

# 1 Problem 1

1D particle in potential  $V(\hat{x}) = U \sin(2\pi\hat{x}/a)$  for  $U > 0$ . Particle is on ring of length  $L = Na$  for  $N$  integer, and satisfies periodic boundary condition  $\Psi(x) = \Psi(x + L)$ .

a.  $\langle x|p \rangle = \frac{e^{ipx/h}}{\sqrt{L}}$ .

$$e^{\frac{i}{\hbar}(xp)} = e^{\frac{i}{\hbar}p(x+L)}$$

$$e^{ixp} = e^{ixp+iLp}$$

(1)

$$e^{iLp} = 1 \rightarrow p = \frac{2\pi}{L}n \text{ for } n \text{ integer.}$$

b. Need to find  $\langle p|V(\hat{x})|p' \rangle$ . Re-express  $V(\hat{x})$  as

$$V(\hat{x}) = U \left[ \frac{e^{2\pi i \hat{x}/a} - e^{-2\pi i \hat{x}/a}}{2i} \right] \text{ and plug in as}$$

$$\langle p|V(\hat{x})|p \rangle = \frac{U}{2i} [\langle p|e^{2\pi i \hat{x}/a}|p \rangle - \langle p|e^{-2\pi i \hat{x}/a}|p \rangle]$$

For each,  $\langle p|e^{\pm 2\pi i \hat{x}/a}|p' \rangle = \int_0^L \frac{e^{-ipx}}{\sqrt{L}} e^{\pm 2\pi i \hat{x}/a} \frac{e^{ip'x}}{\sqrt{L}} dx = \frac{1}{L} \int_0^L e^{-ix(p-p' \mp 2\pi/a)} dx$

(2)

Digressing to the possible solutions to this integral:

$$\text{If } p - p' = \pm \frac{2\pi}{a} \rightarrow \frac{1}{L} \int_0^L e^0 = L/L = 1$$

$$\text{else } p - p' \neq \pm \frac{2\pi}{a} \rightarrow \frac{1}{L} \left[ \frac{e^{-ix(p-p' \mp \frac{2\pi}{a})}}{-i(p-p' \mp \frac{2\pi}{a})} \right] \Big|_0^L = \frac{i}{L} \left[ \frac{e^{iL(-p+p' \pm \frac{2\pi}{a})} - 1}{(p-p' \mp \frac{2\pi}{a})} \right]$$

$$\text{wherein from a. } p = \frac{2\pi n}{L} = \frac{2\pi n}{Na} \text{ therefore } \frac{i}{L} \left[ \frac{e^{i2\pi(-n+n' \pm N)} - 1}{i \frac{2\pi n}{LN a}} \right] = 0$$

(3)

$$\text{Recalling that } e^{i2\pi N} = 1$$

$$\text{As such, } \begin{cases} p - p' = \pm \frac{2\pi}{a} \rightarrow 1 \\ p - p' \neq \pm \frac{2\pi}{a} \rightarrow 0 \end{cases}$$

We enforce the first case  $p - p' = \pm \frac{2\pi}{a}$  such that

$$\langle p|V(\hat{x})|p' \rangle = \frac{U}{2i} [\langle p|e^{2\pi i \hat{x}/a}|p \rangle - \langle p|e^{-2\pi i \hat{x}/a}|p \rangle] = \frac{U}{2i} [\delta_{p-p', \frac{2\pi}{a}} - \delta_{p-p', -\frac{2\pi}{a}}] \quad (4)$$

c. Derive  $|\Psi \rangle$  and reduce it to  $|p = 0 \rangle$  when  $U \rightarrow 0$  to first order in  $U$ . By definition provided in lecture, the wavefn is approximated to  $O(U)$  as below

$$\begin{aligned}
|\Psi\rangle &\approx |0\rangle + \frac{-Q}{E_0 - H^0} V(\hat{x}) |\Psi^0\rangle \\
&= |0\rangle + \frac{-\sum_{p' \neq 0} |p'\rangle \langle p'| V |0\rangle}{E_0 - \frac{p'^2}{2m}}
\end{aligned} \tag{5}$$

