Lista 3 - Quântica B (2013)

1. Counting states

Consider a one-particle quantum mechanical system with a Hilbert space spanned by three orthonormal states $|n\rangle$, with $n = 1, 2, 3$. Three non-interacting particles occcupy these states. Determine how many distinct physical states there are if these particles are: (a) three identical fermions, (b) three identical bosons, (c) two identical fermions and one boson, (d) two identical bosons and one fermion, (e) three distinct fermions, and (f) three distinct bosons.

2. Exchange interaction

Consider a one-dimensional system of two spin-1/2 fermions. The two fermions move in the field of an anharmonic double-well oscillator and interact with each other through a repulsive pair interaction $V(|x|)$. The Hamiltonian for this two-particle system is

$$H = \frac{1}{2m}\left(p_1^2 + p_2^2\right) + U(x_1) + U(x_2) + V(|x_1 - x_2|),$$

where the double-well potential is $U(x) = \frac{U_0}{a^4}\left(x^2 - a^2\right)^2$. As for the pair potential $V(x)$, we will only need to assume that it is repulsive and that it decreases sufficiently fast so that all the integrals involved are convergent. Finally, let $\langle x|R\rangle = \psi_R(x)$ be the harmonic-oscillator ground-state wavefunction centered around $x = a$ and $\langle x|L\rangle = \psi_L(x)$ be the corresponding wave function centered around $x = -a$:

$$\psi_R = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-\frac{(x-a)^2}{2\sigma^2}} \text{ and } \psi_L = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-\frac{(x+a)^2}{2\sigma^2}}, \text{ with } \sigma^2 = \frac{\hbar a}{\sqrt{8mU_0}}.$$

(a) Give a justification for $\psi_{R,L}$. When are they expected to be a good approximation of the true ground-state wavefunctions? Compute the overlap $\ell = \langle L|R\rangle$.

(b) Find the expressions for the matrix elements of the one-particle Hamiltonian $H^{(1)} = \frac{1}{2m}p^2 + U(x)$ in the space spanned by the two single particle kets $|R\rangle$ and $|L\rangle$:

$$H^{(1)}_{\text{eff}} = \begin{pmatrix} \left\langle R\left|H^{(1)}\right|R\right\rangle & \left\langle R\left|H^{(1)}\right|L\right\rangle \\ \left\langle L\left|H^{(1)}\right|R\right\rangle & \left\langle L\left|H^{(1)}\right|L\right\rangle \end{pmatrix}.$$

Now, diagonalize $H^{(1)}_{\text{eff}}$ and find its two Eigenstates $|\pm\rangle$ and corresponding energies $E_\pm$.

(c) What is the maximum number of linearly independent, properly anti-symmetrized two-particle states (including spin)? Construct the two-particle basis using the single particle states $|+,\uparrow\rangle$, $|+,\downarrow\rangle$, $|-,\uparrow\rangle$, and $|-,\downarrow\rangle$.

(d) Calculate the matrix elements of the interaction term (V) of the two-particle Hamiltonian in the unsymmetrized (orbital) basis $|R,R\rangle$, $|R,L\rangle$, $|L,R\rangle$, and $|L,L\rangle$. Now, find an expression for the *appropriately defined* Direct (Coulomb) and Exchange integrals.

(e) Use these expressions (and the overlap ℓ) to compute the energy levels, their quantum numbers and their degeneracies for this two-particle system. Find an expression for the Exchange constant J. (*Hint*: Express your result in terms of $H_{\text{eff}} = \text{const} + J\mathbf{S}_1 \cdot \mathbf{S}_2$, with $\mathbf{S}_i$ being the spin operators.)

3. Free fermions

Consider a system of noninteracting N spin-1/2 particles which are free to move in a smooth one-dimentional ring of length L. The one-particle wavefunctions are

$$\langle x, \sigma|\psi\rangle = \psi_{n,\sigma}(x),$$

with $\sigma = \uparrow, \downarrow$ representing the spin, and n a quantum number to be defined. Assume that $N/2$ is an odd integer.

(a) Write down the one-particle states wavefunctions $\psi_{\sigma,n}(x)$ which obey the boundary condition given above. What is the meaning of the quantum number n?

(b) Use the fermionic field operators $a^\dagger_\sigma(x)$ and $a_\sigma(x)$ in position space (which create/annihilate a fermion in with spin σ at position x) to write the Hamiltonian of this free fermion system in the Fock space. Do the same now for the operators in momentum space.

(c) Compute the anticommutators $\left\{\tilde{a}_\sigma(p), \tilde{a}^\dagger_\tau(q)\right\}$ and $\left\{\tilde{a}_\sigma(p), \tilde{a}_\tau(q)\right\}$.

(d) Construct the many-particle ground state $|G\rangle$ for this system in the Fock space. Compute the Fermi energy E_F, namely the energy of the topmost occupied state. How many single-particle states are present in $|G\rangle$?

(e) Show that the wavefunction of the ground state is an $N \times N$ Slater determinant. In addition, show this determinant can be factorized to the product of two $\frac{N}{2} \times \frac{N}{2}$ determinants. (*Hint*: Notice that $\langle x_{i,\sigma} | \psi_{n,\tau} \rangle = \delta_{\sigma,\tau} \psi_{n,\tau}(x_{i,\sigma})$, where $x_{i,\sigma}$ is the position of the i-th particle with spin σ.)

(f) Show that

$$\Psi\left(x_{1,\uparrow}, x_{1,\downarrow}, \ldots, x_{\frac{N}{2},\uparrow}, x_{\frac{N}{2},\downarrow}\right) = L^{-\frac{N}{2}} e^{-i\left(\frac{2\pi}{L}\right)\left(\frac{N-2}{4}\right) N X_{\mathrm{CM}}} \prod_{i<j=1}^{\frac{N}{2}} \left(z_{i,\uparrow} - z_{j,\uparrow}\right)\left(z_{i,\downarrow} - z_{j,\downarrow}\right),$$

where $z_{i,\sigma} = e^{i\frac{2\pi}{L} x_{i,\sigma}}$ and X_{CM} is the position of the center of mass of the system. (*Hint*: Recall the Vandermonde matrix.)

4. Two coupled bosons

Consider a system of two distinct bosonic particles (type A and B) in which only one mode of each is present:

$$H = \epsilon_{\mathrm{A}} a^\dagger a + \epsilon_{\mathrm{B}} b^\dagger b + V a^\dagger b + V^* b^\dagger a.$$

(a) Show that $c \equiv ua - vb$ and $d \equiv v^* a + u^* b$, with $|u|^2 + |v|^2 = 1$ are bosonic operators.

(b) Show that when $\epsilon_{\mathrm{A}} = \epsilon_{\mathrm{B}}$ and $V = V^*$, the choice $u = v = 1/\sqrt{2}$ decouples the system of bosonic particles C and D.

(c) Determine u and v that diagonalizes the system in the general case. Find the Eigenenergies and Eigenvectors of the system.

5. Two coupled fermions

Consider a system of two spin-$1/2$ identical fermionic particles that can occupy three different states of energies E_i, $i = 1, 2, 3$. The matrix elements allowing the transitions between these states are M_{ij}.

(a) Write down the system Hamiltonian in terms of the criation and annihilation operators.

(b) Determine the equation that gives the Eigenenergies of the sytem.

(c) Diagonalize the system for the particular case $E_i = E$ and $M_{ij} = M$, and the spins of the particles are the same.

6. Grand-canonical ensamble

The Grand partition function is given by the trace

$$Z_{\mathrm{G}} = \operatorname{tr} e^{-\beta(H-\mu N)}, \text{ where } H = \sum_i \epsilon_i a_i^\dagger a_i \text{ and } N = \sum_i a_i^\dagger a_i,$$

and the constants β and μ are the inverse of temperature and the chemical potential, respectively. In the following compute the required quantities for both cases of identical bosonic and fermionic particles.

(a) Compute Z_{G}. (*Hint*: Use the trace in the Fock space: $\operatorname{tr} O = \sum_{n_i \ldots n_\infty} \langle n_1 \ldots n_\infty | O | n_1 \ldots n_\infty \rangle$, and recall that in the Grand-canonical ensamble the number of particles is not fixed.)

(b) Compute the average occupation number $\langle n_i \rangle$, such that $\mathcal{N} = \sum_i \langle n_i \rangle$. (*Hint*: Recall the thermodynamic Grand-potential $\Omega(T, V, \mu) = \beta^{-1} \ln Z_{\mathrm{G}}$, and that $\mathcal{N} = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V}$.)

(c) Show that the fractional deviation from the mean occupation number

$$\frac{\left\langle \left(n_i - \langle n_i \rangle\right)^2 \right\rangle}{\langle n_i \rangle^2} = e^{\beta(\epsilon_i - \mu)} = \frac{1}{\langle n_i \rangle} + \zeta,$$

with the $\zeta = \pm 1$ for bosons and fermions, respectively.

7. Holes in a magnetic moment closed shell as an antiparticle (Merzbacher, chap. 22 - 3rd ed.)

Let $a_{j,m}^\dagger$ be a criation operator of fermionic particle with angular momentum j and projection in the z-direction m.

(a) Construct the closed-shell state: a state in which all one-particle states $m = -j$ to $= +j$ are occupied.

