CSE 389D: Mathematical Modeling **Spring 2025**

Problem Set 4

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Problem 4.1

Part a

Recall that the spin operator is given by $\hat{S} = \frac{1}{2}\hbar\sigma$ where $\sigma = \sigma_x u_x + \sigma_y u_y + \sigma_z u_z$. Then we have that the expectation of the spin operator is

$$\langle\Psi|\,\hat{S}\,|\Psi\rangle = \frac{\hbar}{2}\left[\langle\Psi|\,\sigma_x\,|\Psi\rangle\, u_x + \langle\Psi|\,\sigma_y\,|\Psi\rangle\, u_y + \langle\Psi|\,\sigma_z\,|\Psi\rangle\, u_z\right]$$

and we have that

$$\begin{aligned}
\langle\Psi|\,\sigma_x\,|\Psi\rangle = \begin{bmatrix} u^*(r) & d^*(r) \end{bmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{bmatrix} u(r) \\ d(r) \end{bmatrix} &= u^*(r)d(r) + d^*(r)u(r) \\
&= \operatorname{Re}(u^*d) + i\operatorname{Im}(u^*d) + \operatorname{Re}(u^*d) - i\operatorname{Im}(u^*d) \\
&= 2\operatorname{Re}(u^*d)
\end{aligned}$$

and

$$\begin{aligned}
\langle\Psi|\,\sigma_y\,|\Psi\rangle = \begin{bmatrix} u^*(r) & d^*(r) \end{bmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{bmatrix} u(r) \\ d(r) \end{bmatrix} &= -iu^*(r)d(r) + id^*(r)u(r) \\
&= -i\operatorname{Re}(u^*d) + \operatorname{Im}(u^*d) + i\operatorname{Re}(u^*d) + \operatorname{Im}(u^*d) \\
&= 2\operatorname{Im}(u^*d)
\end{aligned}$$

lastly,

$$\begin{aligned}
\langle\Psi|\,\sigma_z\,|\Psi\rangle = \begin{bmatrix} u^*(r) & d^*(r) \end{bmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{bmatrix} u(r) \\ d(r) \end{bmatrix} &= u^*(r)u(r) - d^*(r)d(r) \\
&= |u|^2 - |d|^2
\end{aligned}$$

and hence then expectation value of the spin operator on this spinsor is given by

$$\langle\Psi|\,\hat{S}\,|\Psi\rangle = \frac{\hbar}{2}\left[2\operatorname{Re}(u^*d)u_x + 2\operatorname{Im}(u^*d)u_y + (|u|^2 - |d|^2)u_z\right]$$

Part b

We compute the norm of $\langle\Psi|\,\hat{S}\,|\Psi\rangle$ as

$$\begin{aligned}
|\langle\Psi|\,\hat{S}\,|\Psi\rangle| &= \frac{\hbar}{2}\sqrt{4\operatorname{Re}(u^*d)^2 + 4\operatorname{Im}(u^*d)^2 + |u|^4 - 2|u|^2|d|^2 + |d|^4} \\
&= \frac{\hbar}{2}\sqrt{4|u^*d|^2 + |u|^4 - 2|u|^2|d|^2 + |d|^4} \\
&= \frac{\hbar}{2}\sqrt{4|u|^2|d|^2 + |u|^4 - 2|u|^2|d|^2 + |d|^4} \\
&= \frac{\hbar}{2}\sqrt{|u|^4 + 2|u|^2|d|^2 + |d|^4} \\
&= \frac{\hbar}{2}\sqrt{(|u|^2 + |d|^2)^2} \\
&= \frac{\hbar}{2}\sqrt{|\Psi|^2} = \frac{\hbar}{2}
\end{aligned}$$

Part c

Consider

$$\exp\left(i\varphi\frac{\hat{S}_z}{\hbar}\right) = \sum_{n=0}^{\infty}\frac{\left(i\varphi\frac{\hat{S}_z}{\hbar}\right)^n}{n!} = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\varphi}{2}\right)^n\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}^n$$

note that for n even we have that

$$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}^n = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

and remains unchanged for n odd, thus we can write the above as

$$\exp\left(i\varphi\frac{\hat{S}_z}{\hbar}\right) = \begin{pmatrix}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\varphi}{2}\right)^n & 0\\ 0 & \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i\varphi}{2}\right)^n\end{pmatrix} = \begin{pmatrix}\exp\left(\frac{i\varphi}{2}\right) & 0\\ 0 & \exp\left(-\frac{i\varphi}{2}\right)\end{pmatrix}$$