From last, substitute  $\sum_{p'} |p'\rangle \langle p'| V |0\rangle = \frac{U}{2i} [|\frac{2\pi\hbar}{a}\rangle - |-\frac{2\pi\hbar}{a}\rangle]$  so that  $E_0 = 0$  while  $H^0 = \frac{p^2}{2m} = \frac{(2\pi\hbar/a)^2}{2m} = \frac{\hbar^2}{2ma^2}$ .

$$\begin{aligned}
|\Psi\rangle &\approx |0\rangle + \frac{1}{\frac{p'^2}{2m}} \frac{U}{2i} [|\frac{2\pi\hbar}{a}\rangle - |-\frac{2\pi\hbar}{a}\rangle] \\
&= |0\rangle + \frac{Uma^2 i}{\hbar^2} [|\frac{2\pi\hbar}{a}\rangle - |-\frac{2\pi\hbar}{a}\rangle]
\end{aligned} \tag{6}$$

Which we can verify reduces to  $|0\rangle$  as  $U \rightarrow 0$ .

**d.** To verify as a block wave, we need to express as plane wave  $\times$  periodic function  $f(x) = f(x+a)$ .

Reexpress the results of 1c as below

$$\begin{aligned}
\langle x | \Psi \rangle &= \langle x | 0 \rangle + C \langle x | \frac{2\pi\hbar}{a} \rangle - C \langle x | \frac{-2\pi\hbar}{a} \rangle \approx e^0 + C i e^{2\pi i x} - C i e^{-2\pi i x} \\
&= 1 + 2iC \sin(2\pi x)
\end{aligned} \tag{7}$$

Which is periodic due to the sine function and has a plane wave block attached where  $e^{ikx}$  as  $k \rightarrow 0$ .

**e.**  $p = \pm \frac{\hbar\pi}{a}$  therefore the subspace is  $[\frac{-\hbar\pi}{a}, \frac{\hbar\pi}{a}]$  with elements  $\langle \pm \frac{\hbar\pi}{a} | V | \pm \frac{\hbar\pi}{a} \rangle$ .

$$V = \begin{bmatrix} \langle \frac{\hbar\pi}{a} | V | \frac{\hbar\pi}{a} \rangle & \langle -\frac{\hbar\pi}{a} | V | \frac{\hbar\pi}{a} \rangle \\ \langle \frac{\hbar\pi}{a} | V | -\frac{\hbar\pi}{a} \rangle & \langle -\frac{\hbar\pi}{a} | V | -\frac{\hbar\pi}{a} \rangle \end{bmatrix} = \frac{U}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{8}$$

Therefore eigenvalues are  $\pm \frac{U}{2}$  and the eigenvector is  $\begin{bmatrix} 1 \\ \pm i \end{bmatrix}$ . The resulting wave equation takes the form  $|\Psi\rangle = |\frac{\hbar\pi}{a}\rangle \pm i |-\frac{\hbar\pi}{a}\rangle$  which, normalized, becomes

$$|\Psi_{\pm}\rangle = \frac{1}{\sqrt{2}} \left[ |\frac{\hbar\pi}{a}\rangle \pm i |-\frac{\hbar\pi}{a}\rangle \right] \text{ with eigenenergies } \frac{p^2}{2m} \pm \frac{U}{2} = \frac{\hbar^2\pi^2}{2ma^2} \pm \frac{U}{2} \tag{9}$$

## 2 Problem 2

a. We want  $\vec{A} = 0$  therefore we impose  $\vec{E} = -\partial_z \phi \hat{z} = E \hat{z}$  where we choose  $E$  in  $\hat{z}$ . Therefore the scalar potential is  $\phi = -Ez$  and the Stark correction is

$$\delta H_S = -e\phi = eEz \quad (10)$$

wrt uniform electric field  $\vec{E}$  and elementary charge  $e$ .