(b) Prove that the this state has zero total angular momentum.

(c) If a fermion with a certain magnetic quantum number $m = k$ is missing from this closed-shell state of particles, show that, for angular momentum purposes, this hole state can be treated as the state of a single particle with quantum number $-k$, and effective creation operator $(-1)^{j-k} a_{j,k}$.

8. (Optional) More on exchange (Merzbacher, chap. 22 - 3rd ed.)

Consider the unperturbed states of n spin-1/2 particles, $a^\dagger_{n,\sigma_n} \dots a^\dagger_{k,\sigma_k} \dots a^\dagger_{1,\sigma_1} |0\rangle$, each occupying one of the n equivalent, degenerate orthogonal orbitals labeled by the quantum number k, with $\sigma_k = \pm 1/2$ denoting the spin quantum number associate with the orbital k. Show that in the space of the 2^n unperturbed states a spin-independent two-body interaction may, in first-order perturbation theory, be replaced by the effective exchange (Heisenberg) Hamiltonian

$$H_{\text{eff}} = -\frac{1}{\hbar^2} \sum_{k,\ell} \langle k, \ell \,| V |\, \ell, k \rangle \, \mathbf{S}_k \cdot \mathbf{S}_\ell + \text{const}, \;\; \text{where } \mathbf{S}_k = \frac{\hbar}{2} \sum_{\sigma_k, \tau_k} a^\dagger_{k,\sigma_k} a_{k,\tau_k} \, \langle \sigma_k \,| \boldsymbol{\sigma} |\, \tau_k \rangle$$

is the localized spin operator, and $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli matrices.

ANSWER:

1.

(a) One state, given by the antisymmetrization of $|1,2,3\rangle \rightarrow (|1,2,3\rangle + |2,3,1\rangle + |3,1,2\rangle - |2,1,3\rangle - |3,2,1\rangle - |1,3,2\rangle)/\sqrt{6}$.

(b) One state in which all bosons are in distinct sates (given by the symmetrization of $|1,2,3\rangle$). Six states in which one of the states are not occupied (they are of type $|1,1,2\rangle$). Three states in which all bosons are in the same state: $|n,n,n\rangle$, with $n = 1,2,3$. Thus, total of 10 states.

(c) There are 3 states in the case of two identical fermions. For one single boson, there are three states. Thus, there is a total of $3 \times 3 = 9$ states.

(d) For two identical bosons, there are six states. For one fermion, three states. Thus, $6 \times 3 = 18$ states.

(e) and (f) There are 3 states for each distinct particle. Thus, $3 \times 3 \times 3 = 27$ states.

2.

(a) Notice the similarities between $\psi_{R,L}$ with the ground-state wavefunction of the 1D Harmonic Oscillator $(\frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2)$

$$\psi(x) = \left(\frac{1}{\pi x_0^2}\right)^{1/4} e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2}, \text{ with } x_0^2 = \frac{\hbar}{m\omega}.$$

In our case, we expect that an Harmonic potential be a good description of the double-well potential around each of its minima $\pm a$. Thus, expanding V around $\pm a$ we get

$$V(x \mp a) = \frac{1}{2} \times \frac{8U_0}{a^2}(x \mp a)^2 + \mathcal{O}(x \mp a)^3 \approx \frac{1}{2}m\omega^2 (x \mp a)^2, \text{ with } \omega = \sqrt{\frac{8U_0}{ma^2}}.$$

This is the corresponding frequency in each minima of V which will give the lenght scale σ used in $\psi_{R,L}$. These wavefunctions will be good approximations of the true wavefunctions when the two minima are well separated. This can be quantified by the overlap

$$\ell = \frac{1}{\sqrt{\pi}\sigma}\int \mathrm{d}x e^{-\frac{(x-a)^2+(x+a)^2}{2\sigma^2}} = \frac{1}{\sqrt{\pi}\sigma}\int \mathrm{d}x e^{-\frac{x^2}{\sigma^2}} e^{-\frac{a^2}{\sigma^2}} = e^{-\left(\frac{a}{\sigma}\right)^2}.$$

Thus, the two wells are well separated whenever $\ell \ll 1$, $\Rightarrow$ $a \gg \sigma$, i.e., $a\sqrt{mU_0} \gg \hbar$.

(b) Using reflecion symmetry and that all functions are real, we notice that $\left\langle R \left| H^{(1)} \right| R \right\rangle = \left\langle L \left| H^{(1)} \right| L \right\rangle$ and that $\left\langle R \left| H^{(1)} \right| L \right\rangle = \left\langle L \left| H^{(1)} \right| R \right\rangle$.

We then need to compute

$$
\begin{aligned}
\left\langle R\left|H^{(1)}\right|R\right\rangle =&\frac{1}{\sqrt{\pi}\sigma}\int \mathrm{d}x e^{-\frac{(x-a)^2}{2\sigma^2}}\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{U_0}{a^4}\left(x^2-a^2\right)^2\right)e^{-\frac{(x-a)^2}{2\sigma^2}}\\
=&\frac{1}{\sqrt{\pi}\sigma}\int \mathrm{d}y e^{-\frac{y^2}{2\sigma^2}}\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}y^2}+\frac{U_0}{a^4}y^2\left(y+2a\right)^2\right)e^{-\frac{y^2}{2\sigma^2}}\\
=&\frac{1}{\sqrt{\pi}}\int \mathrm{d}z e^{-\frac{1}{2}z^2}\left(-\frac{\hbar^2}{2m\sigma^2}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+U_0\frac{\sigma^4}{a^4}z^2\left(z+2\frac{a}{\sigma}\right)^2\right)e^{-\frac{1}{2}z^2}\\
=&\frac{1}{\sqrt{\pi}}\int \mathrm{d}z e^{-z^2}\left(-\frac{\hbar^2}{2m\sigma^2}\left(z^2-1\right)+U_0\frac{\sigma^4}{a^4}z^2\left(z+2\frac{a}{\sigma}\right)^2\right)\\
=&\frac{1}{\sqrt{\pi}}\left(\frac{\sqrt{\pi}}{2}\times\frac{\hbar^2}{2m\sigma^2}+U_0\frac{\sigma^4}{a^4}\times\frac{\sqrt{\pi}}{4}\left(3+8\left(\frac{a}{\sigma}\right)^2\right)\right)=\frac{\hbar^2}{4m\sigma^2}+U_0\frac{\sigma^2\left(3\sigma^2+8a^2\right)}{4a^4}\\
=&\hbar\sqrt{\frac{U_0}{2ma^2}}+\hbar\sqrt{\frac{U_0}{8ma^2}}\left(\frac{3\hbar}{4\sqrt{8mU_0a^2}}+2\right)=U_0\left(4\alpha+\frac{3}{4}\alpha^2\right),\\
\left\langle R\left|H^{(1)}\right|L\right\rangle =&\frac{1}{\sqrt{\pi}\sigma}\int \mathrm{d}x e^{-\frac{(x-a)^2}{2\sigma^2}}\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{U_0}{a^4}\left(x^2-a^2\right)^2\right)e^{-\frac{(x+a)^2}{2\sigma^2}}\\
=&\frac{1}{\sqrt{\pi}\sigma}\int \mathrm{d}x e^{-\left(\frac{x^2+a^2}{\sigma^2}\right)}\left(-\frac{\hbar^2}{2m\sigma^4}\left((x+a)^2-\sigma^2\right)+\frac{U_0}{a^4}\left(x^2-a^2\right)^2\right)\\
=&-\frac{\hbar^2}{2m\sigma^4}\left(a^2-\frac{1}{2}\sigma^2\right)e^{-\left(\frac{a}{\sigma}\right)^2}+\frac{U_0}{a^4}\left(a^4-a^2\sigma^2+\frac{3}{4}\sigma^4\right)e^{-\left(\frac{a}{\sigma}\right)^2}\\
=&e^{-\frac{\sqrt{8ma^2U_0}}{\hbar}}\left(-4U_0\left(1-\frac{\hbar}{2\sqrt{8ma^2U_0}}\right)+U_0\left(1-\frac{\hbar}{\sqrt{8ma^2U_0}}+\frac{3\hbar^2}{32a^2mU_0}\right)\right)\\
=&-U_0\left(3-\alpha-\frac{3}{4}\alpha^2\right)e^{-\frac{1}{\alpha}}=-U_0\left(3-\alpha-\frac{3}{4}\alpha^2\right)\ell,
\end{aligned}
$$

where $\alpha^2=\frac{\hbar^2}{8ma^2U_0}$.

Since the matrix is of the simple form

$$H_{\mathrm{eff}}^{(1)}=\begin{pmatrix} A & -\ell B\\ -\ell B & A\end{pmatrix},$$

the Eigenstates are

$$|\pm\rangle=\frac{1}{\sqrt{2}}\left(|R\rangle\pm|L\rangle\right),\ \text{with energies } E_\pm=A\mp\ell B.$$

(Notice that $\langle R|L\rangle=\ell$, thus $\langle\pm|\pm\rangle=1\pm\ell$ and $\langle+|-\rangle=0$.)