Part d

Note that

$$\Psi' = \exp\left(i\varphi\frac{\hat{S}_z}{\hbar}\right)\Psi = \begin{pmatrix}\exp\left(\frac{i\varphi}{2}\right) & 0\\ 0 & \exp\left(-\frac{i\varphi}{2}\right)\end{pmatrix}\begin{bmatrix}u\\ d\end{bmatrix} = \begin{bmatrix}e^{i\varphi/2}u\\ e^{-i\varphi/2}d\end{bmatrix}$$

then we get that

$$\begin{aligned}
\langle\Psi|\,\sigma_x\,|\Psi\rangle &= \begin{bmatrix}e^{-i\varphi/2}u^*(r) & e^{i\varphi/2}d^*(r)\end{bmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{bmatrix}e^{i\varphi/2}u(r)\\ e^{-i\varphi/2}d(r)\end{bmatrix} = e^{-i\varphi}u^*(r)d(r) + e^{i\varphi}d^*(r)u(r) \\
&= \operatorname{Re}(e^{-i\varphi}u^*d) + i\operatorname{Im}(e^{-i\varphi}u^*d) + \operatorname{Re}(e^{-i\varphi}u^*d) - i\operatorname{Im}(e^{-i\varphi}u^*d) \\
&= 2\operatorname{Re}(e^{-i\varphi}u^*d)
\end{aligned}$$

and

$$\begin{aligned}\langle\Psi|\, \sigma_y \,|\Psi\rangle &= \begin{bmatrix} e^{-i\varphi/2}u^*(r) & e^{i\varphi/2}d^*(r)\end{bmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{bmatrix} e^{i\varphi/2}u(r) \\ e^{-i\varphi/2}d(r)\end{bmatrix} = -ie^{i\varphi}u^*(r)d(r) + ie^{i\varphi}d^*(r)u(r) \\ &= -i\,\mathrm{Re}(e^{-i\varphi}u^*d) + \mathrm{Im}(e^{-i\varphi}u^*d) + i\,\mathrm{Re}(e^{-i\varphi}u^*d) + \mathrm{Im}(e^{-i\varphi}u^*d) \\ &= 2\,\mathrm{Im}(e^{-i\varphi}u^*d)\end{aligned}$$

lastly,

$$\begin{aligned}\langle\Psi|\, \sigma_z \,|\Psi\rangle = \begin{bmatrix} e^{-i\varphi/2}u^*(r) & e^{i\varphi/2}d^*(r)\end{bmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{bmatrix} e^{i\varphi/2}u(r) \\ e^{-i\varphi/2}d(r)\end{bmatrix} &= u^*(r)u(r) - d^*(r)d(r) \\ &= |u|^2 - |d|^2\end{aligned}$$

and hence then expectation value of the spin operator on this spinsor is given by

$$\langle\Psi'|\, \hat{S} \,|\Psi'\rangle = \frac{\hbar}{2}\left[2\,\mathrm{Re}(e^{-i\varphi}u^*d)u_x + 2\,\mathrm{Im}(e^{-i\varphi}u^*d)u_y + (|u|^2 - |d|^2)u_z\right]$$

Part e

Suppose that $u^*d = a + bi$ then $a = \frac{1}{2}S_x$ and $b = \frac{1}{2}S_y$ and we have that

$$e^{-i\varphi}u^*d = (a+bi)(\cos(i\varphi) - i\sin(\varphi)) = a\cos(\varphi) + b\sin(\varphi) + i\left(b\cos(\varphi) - a\sin(\varphi)\right)$$

thus

$$S'_x = 2\,\mathrm{Re}(e^{-i\varphi}u^*d) = S_x\cos(\varphi) + S_y\sin(\varphi)$$

and

$$S'_y = 2\,\mathrm{Im}(e^{-i\varphi}u^*d) = S_y\cos(\varphi) - S_x\sin(\varphi)$$

and clearly

$$S'_z = S_z$$

Part f

From the change of coordinates in Part e, we have that $\exp\left(i\varphi\frac{\hat{S}_z}{\hbar}\right)$ is a clockwise rotation about the z-axis by angle φ.

