PHYS 4302

Homework 2

Charles Averill
charles@utdallas.edu

February 2023

Problem 1

In class we considered a "chain" of N sites (states $|n\rangle$) with nearest-neighbor hopping for our quantum particle, as specified by the Hamiltonian matrix elements

$$\langle n|H|n\rangle = \epsilon, \quad \langle n|H|n+1\rangle = \alpha, \quad n = 1, 2, \ldots N. \tag{1}$$

System (1) was "circularly closed" (with the periodic boundary condition) as signified by

$$|N+1\rangle \equiv |1\rangle, \quad \langle N|H|1\rangle = \alpha \tag{2}$$

and therefore corresponded to ring-type molecular structures. We choose α as a real quantity.

We will be now interested in linear-type molecular structures, for which the periodic boundary condition (2) needs to be replaced with the open-ends condition:

$$\langle N|H|1\rangle = 0. \tag{3}$$

A useful analogy can be drawn with the ordinary 1D quantum mechanics of a particle: compare the particle on a ring and in an infinite square well potential.

We realize that now the familiar system of eigenvalue equations for the wave function amplitudes a_n:

$$Ea_n = \epsilon a_n + \alpha \left(a_{n+1} + \alpha_{n-1}\right), \tag{4}$$

would still look the same for all n except the end sites with $n = 1$ and $n = N$, where there are no neighbors on the left or on the right, respectively. We can easily get out of this inconvenience by augmenting our system with "ghost" sites $n = 0$ and $n = N + 1$ while requiring that the amplitudes on those sites must vanish:

$$a_0 = a_{N+1} = 0. \tag{5}$$

With this augmentation, equations (4) apply for all "real" sites $n = 1, 2, \ldots N$.

(a) Show that the wave function amplitudes in the form of a linear combination of standing waves (6) where k is the unspecified wave number, b the given distance between the neighboring sites, A and B the arbitrary coefficients, satisfy our equations (4) for all "real" sites.

$$a_n \propto A\sin(knb) + B\cos(knb)\,, \tag{6}$$

For some eigenvalue E of H, its corresponding eigenvector $|\psi\rangle$ can be written $|\psi\rangle = \sum_{n=1}^{N} a_n|n\rangle$. To determine that the amplitudes of the eigenvector satisfy (4), we have

$$\begin{aligned}
Ea_n &= \epsilon a_n + \alpha\left(a_{n+1} + a_{n-1}\right) \\
&\quad \text{(replacing proportionality with equality because } A \text{ and } B \text{ are arbitrary)} \\
&= \epsilon a_n + \alpha\Big(A\sin\big(k(n+1)b\big) + B\cos\big(k(n+1)b\big) + A\sin\big(k(n-1)b\big) + B\cos\big(k(n-1)b\big)\Big) \text{ by (6)} \\
&= \epsilon a_n + \alpha\Bigg(A\Big(\sin\big(k(n+1)b\big) + \sin\big(k(n-1)b\big)\Big) + B\Big(\cos\big(k(n+1)b\big) + \cos\big(k(n-1)b\big)\Big)\Bigg) \\
&\quad \text{by trigonometric identity } \sin x + \sin y \\
&= \epsilon a_n + \alpha\Big(A\big(2\sin(knb)\cos(kb)\big) + B\big(2\cos(knb)\cos(kb)\big)\Big) \\
&= \epsilon a_n + 2\alpha\cos(kb)\big(A\sin(knb) + B\cos(knb)\big) \\
&= \big(\epsilon + 2\alpha\cos(kb)\big)a_n \\
\to E &= \boxed{\epsilon + 2\alpha\cos(kb)}
\end{aligned}$$

Therefore, the amplitudes of the eigenvector do satisfy equations (4).

(b) Use now the effective boundary conditions (5) and normalize to determine the actual values of parameters in solutions (6).

$$\begin{aligned}
a_n &= A\sin(knb) + B\cos(knb) \\
\to a_0 &= A\sin(0) + B\sin(0) = 0 \to \boxed{B = 0} \\
a_{N+1} &= A\sin\big(k(N+1)b\big) = 0 \to k(N+1)b = 2\pi p, \quad \exists p \ni p \neq 0 \\
\to k_p &= \frac{2\pi p}{b(N+1)} \\
\to a_n &= A_p\sin\big(k_p nb\big)\,, \quad A_p = A_{p+N+1}
\end{aligned}$$

Normalizing:

$$\begin{aligned}
|\psi\rangle &= \sum n = 1^N a_n|n\rangle - > \sum_{n=1}^{N} a_n^2 = 1 \\
1 &= A_p^2 \sum_{n=1}^{N} \sin^2\big(k_p nb\big) \\
&= A_p^2 \sum_{n=1}^{N} \sin^2\left(\frac{2\pi pn}{N+1}\right) \\
A_p &= \frac{2}{\sqrt{2N + 1 - \sin\left(\frac{2\pi pN}{N+1}\right)\csc\left(\frac{2\pi p}{N+1}\right)}}
\end{aligned}$$

(c) Specify the energies E of all stationary states in our linear system and comment on the degeneracy of the levels in the resulting energy spectrum.

$$E = \epsilon + 2\alpha \cos(kb)$$
$$E_p = \epsilon + 2\alpha \cos\left(\frac{2\pi p}{N+1}\right), \quad p \in Z^+$$

Degenerate states have the same energy as one another, so

$$E_p = E_q$$
$$\cos\left(\frac{2\pi p}{N+1}\right) = \cos\left(\frac{2\pi q}{N+1}\right), \text{ or } p = N+1-1$$

For even N, there are $\frac{N}{2}$ energy levels in the energy spectrum, all two-fold degenerate. Otherwise, there are $\frac{N+1}{2}$ energy levels, all two-fold degenerate except for one.