(c) Since we have for single-particle states, 2 fermions can be distrubuted among them in $\begin{pmatrix}4\\2\end{pmatrix}=6$ different ways. These states are obtained by antisymmetring any two-particle state, which sums $4\times4=16$ states. Due to Pauli principle, 10 states cannot be antisymmetrized. It is easy to check that whenever the orbital part of the wavefunction is symmetric, then the spin part is antisymmetric and vice and versa. With respect to the spin, there are three symmetric sates, dubbed triplet, and one antisymmetric state (singlet). They are respectively, $|t_1\rangle=|\uparrow\rangle_1|\uparrow\rangle_2$, $|t_0\rangle=\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2+|\downarrow\rangle_1|\uparrow\rangle_2\right)$, $|t_{-1}\rangle=|\downarrow\rangle_1|\downarrow\rangle_2$, and $|s\rangle=\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2-|\downarrow\rangle_1|\uparrow\rangle_2\right)$. Likewise, the symmetric orbital wavefunctions are $|\mathcal{S}_1\rangle=|+\rangle_1|+\rangle_2$, $|\mathcal{S}_0\rangle=\frac{1}{\sqrt{2}}\left(|+\rangle_1|-\rangle_2+|-\rangle_1|+\rangle_2\right)$, and $|\mathcal{S}_{-1}\rangle=|-\rangle_1|-\rangle_2$, and the antisymmetric one is $|\mathcal{A}\rangle=\frac{1}{\sqrt{2}}\left(|+\rangle_1|-\rangle_2-|-\rangle_1|+\rangle_2\right)$.

Finally, the six states are $|\mathcal{S}_i\rangle\otimes|s\rangle$ and $|\mathcal{A}\rangle\otimes|t_i\rangle$, with $i=-1,\,0,\,1$

(d) Ignoring spin, we have 4 two-particle sates. We are then interested in the matrix elements

$$\langle A,B\,|V|\,C,D\rangle=\int \mathrm{d}x_1\mathrm{d}x_2\psi_A^*\left(x_1\right)\psi_B^*\left(x_2\right)V(|x_1-x_2|)\psi_C\left(x_1\right)\psi_D\left(x_2\right).$$

Since $V(x_1,x_2)=V(|x_1-x_2|)$, then we set $r=x_1-x_2$ and $R=\frac{1}{2}(x_1+x_2)$. Thus,

$$\begin{aligned}\langle A,B\,|V|\,C,D\rangle =&\int \mathrm{d}r\mathrm{d}R\psi_A^*(R+\frac{1}{2}r)\psi_B^*(R-\frac{1}{2}r)V(|r|)\psi_C(R+\frac{1}{2}r)\psi_D(R-\frac{1}{2}r)\\ =&\frac{1}{\pi\sigma^2}\int \mathrm{d}r\mathrm{d}Re^{-\frac{1}{2\sigma^2}\left[\left(R+\frac{1}{2}r-\epsilon_A a\right)^2+\left(R-\frac{1}{2}r-\epsilon_B a\right)^2+\left(R+\frac{1}{2}r-\epsilon_C a\right)^2+\left(R-\frac{1}{2}r-\epsilon_D a\right)^2\right]}V(|r|)\\ =&\frac{1}{\pi\sigma^2}\int \mathrm{d}r\mathrm{d}Re^{-\frac{1}{2\sigma^2}\left[4R^2+r^2+4a^2-2aR(\epsilon_A+\epsilon_B+\epsilon_C+\epsilon_D)-ar(\epsilon_A-\epsilon_B+\epsilon_C-\epsilon_D)\right]}V(|r|)\\ =&\frac{1}{\pi\sigma^2}\int \mathrm{d}r\mathrm{d}Re^{-\frac{1}{2\sigma^2}\left[4\left(R-\frac{1}{2}ap\right)^2-a^2p^2+(r-aq)^2-a^2q^2+4a^2\right]}V(|r|),\end{aligned}$$

where $\epsilon_x=\pm1$ if $x=R,L$, respectively, $2p=\epsilon_A+\epsilon_B+\epsilon_C+\epsilon_D$, and $2q=\epsilon_A-\epsilon_B+\epsilon_C-\epsilon_D$. We are now able to integrate over R yielding

$$\begin{aligned}\langle A,B\,|V|\,C,D\rangle =&\frac{1}{\sqrt{2\pi}\sigma}e^{\frac{1}{2}\left(\frac{a}{\sigma}\right)^2\left(p^2+q^2-4\right)}\int \mathrm{d}re^{-\frac{1}{2\sigma^2}(r-aq)^2}V(|r|)\\ =&\frac{1}{\sqrt{2\pi}\sigma}e^{\frac{1}{2}\left(\frac{a}{\sigma}\right)^2\left(\epsilon_A\epsilon_C+\epsilon_B\epsilon_D-2\right)}\int \mathrm{d}re^{-\frac{1}{2\sigma^2}(r-aq)^2}V(|r|).\end{aligned}$$

Thus,

$$\begin{aligned}V_{RR,RR}=&\frac{1}{\sqrt{2\pi}\sigma}\int \mathrm{d}re^{-\frac{1}{2\sigma^2}r^2}V(|r|)=V_{LL,LL},\\ V_{RR,RL}=&\frac{1}{\sqrt{2\pi}\sigma}e^{-\left(\frac{a}{\sigma}\right)^2}\int \mathrm{d}re^{-\frac{1}{2\sigma^2}(r-a)^2}V(|r|)=V_{RL,RR}=V_{LR,LL}=V_{LL,LR},\\ V_{RR,LR}=&\frac{1}{\sqrt{2\pi}\sigma}e^{-\left(\frac{a}{\sigma}\right)^2}\int \mathrm{d}re^{-\frac{1}{2\sigma^2}(r+a)^2}V(|r|)=\frac{1}{\sqrt{2\pi}\sigma}e^{-\left(\frac{a}{\sigma}\right)^2}\int \mathrm{d}re^{-\frac{1}{2\sigma^2}(r-a)^2}V(|r|)\\ =&V_{LR,RR}=V_{RL,LL}=V_{LL,RL},\\ V_{RR,LL}=&\frac{1}{\sqrt{2\pi}\sigma}e^{-2\left(\frac{a}{\sigma}\right)^2}\int \mathrm{d}re^{-\frac{1}{2\sigma^2}r^2}V(|r|)=V_{LL,RR},\\ V_{RL,RL}=&\frac{1}{\sqrt{2\pi}\sigma}\int \mathrm{d}re^{-\frac{1}{2\sigma^2}(r-2a)^2}V(|r|)=V_{LR,LR},\\ V_{RL,LR}=&\frac{1}{\sqrt{2\pi}\sigma}e^{-2\left(\frac{a}{\sigma}\right)^2}\int \mathrm{d}re^{-\frac{1}{2\sigma^2}r^2}V(|r|)=V_{LR,RL}.\end{aligned}$$

Thus, the matrix elements of V has only 4 independent values. In the basis $|RR\rangle$, $|RL\rangle$, $|LR\rangle$, $|LL\rangle$, it is of type

$$V=\begin{pmatrix} a & \ell b & \ell b & \ell^2 c\\ \ell b & d & \ell^2 c & \ell b\\ \ell b & \ell^2 c & d & \ell b\\ \ell^2 c & \ell b & \ell b & a\end{pmatrix}.$$

We now have to compute the direct and exchange integrals. They are, respectively, $\langle +-|V|+-\rangle/\langle +-|+-\rangle$ and $\langle +-|V|-+\rangle/\sqrt{\langle +-|+-\rangle\langle -+|-+\rangle}$. Thus,

$$\begin{aligned}
V_{\mathrm{D}} =& \frac{1}{(1+\ell)(1-\ell)}\left(\frac{1}{\sqrt{2}}\right)^4 \left(\langle R| + \langle L|\right)_1 \otimes \left(\langle R| - \langle L|\right)_2 V \left(|R\rangle + |L\rangle\right)_1 \otimes \left(|R\rangle - |L\rangle\right)_1 \\
=& \frac{1}{4(1-\ell^2)}\left(V_{RR,RR} - V_{RR,RL} + V_{RR,LR} - V_{RR,LL} - V_{RL,RR} + V_{RL,RL} - V_{RL,LR} + V_{RL,LL}\right. \\
& \left. + V_{LR,RR} - V_{LR,RL} + V_{LR,LR} - V_{LR,LL} - V_{LL,RR} + V_{LL,RL} - V_{LL,LR} + V_{LL,LL}\right) \\
=& \frac{1}{4(1-\ell^2)}\left(a - \ell^2 c + d - \ell^2 c - \ell^2 c + d - \ell^2 c + a\right) = \frac{1}{2(1-\ell^2)}\left(a + d - 2\ell^2 c\right), \\
V_{\mathrm{E}} =& \frac{1}{4(1-\ell^2)}\left(\langle R| + \langle L|\right)_1 \otimes \left(\langle R| - \langle L|\right)_2 V \left(|R\rangle - |L\rangle\right)_1 \otimes \left(|R\rangle + |L\rangle\right)_1 \\
=& \frac{1}{4(1-\ell^2)}\left(V_{RR,RR} + V_{RR,RL} - V_{RR,LR} - V_{RR,LL} - V_{RL,RR} - V_{RL,RL} + V_{RL,LR} + V_{RL,LL}\right. \\
& \left. + V_{LR,RR} + V_{LR,RL} - V_{LR,LR} - V_{LR,LL} - V_{LL,RR} - V_{LL,RL} + V_{LL,LR} + V_{LL,LL}\right) \\
=& \frac{1}{4(1-\ell^2)}\left(a - \ell^2 c - d + \ell^2 c + \ell^2 c - d - \ell^2 c + a\right) = \frac{1}{2(1-\ell^2)}\left(a - d\right).
\end{aligned}$$