$$H = H_0 + \delta H_S = \frac{p^2}{2m} - \frac{e^2}{r} + eEz \quad (11)$$

b. Firstly, we know  $E_0 = -13.6eV$ . The first-order energy is  $E_1 = \langle \phi_{100} | H_S | \phi_{100} \rangle = eE \langle 100 | z | 100 \rangle$  where the expectation of of an odd fcn is 0, therefore  $E_1 = 0$ . The second-order energy is  $E_2 = \sum_{nlm \neq 100} \frac{|\langle \phi_{nlm} | H_S | \phi_{100} \rangle|^2}{E_0 - \frac{-13.6eV}{n^2}}$ . Therefore,

$$E \approx -13.6eV + \sum_{nlm \neq 100} \frac{e^2 E^2 n^2}{-13.6eV(1 - n^2)} |\langle \phi_{nlm} | z | \phi_{100} \rangle|^2 \quad (12)$$

c. Firstly, we can say that  $\hat{R}(\pi)$  behaves functionally like  $\hat{P}$  in that  $\hat{R}(\pi)\hat{R}(\pi) = I = \hat{P}\hat{P}$  where  $I$  is identity. As such, we can confirm our earlier conclusion for  $E_1 = 0$  with an alternative proof that

$$\begin{aligned} \langle nlm | z | 100 \rangle &= \langle nlm | \hat{P}\hat{P}z\hat{P}\hat{P} | 100 \rangle \\ &= (\langle nlm | \hat{P}) (\hat{P}z\hat{P}) (\hat{P} | 100 \rangle) \\ &= ((-1)^l \langle nlm |) (-z) ((-1)^0 | 100 \rangle) = (-1)^{l+1} \langle nlm | z | 100 \rangle \quad (13) \\ &(-1)^{l+1} = 1 \therefore l \text{ is odd to be nonzero} \\ &\langle 100 | z | 100 \rangle = 0 \end{aligned}$$

As such, the first-order energy dies and the second-order energy is restricted to  $nlm \neq 100, l \text{ odd}$ .

Next, we recognize  $\hat{R}^{-1}\hat{R} = I$  and choose a rotation  $\psi = 2\pi\mathbb{I}$  by which  $R(\psi) = e^{-i\hat{L}_z\psi}$ .

As such,

$$\begin{aligned} \langle nlm|z|100 \rangle &= (\langle nlm|\hat{R}^{-1})(\hat{R}z\hat{R}^{-1})(\hat{R}|100 \rangle) \\ &= (\langle nlm|e^{i\hat{L}_z\psi})(z)(e^{-i\hat{L}_z\psi}|100 \rangle) \end{aligned}$$

$$\begin{aligned} \text{Via the theorem described in class, } \Psi_{nlm}(\hat{R}r) &= e^{im\psi}\Psi_{nlm}(r) \\ \text{satisfies } e^{iL_z\psi}|nlm \rangle &= e^{im\psi}|nlm \rangle \end{aligned} \quad (14)$$

$$\begin{aligned} \therefore \langle nlm|z|100 \rangle &= (\langle nlm|e^{i\hat{L}_z\psi})(z)(e^{-i\hat{L}_z\psi}|100 \rangle) = \langle nlm|e^{im\psi}|z|e^0|100 \rangle \\ \langle nlm|z|100 \rangle &= e^{im\psi} \langle nlm|z|100 \rangle \end{aligned}$$

Wherein with  $e^{im(2\pi\mathbb{I})} = 1$ , the only way which this statement is true is if  $m$  is zero. The second-order energy becomes a sum over  $nlm \neq 100$ ,  $l$  odd and  $m=0$ .

**d.**  $H_z = \frac{|e|\hbar}{m_e c} \vec{S} \cdot \vec{B}$  for  $n=1$  is  $|nlm \rangle \rightarrow |100 \rangle \otimes |\uparrow\rangle$  and  $|100 \rangle \otimes |\downarrow\rangle$ . We choose  $\vec{B} = B\hat{z}$  such that  $\vec{S} \rightarrow \hat{S}_z$  so that each  $|\uparrow\rangle, |\downarrow\rangle$  eigenvector has eigenvalue  $+\frac{\hbar}{2}, -\frac{\hbar}{2}$  for  $\hat{S}_z$  such that the eigenenergies are  $\frac{|e|B\hbar}{2m_e c}, \frac{|e|B\hbar}{2m_e c}$  and we add the ground state order -13.6eV to each.