(d) From your derived normalized wave functions, find the probabilities to find our particle at the end sites $n = 1$ and $n = N$ in all stationary states.

$$P\big(|\psi\rangle = |n\rangle\big) = |a_n|^2$$
$$P\big(|\psi\rangle = |1\rangle\big) = |a_1|^2 = \Big(A_p \sin\big(k_p b\big)\Big)^2 = A_p^2 \sin^2\big(k_p b\big)$$
$$= \boxed{A_p^2 \sin^2\left(\frac{2\pi p}{N+1}\right)}$$
$$P\big(|\psi\rangle = |N\rangle\big) = |a_N|^2 = \Big(A_p \sin\big(k_p bN\big)\Big)^2 = A_p^2 \sin^2\big(k_p bN\big)$$
$$= \boxed{A_p^2 \sin^2\left(\frac{2\pi pN}{N+1}\right)}$$

Problem 2

A localized electron has been polarized so that its spin is oriented in the positive z-direction. It is now subject to the application of a constant uniform magnetic field

$$\mathbf{B}_1 = B\hat{x}$$

along x over a period of time of duration τ. After that, it is subject to the application of another magnetic field of the same magnitude B but along y:

$$\mathbf{B}_2 = B\hat{y},$$

also with duration τ.

The Hamiltonian for this electron is $H = -\mu\mathbf{B}$.

(a) What is the probability P that the spin-flip would occur as a result? That is, what is the probability that the spin of the electron would be found oriented in the negative z-direction after the application of the magnetic field is over?

The electron starts with its spin oriented in the positive z-direction. Therefore, its spin is described by the following Pauli spin matrix:

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

whose eigenvalues are $\lambda = \pm\frac{\hbar}{2}$, yielding eigenvectors $|z+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix}, |z-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, of which we are interested in $|z+\rangle$ at the beginning of the event.

The evolution of the particle in the field can be modeled via the operator

$$\begin{aligned}\hat{U}(\tau) &= e^{-iH\tau} = e^{-i(-\mu\mathbf{B}_1)\tau} \\ &= e^{-i(-\mu B\cos(\theta)\sigma_x)\tau} \\ &= e^{i\mu B\frac{\tau}{\hbar}}\cos\left(\mu B\frac{\tau}{\hbar}\right) I - i\sin\left(\mu B\frac{\tau}{\hbar}\right)\sigma_x\end{aligned}$$

We repeat this to find the evolution of the particle in the second field:

$$\begin{aligned}\hat{V}(\tau) &= e^{-iH\tau} = e^{-i(-\mu\mathbf{B}_2\tau)} \\ &= e^{-i\left(-\mu B\cos(\theta)\sigma_y\right)\tau} \\ &= e^{i\mu B\frac{\tau}{\hbar}}\cos\left(\mu B\frac{\tau}{\hbar}\right) I - i\sin\left(\mu B\frac{\tau}{\hbar}\right)\sigma_y\end{aligned}$$

Using these operators we can determine the state of the electron after exposure to the two fields: $|\psi\rangle = \hat{V}(\tau)\hat{U}(\tau)|z+\rangle$. Now, the probability of finding the electron in the $|z-\rangle$ state due to a spin-flip is given by

$$\begin{aligned}P\left(|\psi\rangle = |z-\rangle\right) &= \left|\langle z-|\hat{V}(\tau)\hat{U}(\tau)|z+\rangle\right|^2 \\ &= \left|\langle z+|\hat{V}(\tau)\hat{U}(\tau)\sigma_z|z+\rangle\right|^2 \\ &= \left|\langle z+|\sigma_y\sigma_x|z+\rangle\right|^2\sin^2\left(\mu B\frac{\tau}{\hbar}\right) \\ &= \left|\langle z+|\sigma_z|z+\rangle\right|^2\sin^2\left(\mu B\frac{\tau}{\hbar}\right) \quad \text{(by } \sigma_y\sigma_x = i\sigma_z\text{)} \\ &= \boxed{\sin^2\left(\mu B\frac{\tau}{\hbar}\right)}\end{aligned}$$

(b) Is it possible to find such duration τ that the spin-flip would occur with probability $P = 1$? If yes, what would be the time τ?

$$\begin{aligned}P = 1 &= \sin^2\left(\mu B\frac{\tau}{\hbar}\right) \\ &\rightarrow \mu B\frac{\tau}{\hbar} = n\pi \\ &\rightarrow \boxed{\tau = n\pi\frac{\hbar}{\mu}B}\end{aligned}$$