(e) The possible states are the six ones discussed item (c). For now, let us focus on the orbital degree of freedom. In the 4-states orbital basis, $|\mathcal{S}_i\rangle$ $(i = 1,\, 0,\, -1)$ and $|\mathcal{A}\rangle$, H_1 is diagonal with Eigenenergies $2E_+$, $E_+ + E_-$, $2E_-$, and $E_+ + E_-$, respectively. The interaction in this basis is

$$V = \begin{pmatrix}
\frac{\frac{a+d}{2} + 2\ell b + \ell^2 c}{(1+\ell)^2} & 0 & \frac{a-d}{2(1-\ell^2)} & 0 \\
0 & \frac{a-\ell^2 c}{1-\ell^2} & 0 & 0 \\
\frac{a-d}{2(1-\ell^2)} & 0 & \frac{\frac{a+d}{2} - 2\ell b + \ell^2 c}{(1-\ell)^2} & 0 \\
0 & 0 & 0 & \frac{d-\ell^2 c}{1-\ell^2}
\end{pmatrix}$$

where we needed

$$\begin{aligned}
V|\mathcal{S}_1\rangle &= \left(\frac{1}{\sqrt{2}}\right)^2 V\left(|RR\rangle + |RL\rangle + |LR\rangle + |LL\rangle\right) \\
&= \left(\frac{1}{\sqrt{2}}\right)^2 \left[\left(a + 2\ell b + \ell^2 c\right)\left(|RR\rangle + |LL\rangle\right) + \left(d + 2\ell b + \ell^2 c\right)\left(|RL\rangle + |LR\rangle\right)\right] \\
&= \left(\frac{a+d}{2} + 2\ell b + \ell^2 c\right)|\mathcal{S}_1\rangle + \left(\frac{a-d}{2}\right)|\mathcal{S}_{-1}\rangle, \\
V|\mathcal{S}_{-1}\rangle &= \left(\frac{1}{\sqrt{2}}\right)^2 V\left(|RR\rangle - |RL\rangle - |LR\rangle + |LL\rangle\right) \\
&= \left(\frac{1}{\sqrt{2}}\right)^2 \left[\left(a - 2\ell b + \ell^2 c\right)\left(|RR\rangle + |LL\rangle\right) - \left(d - 2\ell b + \ell^2 c\right)\left(|RL\rangle + |LR\rangle\right)\right] \\
&= \left(\frac{a-d}{2}\right)|\mathcal{S}_1\rangle + \left(\frac{a+d}{2} - 2\ell b + \ell^2 c\right)|\mathcal{S}_{-1}\rangle, \\
V|\mathcal{S}_0\rangle &= \left(\frac{1}{\sqrt{2}}\right)^4 V\left(2|RR\rangle - 2|LL\rangle\right) = \left(a - \ell^2 c\right)|\mathcal{S}_0\rangle, \\
V|\mathcal{A}\rangle &= \left(\frac{1}{\sqrt{2}}\right)^4 V\left(2|RL\rangle - 2|LR\rangle\right) = \left(d - \ell^2 c\right)|\mathcal{S}_0\rangle.
\end{aligned}$$

Thus, we already have two of the Eigenstates: $|\mathcal{A}\rangle$ with $E_{\mathcal{A}} = E_+ + E_- + V_{\mathrm{D}} - V_{\mathrm{E}}$, and $|\mathcal{S}_0\rangle$ with $E_{\mathcal{S}_0} = E_+ + E_- + V_{\mathrm{D}} + V_{\mathrm{E}}$. Actually, this corresponds for 4 states when spin is considered: $|\mathcal{A}\rangle \otimes |t_i\rangle$, $i = 1,\, 0,\, -1$ and $|\mathcal{S}_0\rangle \otimes |s\rangle$. Notice that this states are degenerate if only $H^{(1)}$ is considered. The degeneracy is lifted by the interaction V splitting this four states into triplet and singlet states. With respect with these two states, the Hamiltonian can be recast as

$$H_{\mathrm{eff}} = \mathrm{const} + J\mathbf{S}_1 \cdot \mathbf{S}_2,$$

where $\mathbf{S}_i$ are spin operators. Notice the Eigenstates of H_{eff} are spin singlet $|s\rangle$ and triplet $|t_i\rangle$ with energies const$-\frac{3\hbar^2}{4}J$ and const$+\frac{\hbar^2}{4}J$, respectively. In order to recast the spectrum of $|\mathcal{S}_0\rangle \otimes |s\rangle$ and $|\mathcal{A}\rangle \otimes |t_i\rangle$, we set const $= E_+ + E_- + V_{\text{D}} - \frac{1}{2}V_{\text{E}}$ and the exchange constant

$$J\hbar^2 = -2V_{\text{E}} = \frac{d-a}{1-\ell^2} = \frac{-1}{\sqrt{2\pi}\,(1-\ell^2)\,\sigma}\int \mathrm{d}r \left(e^{-\frac{1}{2\sigma^2}r^2} - e^{-\frac{1}{2\sigma^2}(r-2a)^2}\right) V(|r|).$$

If $V(r)$ is positive and monotonically decreasing, this means that it costs energy for the particles to be close to each other. Thus, it is energetically favorable to their orbital wavefunction to be antisymmetric [meaning $\psi(R, r=0)=0$]. In this case, the spin part of the wavefunction has to be symmetric, i.e., a triplet. The triplet state is favorable whenever $J<0$. This is indeed the case as can be seen from the expression for J. On the other hand, if $V<0$ and drecreases (in magnitude) monotonically, then we expect the orbital part to be symmetric [yielding $\psi(R, r=0) \neq 0$]. Thus, the spin part has to be antisymmetric and, as a consequence, $J>0$.

Finally, we now have to diagonalize the subspace spanned by $|\mathcal{S}_{\pm 1}\rangle$. The related matrix is

$$\begin{pmatrix} \frac{2E_+ + \frac{a+d}{2} + \ell^2 c + 2\ell b}{(1+\ell)^2} & \frac{a-d}{2(1-\ell^2)} \\ \frac{a-d}{2(1-\ell^2)} & \frac{2E_- + \frac{a+d}{2} + \ell^2 c - 2\ell b}{(1-\ell)^2} \end{pmatrix} = \begin{pmatrix} A & C \\ C & B \end{pmatrix}, \quad \Rightarrow \quad \lambda^2 - (A+B)\,\lambda + AB - C^2 = 0.$$

The Eigenenergies are $\frac{1}{2}(A+B\pm\Delta)$ with $\Delta = \sqrt{(A-B)^2 + 4C^2}$, and (unnormalized) Eigenvectors $[(A-B\pm\Delta)\,|{+}{+}\rangle + 2C\,|{-}{-}\rangle] \otimes |s\rangle$.

3.

(a) The wavefunctions are those of free particles, $\psi = e^{ikx}/\sqrt{L}$, with periodic boundary conditions $\psi(x) = \psi(x+L)$. Thus,

$$e^{ikL} = 1, \quad \Rightarrow \quad k_n = \frac{2\pi}{L}n, \text{ with } n \in \mathbb{Z}. \quad \Rightarrow \quad \psi_{n,\sigma} = \frac{1}{\sqrt{L}} e^{ik_n x}\sigma.$$

The quantum number n labels the momentum $\hbar k_n$ which, due to translational symmetry, is a good quantum number. Moreover, notice the enegies of these states are $E_n = \frac{1}{2m}\hbar^2\left(\frac{2\pi}{L}\right)^2 n^2$. Thus, since $E_n = E_{-n}$, the degeneracy is twofold for all states $n \neq 0$. The $k_n = 0$ state is nondegerante. If spin is considered, all these degeneracies are multiplied by 2.

