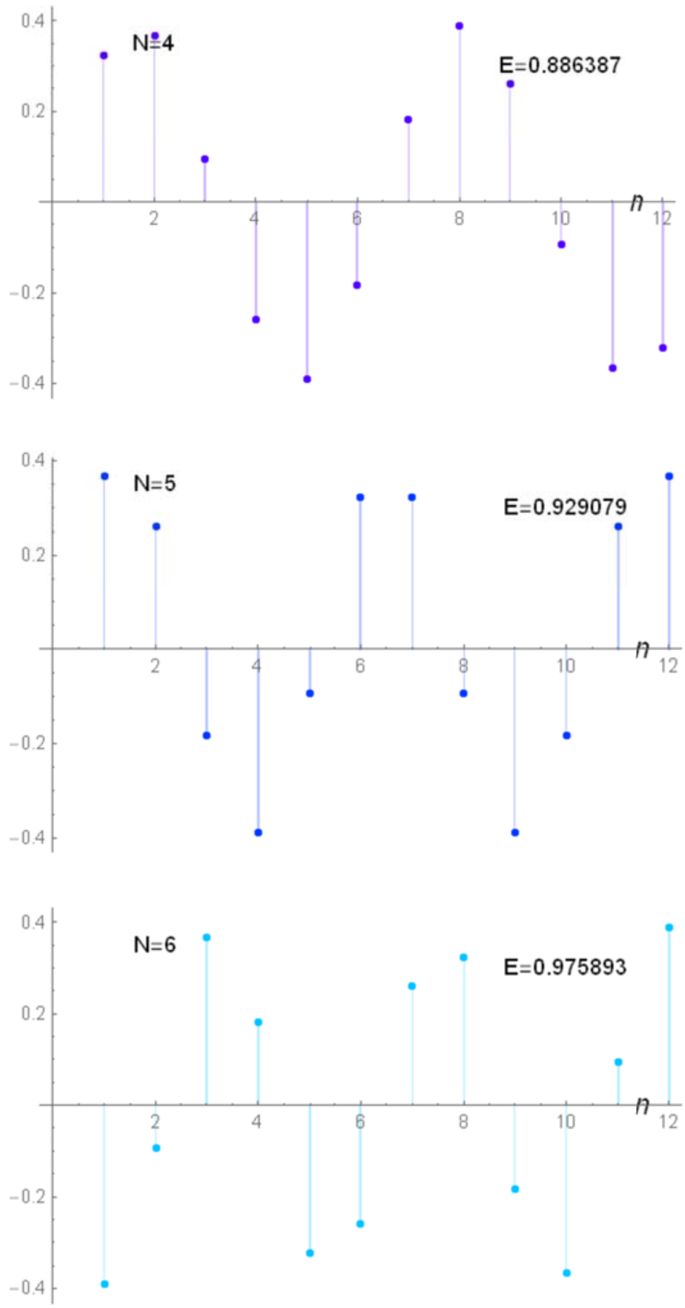
```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

H1 = {{1, -a, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
      {-a, 1, -a, 0, 0, 0, 0, 0, 0, 0, 0, 0},
      {0, -a, 1, -a, 0, 0, 0, 0, 0, 0, 0, 0},
      {0, 0, -a, 1, -a, 0, 0, 0, 0, 0, 0, 0},
      {0, 0, 0, -a, 1, -a, 0, 0, 0, 0, 0, 0},
      {0, 0, 0, 0, -a, 1, -a, 0, 0, 0, 0, 0},
      {0, 0, 0, 0, 0, -a, 1, -a, 0, 0, 0, 0},
      {0, 0, 0, 0, 0, 0, -a, 1, -a, 0, 0, 0},
      {0, 0, 0, 0, 0, 0, 0, -a, 1, -a, 0, 0},
      {0, 0, 0, 0, 0, 0, 0, 0, -a, 1, -a, 0},
      {0, 0, 0, 0, 0, 0, 0, 0, 0, -a, 1, -a},
      {0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -a, 1}};

H11 = H1 /. {a → 0.1};

eq1 = Eigensystem[H11];

Pt[n_] := Module[{f1, f2, n1}, n1 = n;
  f1 = ListPlot[Normalize[eq1[[2, n]]],
     PlotStyle → {Hue[0.09 (n - 1)], Thick},
     Filling → Axis];
  f2 = Graphics[
     {Text[Style["E=" <> ToString[eq1[[1, n]]],
         Black, 12], {10, 0.3}],
      Text[Style["N=" <> ToString[12 - n1 + 1],
         Black, 12], {2, 0.35}],
      Text[Style["n", Black, Italic, 15],
       {11.5, 0}]}]; Show[f1, f2]];
```