Problem 4.2

Part a

Recall that

$$\chi_\uparrow = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \chi_\downarrow = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

and note that

$$\chi_\uparrow \otimes \chi_\uparrow = \begin{bmatrix}1\\0\end{bmatrix} \otimes \begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}$$

$$\chi_\uparrow \otimes \chi_\downarrow = \begin{bmatrix}1\\0\end{bmatrix} \otimes \begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$$

$$\chi_\downarrow \otimes \chi_\uparrow = \begin{bmatrix}0\\1\end{bmatrix} \otimes \begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}0\\0\\1\\0\end{bmatrix}$$

$$\chi_\downarrow \otimes \chi_\downarrow = \begin{bmatrix}0\\1\end{bmatrix} \otimes \begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

and hence we see that

$$\psi(\mathbf{r}_1, \mathbf{r}_2; 1)\chi_\uparrow \otimes \chi_\uparrow + \psi(\mathbf{r}_1, \mathbf{r}_2; 2)\chi_\uparrow \otimes \chi_\downarrow + \psi(\mathbf{r}_1, \mathbf{r}_2; 3)\chi_\downarrow \otimes \chi_\uparrow + \psi(\mathbf{r}_1, \mathbf{r}_2; 4)\chi_\downarrow \otimes \chi_\downarrow$$

becomes

$$\psi(\mathbf{r}_1, \mathbf{r}_2; 1)\begin{bmatrix}1\\0\\0\\0\end{bmatrix} + \psi(\mathbf{r}_1, \mathbf{r}_2; 2)\begin{bmatrix}0\\1\\0\\0\end{bmatrix} + \psi(\mathbf{r}_1, \mathbf{r}_2; 3)\begin{bmatrix}0\\0\\1\\0\end{bmatrix} + \psi(\mathbf{r}_1, \mathbf{r}_2; 4)\begin{bmatrix}0\\0\\0\\1\end{bmatrix} = \begin{bmatrix}\psi(\mathbf{r}_1, \mathbf{r}_2; 1)\\\psi(\mathbf{r}_1, \mathbf{r}_2; 2)\\\psi(\mathbf{r}_1, \mathbf{r}_2; 3)\\\psi(\mathbf{r}_1, \mathbf{r}_2; 4)\end{bmatrix}$$

Part b

Consider the spin operator for the two electron systems defined by

$$\hat{S}_{\text{tot}} = \hat{S} \otimes I + I \otimes \hat{S}$$

where $\hat{S} = \hbar/2\hat{\sigma}$. Then we have that

$$\hat{S} \otimes I = \frac{\hbar}{2}\begin{bmatrix}\sigma_x\\\sigma_y\\\sigma_z\end{bmatrix} \otimes \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} = \frac{\hbar}{2}\begin{bmatrix}0 & I\\I & 0\\0 & -iI\\iI & 0\\I & 0\\0 & -I\end{bmatrix}$$

and

$$I \otimes \hat{S} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \frac{\hbar}{2} \begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} \sigma_x & 0 \\ \sigma_y & 0 \\ \sigma_z & 0 \\ 0 & \sigma_x \\ 0 & \sigma_y \\ 0 & \sigma_z \end{bmatrix}$$

thus

$$\hat{S}_{\text{tot}} = \frac{\hbar}{2} \begin{bmatrix} 0 & I \\ I & 0 \\ 0 & -iI \\ iI & 0 \\ I & 0 \\ 0 & -I \end{bmatrix} + \frac{\hbar}{2} \begin{bmatrix} \sigma_x & 0 \\ \sigma_y & 0 \\ \sigma_z & 0 \\ 0 & \sigma_x \\ 0 & \sigma_y \\ 0 & \sigma_z \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} \sigma_x & I \\ \sigma_y + I & 0 \\ \sigma_z & -iI \\ iI & \sigma_x \\ I & \sigma_y \\ 0 & \sigma_z - I \end{bmatrix}$$

or after expanding each the σ_i terms we have that

$$\hat{S}_{\text{tot}} = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & -i & 0 & 0 \\ i & 1 & 0 & 0 \\ 1 & 0 & -i & 0 \\ 0 & -1 & 0 & -i \\ i & 0 & 0 & 1 \\ 0 & i & 1 & 0 \\ 1 & 0 & 0 & -i \\ 0 & 1 & i & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{bmatrix}$$

then we get that

$$(\hat{S}_{\text{tot}})_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & -i \\ 0 & -1 & i & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix}$$