(b) Since $H = \frac{1}{2m}p^2$, it is very simple to express H in terms of $\tilde{a}_\sigma(p)$:

$$H = \int \frac{\mathrm{d}p\mathrm{d}q}{(2\pi\hbar)^2} \sum_{\sigma,\tau} \tilde{a}_\sigma^\dagger(p) \left\langle p,\sigma \left| \frac{1}{2m}p^2 \right| q\tau \right\rangle \tilde{a}_\tau(q) = \int \frac{\mathrm{d}p\mathrm{d}q}{(2\pi\hbar)^2} \sum_{\sigma,\sigma'} \tilde{a}_\sigma^\dagger(p)\delta_{\sigma,\tau}\frac{q^2}{2m}\langle p|q\rangle\, \tilde{a}_\tau(q)$$
$$= \sum_\sigma \int \frac{\mathrm{d}p}{2\pi\hbar}\tilde{a}_\sigma^\dagger(p)\frac{p^2}{2m}\tilde{a}_\sigma(p), \text{ where } \langle p|q\rangle = 2\pi\hbar\delta(p-q).$$

In the position space, either we inverse Fourier transform the operators $\tilde{a}$ and $\tilde{a}^\dagger$, or, simply

$$H = \int \mathrm{d}x\mathrm{d}y \sum_{\sigma,\tau} a_\sigma^\dagger(x) \left\langle x,\sigma \left| \frac{1}{2m}p^2 \right| y\tau \right\rangle a_\tau(y) = \int \mathrm{d}x\mathrm{d}x' \sum_{\sigma,\tau} a_\sigma^\dagger(x)\delta_{\sigma,\tau}\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}y^2}\right)\langle x|y\rangle\, a_\tau(y)$$
$$= \sum_\sigma \int \mathrm{d}x a_\sigma^\dagger(x)\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)a_\sigma(x), \text{ where } \langle x|y\rangle = \delta(x-y).$$

(c) This can be done straightforwardly,

$$\{\tilde{a}_\sigma(p), \tilde{a}_\tau^\dagger(q)\} = \int \mathrm{d}x\mathrm{d}y\, \{\tilde{a}_\sigma(x), \tilde{a}_\tau^\dagger(y)\}\, e^{-i\frac{px}{\hbar}}e^{i\frac{qy}{\hbar}} = \int \mathrm{d}x\mathrm{d}y\delta_{\sigma,\tau}\delta(x-y)\, e^{-i\frac{px}{\hbar}}e^{i\frac{qy}{\hbar}}$$
$$= \delta_{\sigma,\tau}\int \mathrm{d}x e^{-i\frac{(p-q)x}{\hbar}} = 2\pi\hbar\delta(p-q)\,\delta_{\sigma,\tau}.$$

Notice in this convention, that both$\tilde{a}(p)$ and $a(x)$ has dimension of square root of length. Because the problem is in a finite-size ring, one could make this operators dimensionless and the integrals should be normalized by L. Finally, because $\{a_\sigma(x), a_\tau(y)\} = 0$, we have that $\{\tilde{a}_\sigma(p), \tilde{a}_\tau(q)\} = 0$.

(d) Because $\frac{1}{2}N$ is odd, we write $N = 4K + 2$ with K being integer. To construct the ground state, we add 2 fermions in the $n = 0$ sates. Then, $N - 2 = 4K$ fermions remains to fill the other states. Noticing that a $n \neq 0$ energy-level is degenerate with the $-n$ level, and that each of these levels can accomodate 2 fermions (with opposite spins), then there remains K levels to be filled, i.e., $E_F = E_K = \frac{1}{2m}\hbar^2 \left(\frac{2\pi}{L}\right)^2 K^2 = \frac{1}{2m}\hbar^2 \left(\frac{2\pi}{L}\right)^2 \left(\frac{N-2}{4}\right)^2$. The ground state is

$$|G\rangle = a^\dagger_{0,\uparrow} a^\dagger_{0,\downarrow} \prod_{i=\frac{N-2}{4}}^{1} a^\dagger_{i,\uparrow} a^\dagger_{i,\downarrow} a^\dagger_{-i,\uparrow} a^\dagger_{-i,\downarrow} |0\rangle \,,$$

where $a^\dagger_{n,\sigma}$ creates a fermion the wavefunction of which is $\psi_{n,\sigma}(x)$.

(e) The wavefunction of a many-particle fermionic system is generically written as a slater determinant

$$\Psi = \begin{vmatrix} \psi_1(x_1) & \psi_2(x_1) & \ldots & \psi_N(x_1) \\ \psi_1(x_2) & \psi_2(x_2) & \ldots & \psi_N(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_1(x_N) & \psi_2(x_N) & \ldots & \psi_N(x_N) \end{vmatrix},$$

where $\psi_j(x_i) = \langle x_i|\psi_j\rangle$. If we want to connect this with our problem where spin is explicitly involved, then $\langle x_i|\psi_j\rangle \to \langle x_{i,\sigma}|\psi_{j,\tau}\rangle = \delta_{\sigma,\tau}\psi_{j,\sigma}(x_{i,\sigma}) = \delta_{\sigma,\tau}\psi_j(x_{i,\sigma})$. Thus,

$$\Psi = \begin{vmatrix} \psi_0(x_{1,\uparrow}) & 0 & \psi_1(x_{1,\uparrow}) & 0 & \psi_{-1}(x_{1,\uparrow}) & 0 & \ldots & \psi_{-K}(x_{1,\uparrow}) & 0 \\ 0 & \psi_0(x_{1,\downarrow}) & 0 & \psi_1(x_{1,\downarrow}) & 0 & \psi_{-1}(x_{1,\downarrow}) & \ldots & 0 & \psi_{-K}(x_{1,\downarrow}) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \psi_0\left(x_{\frac{N}{2},\downarrow}\right) & \ldots & \psi_1\left(x_{\frac{N}{2},\downarrow}\right) & 0 & \psi_{-1}\left(x_{\frac{N}{2},\downarrow}\right) & \ldots & 0 & \psi_{-K}\left(x_{\frac{N}{2},\downarrow}\right) \end{vmatrix}.$$

This matrix can be rearranged in the following way: set all the spin-up states to appear before the spin-down states. [It is equivalent as doing $\frac{1}{2}N$ permutations of lines and rows, which leaves the determinant unchanged, or rewritting the ground state as

$$|G\rangle = \left(a^\dagger_{0,\uparrow} \prod_{i=\frac{N-2}{4}}^{1} a^\dagger_{i,\uparrow} a^\dagger_{-i,\uparrow}\right) \left(a^\dagger_{0,\downarrow} \prod_{i=\frac{N-2}{4}}^{1} a^\dagger_{i,\downarrow} a^\dagger_{-i,\downarrow}\right) |0\rangle \,.]$$

Moreover, notice that that resulting matrix will be block diagonal. Thus, it can be factorized as

$$\begin{vmatrix} \psi_0(x_{1,\uparrow}) & \psi_1(x_{1,\uparrow}) & \psi_{-1}(x_{1,\uparrow}) & \ldots & \psi_{-K}(x_{1,\uparrow}) \\ \psi_0(x_{2,\uparrow}) & \psi_1(x_{2,\uparrow}) & \psi_{-1}(x_{2,\uparrow}) & \ldots & \psi_{-K}(x_{2,\uparrow}) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \psi_0\left(x_{\frac{N}{2},\uparrow}\right) & \psi_1\left(x_{\frac{N}{2},\uparrow}\right) & \psi_{-1}\left(x_{\frac{N}{2},\uparrow}\right) & \ldots & \psi_{-K}\left(x_{\frac{N}{2},\uparrow}\right) \end{vmatrix} \begin{vmatrix} \psi_0(x_{1,\downarrow}) & \psi_1(x_{1,\downarrow}) & \psi_{-1}(x_{1,\downarrow}) & \ldots & \psi_{-K}(x_{1,\downarrow}) \\ \psi_0(x_{2,\downarrow}) & \psi_1(x_{2,\downarrow}) & \psi_{-1}(x_{2,\downarrow}) & \ldots & \psi_{-K}(x_{2,\downarrow}) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \psi_0\left(x_{\frac{N}{2},\downarrow}\right) & \psi_1\left(x_{\frac{N}{2},\downarrow}\right) & \psi_{-1}\left(x_{\frac{N}{2},\downarrow}\right) & \ldots & \psi_{-K}\left(x_{\frac{N}{2},\downarrow}\right) \end{vmatrix}.$$

(f) Finally, we can compute these determinants given that we know the wavefucntion ψ_n:

$$\Psi = \left(\frac{1}{\sqrt{L}}\right)^N \begin{vmatrix} z^0_{1,\uparrow} & z^1_{1,\uparrow} & z^{-1}_{1,\uparrow} & \ldots & z^{-K}_{1,\uparrow} \\ z^0_{2,\uparrow} & z^1_{2,\uparrow} & z^{-1}_{2,\uparrow} & \ldots & z^{-K}_{2,\uparrow} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ z^0_{\frac{1}{2}N,\uparrow} & z^1_{\frac{1}{2}N,\uparrow} & z^{-1}_{\frac{1}{2}N,\uparrow} & \ldots & z^{-K}_{\frac{1}{2}N,\uparrow} \end{vmatrix} \begin{vmatrix} z^0_{1,\downarrow} & z^1_{1,\downarrow} & z^{-1}_{1,\downarrow} & \ldots & z^{-K}_{1,\downarrow} \\ z^0_{2,\downarrow} & z^1_{2,\downarrow} & z^{-1}_{2,\downarrow} & \ldots & z^{-K}_{2,\downarrow} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ z^0_{\frac{1}{2}N,\downarrow} & z^1_{\frac{1}{2}N,\downarrow} & z^{-1}_{\frac{1}{2}N,\uparrow} & \ldots & z^{-K}_{\frac{1}{2}N,\downarrow} \end{vmatrix}$$

$$= \left(\frac{1}{\sqrt{L}}\right)^N \begin{vmatrix} z^{-K}_{1,\uparrow} & \ldots & z^0_{1,\uparrow} & \ldots & z^K_{1,\uparrow} \\ z^{-K}_{2,\uparrow} & \ldots & z^0_{2,\uparrow} & \ldots & z^K_{2,\uparrow} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ z^{-K}_{\frac{1}{2}N,\uparrow} & \ldots & z^0_{\frac{1}{2}N,\uparrow} & \ldots & z^K_{\frac{1}{2}N,\uparrow} \end{vmatrix} \begin{vmatrix} z^{-K}_{1,\downarrow} & \ldots & z^0_{1,\downarrow} & \ldots & z^K_{1,\downarrow} \\ z^{-K}_{2,\downarrow} & \ldots & z^0_{2,\downarrow} & \ldots & z^K_{2,\downarrow} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ z^{-K}_{\frac{1}{2}N,\downarrow} & \ldots & z^0_{\frac{1}{2}N,\downarrow} & \ldots & z^K_{\frac{1}{2}N,\downarrow} \end{vmatrix}.$$