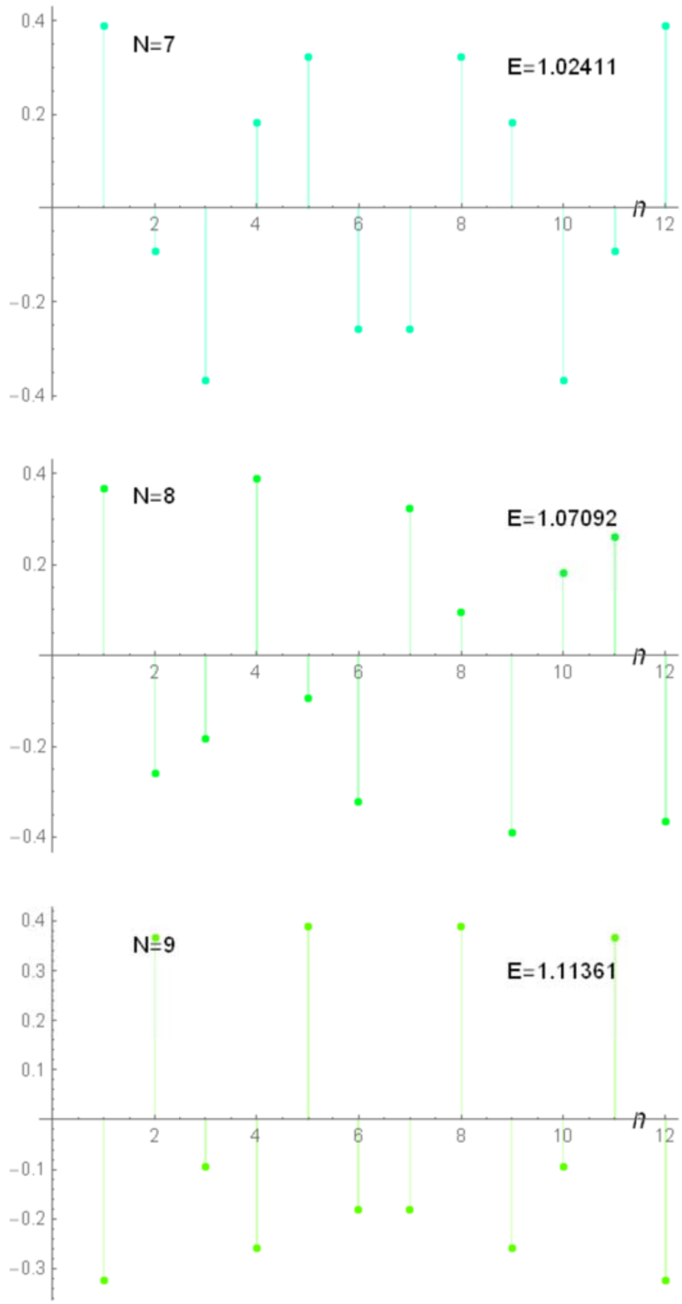
Ground state $E = E_0 - 2\Delta \approx 0.80$



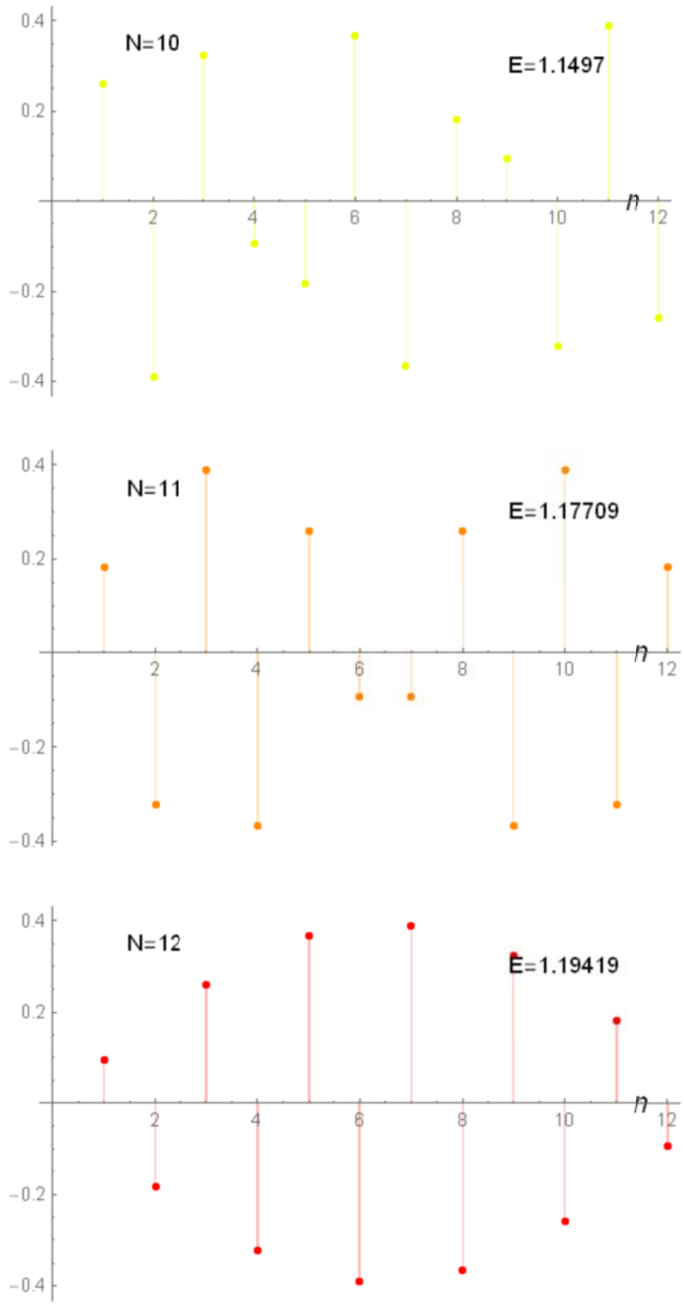




N=4
E=0.886387
N=5
E=0.929079
N=6
E=0.975893
n



N=7
E=1.02411
N=8
E=1.07092
N=9
E=1.11361
n



Highest state $E = E_0 + 2\Delta \approx 1.20$

REFERENCES

R.P. Feynman, R. Leighton, and M. Sands

Pekka: Advanced Quantum Mechanics

R. Shankar, *Principles of Quantum Mechanics*, 2nd edition (Plenum Press, 1994).