Chapter 4

4.1

Using a generalized commutator

$$\left[\hat{A}, \hat{B}\right]_{\zeta} = \hat{A}\hat{B} - \zeta\hat{B}\hat{A}$$

where $\zeta = \pm 1$ for bosons/fermions, the operator $\hat{\rho}(\mathbf{x})\hat{\rho}(\mathbf{y})$ can be written as

$$\begin{aligned}
\hat{\rho}(\mathbf{x})\hat{\rho}(\mathbf{y}) &= \hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}^{\dagger}(\mathbf{y})\hat{\psi}(\mathbf{y}) \\
&= \hat{\psi}^{\dagger}(\mathbf{x})\Big(\delta^{(3)}(\mathbf{x}-\mathbf{y}) + \zeta\hat{\psi}^{\dagger}(\mathbf{y})\hat{\psi}(\mathbf{x})\Big)\hat{\psi}(\mathbf{y}) \\
\hat{\rho}(\mathbf{x})\hat{\rho}(\mathbf{y}) &= \zeta^2\hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}^{\dagger}(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) + \delta^{(3)}(\mathbf{x}-\mathbf{y})\hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}(\mathbf{y})
\end{aligned}$$

which yields the "wrong" potential shown below. Since for bosons and fermions $\zeta^2 = 1$, the result is the same for both

$$\begin{aligned}
\hat{V}_{\text{wrong}} &= \frac{1}{2}\int \mathrm{d}^3x\,\mathrm{d}^3y\,V(\mathbf{x},\mathbf{y})\hat{\rho}(\mathbf{x})\hat{\rho}(\mathbf{y}) \\
&= \frac{\zeta^2}{2}\int \mathrm{d}^3x\,\mathrm{d}^3y\,\hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}^{\dagger}(\mathbf{y})V(\mathbf{x},\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) + \frac{1}{2}\int \mathrm{d}^3x\,V(\mathbf{x},\mathbf{x})\hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}(\mathbf{x}) \\
&\boxed{\hat{V}_{\text{wrong}} = \hat{V} + \frac{1}{2}\int \mathrm{d}^3x\,V(\mathbf{x},\mathbf{x})\hat{\rho}(\mathbf{x})}
\end{aligned}$$

4.2

The single particle density matrix

$$\hat{\rho}_1(\mathbf{x}-\mathbf{y}) = \left\langle \hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}(\mathbf{y})\right\rangle$$

can be written in terms of creation and annihilation operators as follows

$$\hat{\rho}_1(\mathbf{x}-\mathbf{y}) = \left\langle \frac{1}{\sqrt{\mathcal{V}}}\sum_{\mathbf{q}}\hat{a}^{\dagger}_{\mathbf{q}}e^{-i\mathbf{q}\cdot\mathbf{x}}\frac{1}{\sqrt{\mathcal{V}}}\sum_{\mathbf{p}}\hat{a}_{\mathbf{p}}e^{i\mathbf{p}\cdot\mathbf{y}}\right\rangle$$

$$\boxed{\hat{\rho}_1(\mathbf{x}-\mathbf{y}) = \frac{1}{\mathcal{V}}\sum_{\mathbf{p},\mathbf{q}}e^{-i(\mathbf{q}\cdot\mathbf{x}-\mathbf{p}\cdot\mathbf{y})}\left\langle\hat{a}^{\dagger}_{\mathbf{q}}\hat{a}_{\mathbf{p}}\right\rangle}$$

4.3

The Hubbard Hamiltonian for a two spin system in which the spins are anti-aligned is given by

$$\hat{H} \to \begin{pmatrix} U & -t & -t & 0 \\ -t & 0 & 0 & -t \\ -t & 0 & 0 & -t \\ 0 & -t & -t & U \end{pmatrix}$$

The eigenvalues of this Hamiltonian can be found as follows

$$\begin{vmatrix} U-E & -t & -t & 0 \\ -t & -E & 0 & -t \\ -t & 0 & -E & -t \\ 0 & -t & -t & U-E \end{vmatrix} = 0$$

$$(U-E)\Big\{-E\Big[-E(U-E)-t^2\Big]-t\Big[-tE\Big]\Big\}+t\Big\{-t\Big[-E(U-E)-t^2\Big]-t\Big[t^2\Big]\Big\}$$
$$-t\Big\{-t\Big[-t^2\Big]+E\Big[-t(U-E)\Big]-t\Big[t^2\Big]\Big\}=0$$
$$(U-E)\Big\{E^2(U-E)+Et^2+Et^2\Big\}+t\Big\{Et(U-E)+t^3-t^3\Big\}+t\Big\{-t^3+Et(U-E)+t^3\Big\}=0$$
$$E^2(U-E)^2+2Et^2(U-E)+Et^2(U-E)+Et^2(U-E)=0$$
$$E(U-E)\Big[E(U-E)+4t^2\Big]=0$$
$$\boxed{E=0,U,\frac{U}{2}\pm\frac{1}{2}\left(U^2+16t^2\right)^{1/2}}$$

The eigenvectors corresponding to these values are as follows

$$\begin{aligned}
|E_0\rangle &= \frac{1}{\sqrt{2}}\Big[\,|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle\,\Big] \\
|E_U\rangle &= \frac{1}{\sqrt{2}}\Big[\,|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle\,\Big] \\
|E_+\rangle &= N\Big[\,|\uparrow\downarrow,0\rangle+\left(\frac{U}{4t}-\frac{1}{4t}\left(U^2+16t^2\right)^{1/2}\right)\Big(|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle\Big)+|0,\uparrow\downarrow\rangle\,\Big] \\
|E_-\rangle &= N\Big[\,|\uparrow\downarrow,0\rangle+\left(\frac{U}{4t}+\frac{1}{4t}\left(U^2+16t^2\right)^{1/2}\right)\Big(|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle\Big)+|0,\uparrow\downarrow\rangle\,\Big]
\end{aligned}$$

where N is just a normalization constant. In the limit as $t \to 0$, the energy eigenvalues become degenerate

$$\boxed{E=0,0,U,U}$$

In the limit $\dfrac{t}{U} \ll 1,\ t \neq 0$, we have

$$\begin{aligned}
E_\pm &= \frac{U}{2}\pm\frac{U}{2}\left[1+\left(\frac{4t}{U}\right)^2\right]^{1/2} \\
&\approx \frac{U}{2}\pm\frac{U}{2}\left[1+\frac{1}{2}\left(\frac{4t}{U}\right)^2\right] \\
E_\pm &= \frac{U}{2}\pm\frac{U}{2}\pm\frac{8t^2}{U}
\end{aligned}$$

and therefore

$$\boxed{E=0,U,U+4U\left(\frac{t}{U}\right)^2,-4U\left(\frac{t}{U}\right)^2}$$