We now factorize the first value in each row in order to construct the corresponding Vandermond matrix:

$$\begin{aligned}\Psi &= L^{-\frac{N}{2}}\prod_{i=1}^{\frac{1}{2}N} z_{i,\uparrow}^{-K} z_{i,\downarrow}^{-K} \begin{vmatrix} 1 & \dots & z_{1,\uparrow}^{K} & \dots & z_{1,\uparrow}^{2K} \\ 1 & \dots & z_{2,\uparrow}^{K} & \dots & z_{2,\uparrow}^{2K} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & z_{\frac{1}{2}N,\uparrow}^{K} & \dots & z_{\frac{1}{2}N,\uparrow}^{2K} \end{vmatrix} \begin{vmatrix} 1 & \dots & z_{1,\downarrow}^{K} & \dots & z_{1,\downarrow}^{2K} \\ 1 & \dots & z_{2,\downarrow}^{K} & \dots & z_{2,\downarrow}^{2K} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & z_{\frac{1}{2}N,\downarrow}^{K} & \dots & z_{\frac{1}{2}N,\downarrow}^{2K} \end{vmatrix} \\ &= L^{-\frac{N}{2}}\prod_{i=1}^{\frac{1}{2}N} z_{i,\uparrow}^{-K} z_{i,\downarrow}^{-K} \prod_{1\le i<j\le \frac{N}{2}} \left(z_{i,\uparrow}-z_{j,\uparrow}\right) \prod_{1\le i<j\le \frac{N}{2}} \left(z_{i,\downarrow}-z_{j,\downarrow}\right), \\ &= L^{-\frac{N}{2}} e^{-i\left(\frac{2\pi}{L}\right)\left(\frac{N-2}{4}\right)NX_{\mathrm{CM}}} \prod_{1\le i<j\le \frac{N}{2}} \left(z_{i,\uparrow}-z_{j,\uparrow}\right)\left(z_{i,\downarrow}-z_{j,\downarrow}\right),\end{aligned}$$

where $NX_{\mathrm{CM}} = \sum_{i=1}^{\frac{1}{2}N}\left(x_{i,\uparrow}+x_{i,\downarrow}\right).$

4.

(a) We need to show that $[c,c]=[d,d]=[c,d]=0$, which is straightfoward since $[a,a]=[b,b]=[a,b]=0$. Let us show that

$$\left[c,d^\dagger\right] = \left[ua-vb, va^\dagger+ub^\dagger\right] = uv\left(\left[a,a^\dagger\right]-\left[b,b^\dagger\right]\right)=0,$$

since $\left[a,b^\dagger\right]=0$. Finally, we need to show that $\left[c,c^\dagger\right]=\left[d,d^\dagger\right]=1$.

$$\begin{aligned}\left[c,c^\dagger\right] &= |u|^2\left[a,a^\dagger\right]+|v|^2\left[b,b^\dagger\right] = |u|^2+|v|^2=1,\\ \left[d,d^\dagger\right] &= |v|^2\left[a,a^\dagger\right]+|u|^2\left[b,b^\dagger\right] = |v|^2+|u|^2=1.\end{aligned}$$

(b) In this case, $a=\frac{1}{\sqrt{2}}(c+d)$ and $b=\frac{1}{\sqrt{2}}(-c+d)$. Thus,

$$H=\epsilon\left(a^\dagger a+b^\dagger b\right)+V\left(a^\dagger b+b^\dagger a\right)=(\epsilon-V)\,c^\dagger c+(\epsilon+V)\,d^\dagger d=H_{\mathrm{C}}+H_{\mathrm{D}}.$$

(c) In the general case, $a=u^*c+vd$ and $b=ud-v^*c$. Inserting this on the Hamiltonian yields,

$$\begin{aligned}H =&\epsilon_A\left(|u|^2c^\dagger c+|v|^2d^\dagger d\right)+\epsilon_B\left(|v|^2c^\dagger c+|u|^2d^\dagger d\right)+V\left(-uv^*c^\dagger c+uv^*d^\dagger d\right)+V^*\left(-u^*vc^\dagger c+u^*vd^\dagger d\right)\\ &+\left[\left(\epsilon_A-\epsilon_B\right)uv+Vu^2-V^*v^2\right]c^\dagger d+\left[\left(\epsilon_A-\epsilon_B\right)u^*v^*+V^*u^{*2}-Vv^{*2}\right]d^\dagger c.\end{aligned}$$

Notice that the first four terms are decoupled and the C and D bosons are compled only via the last two terms. Setting them to zero yields,

$$\left(\epsilon_A-\epsilon_B\right)uv+Vu^2-V^*v^2=0,$$

in addition to $|u|^2+|v|^2=1$. This two equations determines u and v. The algebra is tedious and will not be done here.

The Eigenenergies are obtained from the decoupled Hamiltonian

$$H=\left(\epsilon_C-V'\right)c^\dagger c+\left(\epsilon_D+V'\right)d^\dagger d,$$

with $\epsilon_C=\epsilon_A|u|^2+\epsilon_B|v|^2$, $\epsilon_D=\epsilon_A|v|^2+\epsilon_B|u|^2$, and $V'=2\Re(Vuv^*)$. The Eigenenergies are then $E_{n_C,n_D}=\epsilon_C n_C+\epsilon_D n_D+V'\left(n_D-n_C\right)$, with $n_C\ge 0$ and $n_D\ge 0$ integers. The Eigenstates are

$$||n_C,n_D\rangle = \frac{\left(c^\dagger\right)^{n_C}\left(d^\dagger\right)^{n_D}}{\sqrt{n_C!n_D!}}|0\rangle\,.$$

This can be connected to the original states $|n_A,n_B\rangle$ via the relations $c^\dagger=u^*a^\dagger-v^*b^\dagger$ and $d^\dagger=va^\dagger+ub^\dagger$:

$$\begin{aligned}||n_C,n_D\rangle &= \frac{1}{\sqrt{n_C!n_D!}}\left(\sum_{i=0}^{n_C}(-1)^i\binom{n_C}{i}\left(u^*a^\dagger\right)^{n_C-i}\left(v^*b^\dagger\right)^i\right)\left(\sum_{j=0}^{n_D}\binom{n_D}{j}\left(va^\dagger\right)^{n_D-j}\left(ub^\dagger\right)^j\right)|0\rangle\\ &= \frac{1}{\sqrt{n_C!n_D!}}\sum_{i=0}^{n_C}\sum_{j=0}^{n_D}(-1)^i\binom{n_C}{i}\binom{n_D}{j}u^j\left(u^*\right)^{n_C-i}v^{n_D-j}\left(v^*\right)^i\left(a^\dagger\right)^{n_C+n_D-i-j}\left(b^\dagger\right)^{i+j}|0\rangle\\ &= \frac{1}{\sqrt{n_C!n_D!}}\sum_{i=0}^{n_C}\sum_{j=0}^{n_D}(-1)^i\binom{n_C}{i}\binom{n_D}{j}u^j\left(u^*\right)^{n_C-i}v^{n_D-j}\left(v^*\right)^i|n_C+n_D-i-j,i+j\rangle\,.\end{aligned}$$

5.

(a) In first quantization, the 1-particle Hamiltonian reads

$$H_{1-\text{particle}}=\begin{pmatrix} E_1 & M_{21} & M_{31}\\ M_{12} & E_2 & M_{32}\\ M_{13} & M_{23} & E_3\end{pmatrix},$$

where $M_{ij}=M^*_{ji}$. Let $a^\dagger_{i,\sigma}$ be the criation operator of a fermion of spin σ at state i. Then,

$$\begin{aligned} H &= \sum_{i,\sigma}\sum_{j,\tau}\langle i,\sigma\left|H_{1-\text{particle}}\right|j,\tau\rangle\, a^\dagger_{i,\sigma}a_{j,\tau}=\sum_{i,\sigma}\sum_{j,\tau}\langle i\left|H_{1-\text{particle}}\right|j\rangle\, a^\dagger_{i,\sigma}a_{j,\tau}\delta_{\sigma,\tau}\\ &=\sum_{i,\sigma}E_i a^\dagger_{i,\sigma}a_{i,\sigma}+\sum_{i\neq j,\sigma}M_{i,j}a^\dagger_{i,\sigma}a_{j,\tau}.\end{aligned}$$

(b) Let us consider the case in which the two fermions have (i) opposite and (ii) same spins.

