Problem J13Q.2

(a) For a single particle with these boundary conditions, the eigenstates are

$$\psi_n(x) := \frac{e^{2i\pi nx/L}}{\sqrt{L}}$$

for $n \in \mathbb{Z}$, with corresponding energy

$$E_n := \frac{\hbar^2}{2m}\left(\frac{2\pi n}{L}\right)^2 = E_1 n^2.$$

The spins of the particles may couple to give spin $0, 1$, or 2.

The total wavefunction must be symmetric. In the total spin-0 and spin-2 case, the spin wavefunction is symmetric, so the spatial wavefunction must be symmetric. In this case the spatial ground state is

$$\Psi_{00}(x_1, x_2) = \psi_0(x_1)\psi_0(x_2) = \frac{1}{L},$$

with zero energy. The first excited state is two-fold (spatially) degenerate, with basis

$$\begin{aligned}\Psi_{\pm}^{(+)}(x_1, x_2) &:= \frac{\psi_{\pm 1}(x_1)\psi_0(x_2) + \psi_0(x_1)\psi_{\pm 1}(x_2)}{\sqrt{2}} \\ &= \frac{e^{\pm 2\pi i x_1/L} + e^{\pm 2\pi i x_2/L}}{L\sqrt{2}},\end{aligned}$$

each with energy $E_1 = 2\pi^2\hbar^2/mL^2$. In the spin-2 case, the above degeneracies must be multiplied by 5.

In the total spin-1, case, the spatial wavefunction must be antisymmetric. Thus the ground state in this case is two-fold spatially degenerate (six-fold including spin), with spatial basis

$$\begin{aligned}\Psi_{\pm}^{(-)}(x_1, x_2) &:= \frac{\psi_{\pm 1}(x_1)\psi_0(x_2) - \psi_0(x_1)\psi_{\pm 1}(x_2)}{\sqrt{2}} \\ &= \frac{e^{\pm 2\pi i x_1/L} - e^{\pm 2\pi i x_2/L}}{L\sqrt{2}}\end{aligned}$$

and energy E_1. There is a non-degenerate (three-fold degenerate including spin) first excited state

$$\begin{aligned}\Psi_{1,-1}^{(-)}(x_1, x_2) &:= \frac{\psi_1(x_1)\psi_{-1}(x_2) - \psi_{-1}(x_1)\psi_1(x_2)}{\sqrt{2}} \\ &= \frac{i\sqrt{2}}{L}\sin\left(2\pi\frac{x_1 - x_2}{L}\right).\end{aligned}$$

(b) The interaction does not affect the total spin-1 case, since the spatial wavefunction is antisymmetric and so there is always zero amplitude on the manifold $x_1 = x_2$.

For the total spin-0 and spin-2 case, the ground state remains non-degenerate, since it is protected by a gap $E_1 > 0$ from the first excited state manifold.

The twofold-degenerate first excited state splits under a small interaction g. Under first-order degenerate perturbation theory, we compute the matrix elements

$$V \sim \frac{g}{L}\begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}$$

with respect to the basis $\Psi_+^{(+)}, \Psi_-^{(+)}$, so the new first and second excited states are

$$\Psi_a := \frac{\Psi_+^{(+)} + \Psi_-^{(+)}}{\sqrt{2}} \quad \text{and} \quad \Psi_b := \frac{\Psi_+^{(+)} - \Psi_-^{(+)}}{\sqrt{2}}$$

with energies $E_a = E_1 + 2g/L$ and $E_b = E_1 - 2g/L$, respectively. In the case $g > 0$, the state E_b is the new lowest excited state. In the case $g < 0$, the state E_a is the new lowest excited state.

(c) For $g = 0$, the ground state is sixfold degenerate with wavefunction

$$|\Psi_{00}\rangle \otimes |S\rangle\,,$$

where $|S\rangle$ is any linear combination of spin states with total spin 0 or 2.

For $g \neq 0$, the ground state is again sixfold-degenerate of the form $|\Psi\rangle \otimes |S\rangle$, where $|\Psi\rangle$ is the unique spatial ground state. To determine the spatial wavefunction, we may unwrap the coordinates x_1, x_2 and deal with a lattice potential

$$V(x_1, x_2) = g \sum_{r \in L\mathbb{Z}} \delta(x_1 - x_2 - r).$$

Defining the new coordinates $u := x_1 + x_2$ and $v := x_1 - x_2$, the Hamiltonian becomes

$$H = -\frac{\hbar^2}{4m}\partial_u^2 - \frac{\hbar^2}{4m}\partial_v^2 + g \sum_{r \in L\mathbb{Z}} \delta(v - r).$$

This Hamiltonian is now separable, and its ground state has no u-dependence.

The ground-state wavefunction for v must be L-periodic, so we need only solve for $\Psi(v)$ on $[0, L]$. For $g < 0$ this must be of the form

$$\Psi(v) = \cosh(k\,(v - L/2)),$$

and for $g > 0$ we must have

$$\Psi(v) = \cos(k\,(v - L/2)).$$

In the first case the energy is $E = -\hbar^2 k^2/4m$, and there is a boundary condition

$$\Psi'(L) - \Psi'(0) = \frac{4mg}{\hbar^2}\Psi(0)$$

from integrating the Schrödinger equation. This equation expands to

$$2k\tanh(kL/2) + \frac{4mg}{\hbar^2} = 0,$$

which yields a unique solution $k > 0$ for every $g < 0$.

For the case $g > 0$, the ground-state energy is $E = \hbar^2 k^2/4m$, and the boundary condition becomes

$$2k\tan(kL/2) - \frac{4mg}{\hbar^2} = 0,$$

which again yields a solution $k > 0$ for any $g < 0$. In this case there are multiple solutions, and the ground state corresponds to the minimal k.

As expected, in both cases $k \to 0$ as $g \to 0$, and the ground state reduces to a uniform distribution.