(i) This is the simpler case as we can consider the fermions distinct particles. Thus, we only need to solve the problem of one particle and second quantization is not necessary. Let λ_i (with $i=1,2,3$) be the Eigenvalues of $H_{1-\text{particle}}$, i.e.,

$$\begin{vmatrix} E_1-\lambda_i & M_{21} & M_{31}\\ M_{12} & E_2-\lambda_i & M_{32}\\ M_{13} & M_{23} & E_3-\lambda_i\end{vmatrix}=0.$$

Then, the nine Eigenenergies of the systems are

$$E_{n_1,n_2}=\lambda_{n_1}+\lambda_{n_2},$$

where n_i labels the Eigenstate occupied by the i-th particle.

(ii) When the fermions have the same spin (say, spin-up), it is like there is no spin at all and we have only two identical fermionic particles. In this way, there are only three possible states: $|1\rangle=|1,1,0\rangle$, $|2\rangle=|1,0,1\rangle$, and $|3\rangle=|0,1,1\rangle$. In this basis, the Hamiltonian reads

$$H=\begin{pmatrix} E_1+E_2 & M_{23} & -M_{13}\\ M^*_{23} & E_1+E_3 & M_{12}\\ -M^*_{13} & M^*_{12} & E_2+E_3\end{pmatrix}.$$

Notice the minus sign coming from anticommutation relation: $M_{13}a^\dagger_{1,\sigma}a_{3,\sigma}|3\rangle=M_{13}a^\dagger_{1,\sigma}a_{3,\sigma}|0,1,1\rangle=-M_{13}a^\dagger_{1,\sigma}|0,1,0\rangle=-M_{13}|1,1,0\rangle=-M_{13}|1\rangle$. The three Eigenenergies of the system comes from the Eigenvalues of the above matrix. (Recall there are other 3 states corresponding to the case in which the particles have spin-down.)

(c) In the particular case of $E_i=E$ and $M_{ij}=M$, we have that:

(i)

$$(E-\lambda)^3+2M^3-3M^2(E-\lambda)=0=\lambda'^3+2M^3-3M^2\lambda'=\lambda''^3-3\lambda''+2.$$

Notice that $\lambda''=1$ is solution. Thus, $\lambda'=M=E-\lambda$ and $\lambda_1=E-M$. The other two eigenvalues are $\lambda_2=\lambda_1=E-M$ and $\lambda_3=E+2M$.

Now we have to contruct the Eigenstates which follows from the receipt of problem 3.

(ii) In this case, the secular equation becomes

$$(2E-\lambda)^3-2M^3-3M^2(2E-\lambda)=0=\lambda'^3-2M^3-3M^2\lambda'=\lambda''^3-3\lambda''-2.$$

Notice that $\lambda''=2$ is solution. Thus, $\lambda'=2M=2E-\lambda$ and $\lambda_1=2(E-M)$. The other Eigenvalues are $\lambda_2=\lambda_3=2E+M$.

The corresponding Eigenstates are

$$\begin{aligned}|\lambda_1\rangle &= \frac{1}{\sqrt{3}}\left(|1\rangle-|2\rangle+|3\rangle\right)=\frac{1}{\sqrt{3}}\left(|1,1,0\rangle-|1,0,1\rangle+|0,1,1\rangle\right),\\ |\lambda_2\rangle &= \frac{1}{\sqrt{2}}\left(|1\rangle-|3\rangle\right)=\frac{1}{\sqrt{2}}\left(|1,1,0\rangle-|0,1,1\rangle\right),\\ |\lambda_3\rangle &= \frac{1}{\sqrt{2}}\left(|1\rangle+|2\rangle\right)=\frac{1}{\sqrt{2}}\left(|1,1,0\rangle+|1,0,1\rangle\right).\end{aligned}$$

These are antisymmetric states. Thus, the Eigenstates (considering spin) are $|\lambda_i\rangle \otimes |\uparrow\rangle_1 \otimes |\uparrow\rangle_2$ and $|\lambda_i\rangle \otimes |\downarrow\rangle_1 \otimes |\downarrow\rangle_2$.

6.
(a) The partition function is

$$Z_{\mathrm{G}} = \sum_{n_1,\ldots,n_\infty} \left\langle n_1 \ldots n_\infty \left| e^{-\beta(H-\mu N)} \right| n_1 \ldots n_\infty \right\rangle = \sum_{n_1,\ldots,n_\infty} e^{-\beta\left(\sum_i \epsilon_i n_i - \mu \mathcal{N}\right)}.$$

Notice that $\mathcal{N}$ is not constant and cannot be taken away from the sum. Moreover, the sum is irrestricted because $\mathcal{N}$ is not fixed.

Let us focus now on the case of bosons. First, we perform the sum over $n_j = 0, 1, \ldots, \infty$. Thus,

$$\begin{aligned} Z_{\mathrm{G}} &= \sum_{n_1,\ldots,n_{j-1},n_{j+1},\ldots n_\infty} e^{-\beta\left(\sum_{i\neq j}(\epsilon_i-\mu)n_i\right)} \left(\sum_{n_j=0}^{\infty} e^{-\beta(\epsilon_j-\mu)n_j}\right) \\ &= \sum_{n_1,\ldots,n_{j-1},n_{j+1},\ldots n_\infty} e^{-\beta\left(\sum_{i\neq j}(\epsilon_i-\mu)n_i\right)} \left(\frac{1}{1-e^{-\beta(\epsilon_j-\mu)}}\right). \end{aligned}$$

Repeating the same process for all the remaining n_i, we arrive at

$$Z_{\mathrm{G,bosons}} = \prod_{i=1}^{\infty} \left(1 - e^{-\beta(\epsilon_i-\mu)}\right)^{-1}.$$

For fermions, on the other hand, $n_j = 0$ or 1. Thus, the single energy-level sum becomes $\sum_{n_j=0}^{1} e^{-\beta(\epsilon_j-\mu)n_j} = 1 + e^{-\beta(\epsilon_j-\mu)}$. Thus,

$$Z_{\mathrm{G,fermions}} = \prod_{i=1}^{\infty} \left(1 + e^{-\beta(\epsilon_i-\mu)}\right).$$

(b) In general, we write

$$Z_{\mathrm{G}} = \prod_{i=1}^{\infty} \left(1 - \zeta e^{-\beta(\epsilon_i-\mu)}\right)^{-\zeta},$$

with $\zeta = \pm 1$ for bosons and fermions, respectively. Then,

$$\Omega = -\frac{1}{\beta}\ln Z_{\mathrm{G}} = \frac{\zeta}{\beta}\sum_{i=1}^{\infty} \ln\left(1 - \zeta e^{-\beta(\epsilon_i-\mu)}\right).$$

Using that

$$\begin{aligned} \mathcal{N} = \sum_{i=1}^{\infty} \langle n_i \rangle = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} &= -\frac{\zeta}{\beta}\sum_{i=1}^{\infty} \frac{1}{1-\zeta e^{-\beta(\epsilon_i-\mu)}} \times \left(-\zeta\beta e^{-\beta(\epsilon_i-\mu)}\right) \\ &= \sum_{i=1}^{\infty} \frac{1}{1-\zeta e^{-\beta(\epsilon_i-\mu)}} \times \left(e^{-\beta(\epsilon_i-\mu)}\right) = \sum_{i=1}^{\infty} \frac{1}{e^{\beta(\epsilon_i-\mu)} - \zeta}. \end{aligned}$$

Thus,

$$\langle n_i \rangle = \frac{1}{e^{\beta(\epsilon_i-\mu)} - \zeta}.$$

(c) The straightforward way would be computing

$$\begin{aligned} \left\langle \left(\sum_i n_i\right)^2 \right\rangle &= \frac{1}{Z_{\mathrm{G}}}\mathrm{tr}\left(e^{-\beta\left(H-\mu\sum_i n_i\right)}\left(\sum_i n_i\right)^2\right) = \frac{\beta^{-2}}{Z_{\mathrm{G}}}\frac{\partial^2 Z_{\mathrm{G}}}{\partial \mu^2} = \frac{1}{\beta^2}\left[\left(\frac{\partial \ln Z_{\mathrm{G}}}{\partial \mu}\right)^2 + \frac{\partial^2 \ln Z_{\mathrm{G}}}{\partial \mu^2}\right] \\ &= \sum_i \langle n_i^2 \rangle + \sum_{i\neq j} \langle n_i \rangle \langle n_j \rangle = \left(\frac{\partial \Omega}{\partial \mu}\right)^2 + \frac{1}{\beta}\frac{\partial^2 \Omega}{\partial \mu^2} = \left(\sum_{i=1}^{\infty} \langle n_i \rangle\right)^2 + \frac{1}{\beta}\frac{\partial^2 \Omega}{\partial \mu^2}. \end{aligned}$$

Thus,

$$\sum_i \left(\langle n_i^2\rangle - \langle n_i\rangle^2\right) = \sum_i \left\langle \left(n_i^2 - \langle n_i\rangle^2\right)\right\rangle = \frac{1}{\beta}\frac{\partial^2 \Omega}{\partial \mu^2} = -\frac{1}{\beta}\frac{\partial}{\partial\mu}\sum_i \langle n_i\rangle .$$
$$= -\frac{1}{\beta}\sum_i \frac{\partial}{\partial\mu}\langle n_i\rangle = \sum_i \langle n_i\rangle^2 e^{\beta(\epsilon_i-\mu)}.$$

Therefore,

$$\frac{\left\langle \left(n_i^2 - \langle n_i\rangle^2\right)\right\rangle}{\langle n_i\rangle^2} = \frac{\langle n_i^2\rangle - \langle n_i\rangle^2}{\langle n_i\rangle^2} = e^{\beta(\epsilon_i-\mu)} = \frac{1}{\langle n_i\rangle} + \zeta.$$

Moreover, there is a more elegant way to show all of this which is by directly using the operator algebra. For fermions, $n^2 = a^\dagger a a^\dagger a = a^\dagger\left(1 - a^\dagger a\right)a = n - a^{\dagger 2}a^2 = n$. Hence,

$$\frac{\langle n_i^2\rangle - \langle n_i\rangle^2}{\langle n_i\rangle^2} = \frac{\langle n_i\rangle - \langle n_i\rangle^2}{\langle n_i\rangle^2} = \frac{1}{\langle n_i\rangle} - 1.$$

For bosons, this is not so simple (since $a^2 \neq 0$). We have that $n^2 = a^\dagger a a^\dagger a = a^\dagger\left(1 + a^\dagger a\right)a = n + a^{\dagger 2}a^2$. Thus, $\langle n^2\rangle = \langle n\rangle + \langle a^{\dagger 2}a^2\rangle$. This second term can be computed using the Wick's theorem $\langle a^{\dagger 2}a^2\rangle = 2\langle a^\dagger a\rangle^2 = 2\langle n\rangle^2$ .Therefore,

$$\frac{\langle n_i^2\rangle - \langle n_i\rangle^2}{\langle n_i\rangle^2} = \frac{\langle n_i\rangle + \langle n_i\rangle^2}{\langle n_i\rangle^2} = \frac{1}{\langle n_i\rangle} + 1.$$

7.

(a) Let a generic state be labeled by $|n_j, n_{j-1}, \ldots, n_{-j+1}, n_{-j}\rangle$. The closed shell state is thus

$$|\mathrm{cs}\rangle = |1, 1, \ldots, 1\rangle = \prod_{i=-j}^{j} a_{j,i}^\dagger |0\rangle .$$

(b) In second quantization, the total angular momentum operator is

$$\mathbf{J} = \sum_{i=-j}^{j}\sum_{k=-j}^{j} \langle i|\mathbf{J}|k\rangle a_{j,i}^\dagger a_{j,k} = \sum_{i,k} \mathbf{J}_{i,k} a_{j,i}^\dagger a_{j,k},$$

where $|i\rangle = a_{j,i}^\dagger|0\rangle$ (and notice $\mathbf{J}_{i,k}$ is not an operator.)

Now let us compute

$$\mathbf{J}|\mathrm{cs}\rangle = \sum_{i,k}\mathbf{J}_{i,k}a_{j,i}^\dagger a_{j,k}|\mathrm{cs}\rangle = \sum_{i,k}\mathbf{J}_{i,k}\delta_{i,k}|\mathrm{cs}\rangle = \mathbf{J}_{\mathrm{cs}}|\mathrm{cs}\rangle, \text{ where } \mathbf{J}_{\mathrm{cs}} = \sum_{k=-j}^{j}\mathbf{J}_{k,k}.$$

Our task now is to show that $\mathbf{J}_{\mathrm{cs}} = 0$. Let us start with the z-component:

$$J^z|k\rangle = \hbar k|k\rangle, \quad \Rightarrow \quad J^z_{k,k} = \hbar k. \text{ Thus, } J^z_{\mathrm{cs}} = \sum_{k=-j}^{j} J^z_{k,k} = 0.$$

With respect to the x-component, recall that $J^x|k\rangle = \frac{1}{2}\left(J^+ + J^-\right)|k\rangle = \alpha|k+1\rangle + \beta|k-1\rangle$, where $\alpha = \frac{1}{2}\hbar\sqrt{(j-k)(j+k+1)}$ and $\beta = \frac{1}{2}\hbar\sqrt{(j+k)(j-k+1)}$. Thus, $J^x_{k,k} = 0$, and consequently, $J^x_{\mathrm{cs}} = 0$. Analogously, $J^y_{\mathrm{cs}} = 0$.

(c) The hole state is

$$|\bar{k}\rangle = |1, 1\ldots, 1, 0, 1, \ldots 1\rangle = \prod_{i=-j}^{k-1}\prod_{i=k+1}^{j} a_{j,i}^\dagger|0\rangle .$$

Likewise, this state can be rewritten as

$$\begin{aligned}\left|\bar{k}\right\rangle &= a^{\dagger}_{j,j}\dots a^{\dagger}_{j,k+1}a^{\dagger}_{j,k-1}\dots a^{\dagger}_{j,-j}\left|0\right\rangle = a^{\dagger}_{j,j}\dots a^{\dagger}_{j,k+1}a_{j,k}a^{\dagger}_{j,k}a^{\dagger}_{j,k-1}\dots a^{\dagger}_{j,-j}\left|0\right\rangle \\ &= (-1)^{j-k}\,a_{j,k}\left(a^{\dagger}_{j,j}\dots a^{\dagger}_{j,k+1}a^{\dagger}_{j,k}a^{\dagger}_{j,k-1}\dots a^{\dagger}_{j,-j}\left|0\right\rangle\right) = (-1)^{j-k}\,a_{j,k}\left|\text{cs}\right\rangle.\end{aligned}$$

Thus, if we consider $\left|\text{cs}\right\rangle$ as the vacuum of the theory, the state $\left|\bar{k}\right\rangle$ is created upon acting an effective creation operator $(-1)^{j-k}\,a_{j,k}$ on this vacuum.

Now, let us apply

$$\begin{aligned}\mathbf{J}\left|\bar{k}\right\rangle &= \sum_{i,m}\mathbf{J}_{i,m}a^{\dagger}_{j,i}a_{j,m}\left|\bar{k}\right\rangle = \sum_{i,m}\mathbf{J}_{i,m}\delta_{m,i}\left(1-\delta_{k,i}\right)\left|\bar{k}\right\rangle + \sum_{i,m}\mathbf{J}_{i,m}\delta_{k,i}\left(1-\delta_{k,m}\right)\left|\bar{m}\right\rangle \\ &= \left(\sum_{i\neq k}\mathbf{J}_{i,i}\right)\left|\bar{k}\right\rangle + \left(\sum_{m\neq k}\mathbf{J}_{k,m}\left|\bar{m}\right\rangle\right) = \left(\sum_{i\neq k}J^{z}_{i,i}\hat{z}\right)\left|\bar{k}\right\rangle + \left(\sum_{m\neq k}J^{x}_{k,m}\hat{x}\left|\bar{m}\right\rangle + \sum_{m\neq k}J^{y}_{k,m}\hat{y}\left|\bar{m}\right\rangle\right).\end{aligned}$$

In the last passage, we used that $J^{x,y}_{k,k} = 0 = J^{z}_{k,m\neq k}$. Notice that the diagonal term is just like $J^{z}\left|\bar{k}\right\rangle = \hbar m_{\bar{k}}\left|\bar{k}\right\rangle$. The corresponding angular momentum in the z-direction is

$$m_{\bar{k}} = \sum_{i\neq k} i = \left(\sum_{i=-j}^{j} i\right) - k = 0 - k = -k.$$

We now work on the off-diagona terms. It is actually simpler to work with the ladder operator

$$J^{+}\left|\bar{k}\right\rangle = \sum_{i,m}J^{+}_{i,m}a^{\dagger}_{j,i}a_{j,m}\left|\bar{k}\right\rangle = \left(\sum_{i\neq k}J^{+}_{i,i}\right)\left|\bar{k}\right\rangle + \left(\sum_{m\neq k}J^{+}_{k,m}\left|\bar{m}\right\rangle\right).$$

The matrix element

$$\left\langle k\left|J^{+}\right|m\right\rangle = \hbar\sqrt{(j-m)\,(j+m+1)}\left\langle k|m+1\right\rangle = \hbar\sqrt{(j-m)\,(j+m+1)}\delta_{m,k-1}.$$

Hence,

$$J^{+}\left|\bar{k}\right\rangle = \hbar\sqrt{(j-k+1)\,(j+k)}\left|\overline{k-1}\right\rangle = \hbar\sqrt{(j-m_{\bar{k}})\,(j+m_{\bar{k}}+1)}\left|\overline{k}+1\right\rangle.$$

Likewise,

$$J^{-}\left|\bar{k}\right\rangle = \hbar\sqrt{(j+m_{\bar{k}})\,(j-m_{\bar{k}}+1)}\left|\overline{k}-1\right\rangle.$$

Comparing with

$$J^{z}\left|k\right\rangle = \hbar m_{k}\left|k\right\rangle, \text{ and } J^{\pm}\left|k\right\rangle = \hbar\sqrt{(j\mp m_{k})\,(j\pm m_{k}+1)}\left|k+1\right\rangle,$$

we conclude that $\left|\bar{k}\right\rangle$ is like a state $\left|-k\right\rangle$.