2. In this problem we will calculate the approximate ground state energy of a gas of N weakly interacting spin-1/2 particles of mass m in a one-dimensional harmonic oscillator potential

$$V(X) = \frac{1}{2}m\omega^2 X^2.$$

The potential for interactions between particles is

$$U_{12} = u_0 I_{12},$$

where u_0 is a constant number and I_{12} is the identity: the interaction is constant and independent of particle separation.

(a) (10) Write each term of the Hamiltonian in terms of creation and annihilation operators $a^\dagger_{n_i,\sigma_i}$, a_{n_i,σ_i}, which respectively create and destroy particles in the state $|\phi_{n_i}\rangle|\sigma_i\rangle$. Note that $n_i = 0, 1, 2, 3, \ldots$ in this notation is not the number of particles! To do this, first express the Hamiltonian in terms of the field operators $\psi^\dagger_\sigma(x)$, $\psi_\sigma(x)$:

$$\psi_\sigma(x) = \sum_n \langle x|n\rangle a_{n,\sigma}$$
$$\psi^\dagger_\sigma(x) = \sum_n \langle n|x\rangle a^\dagger_{n,\sigma}$$

where the $\langle x|n\rangle \equiv \Psi_n(\sqrt{m\omega/\hbar}x)$ are the eigenfunctions of the 1D harmonic oscillator. These are the usual Hermite functions which are real and obey:

$$\frac{d}{dx}\Psi_n(x) = \sqrt{\frac{n}{2}}\Psi_{n-1}(x) - \sqrt{\frac{n+1}{2}}\Psi_{n+1}(x),$$
$$x\Psi_n(x) = \sqrt{\frac{n}{2}}\Psi_{n-1}(x) + \sqrt{\frac{n+1}{2}}\Psi_{n+1}(x),$$
$$\int_{-\infty}^{\infty}\Psi_n(\sqrt{m\omega/\hbar}x)\Psi_m(\sqrt{m\omega/\hbar}x)dx = \delta_{nm}.$$

The non-interacting term should be proportional to $E_n(n+1/2)$ where you must determine E_n.

(b) (10) Use the hamiltonian that you wrote down to determine an expression for the ground state energy, assuming that the ground state is the Hartree-Fock state, i.e.:

$$|\Psi_g^{HF}\rangle = a^\dagger_{0,+}a^\dagger_{0,-}a^\dagger_{1,+}a^\dagger_{1,-}\ldots a^\dagger_{(N/2-1),+}a^\dagger_{(N/2-1),-}|0\rangle. \quad (3)$$

You can assume N is an even number.

Let $|\phi_{n_i}\rangle|\sigma_i\rangle \equiv |\phi_{n_i};\sigma_i\rangle$

$k = \sqrt{\frac{m\omega}{\hbar}}$

- Starting with the K.E term,

$$T_i^N = \sum_{i=1}^{N}\frac{P_i^2}{2m} = \sum_{i=1}^{N} T_i$$, Let's second quantize T_i

Using the fact that if $\hat{A} = \sum_{i=1}^{N} A_i$, with A_i acts on on a single particle 'i', then:

$$A^N_{(1)} = \sum_{k_\alpha,k_\beta}\langle k_\alpha|A_i(\vec{x},\vec{P},\vec{S})|k_\beta\rangle a^\dagger_{k_\alpha}a_{k_\beta}$$

In our case, we also have spin for the states,

$$A^N_{(1)} = \sum_{\substack{k_\alpha\\k_\beta}}\sum_{\substack{\sigma_\alpha\\\sigma_\beta}}\langle k_\alpha,\sigma_\alpha|A_i(\vec{X},\vec{P},\vec{S})|k_\beta,\sigma_\beta\rangle a^\dagger_{\substack{k_\alpha\\\sigma_\alpha}}a_{\substack{k_\beta\\\sigma_\beta}}$$

$$\therefore T_i^N = \sum_{\substack{\sigma_1\\\sigma_2}}\int dx_1\,dx_2\,\langle x_1,\sigma_1|\frac{P^2}{2m}|x_2,\sigma_2\rangle\,\psi^\dagger_{\sigma_1}(x_1)\,\psi_{\sigma_2}(x_2)$$

$$= \sum_{\substack{\sigma_1\\\sigma_2}}\int dx_1\,dx_2\,\langle x_1,\sigma_1|\left(\frac{-\hbar^2\nabla^2_{x_2}}{2m}\right)|x_2,\sigma_2\rangle\,\psi^\dagger_{\sigma_1}(x_1)\,\psi_{\sigma_2}(x_2)$$

$$= \sum_{\substack{\sigma_1 \\ \sigma_2}} \int dx_1\, dx_2 \langle x_1, \sigma_1 | x_2, \sigma_2 \rangle \Psi^\dagger_{\sigma_1}(x_1) \left(\frac{-\hbar^2 \nabla^2_{x_2}}{2m} \right) \Psi_{\sigma_2}(x_2)$$

Integration by parts + Dirac δ function from $\langle x_1, \sigma_1 | x_2, \sigma_2 \rangle = \delta_{\sigma_1 \sigma_2} \delta(x_1 - x_2)$

$$= \frac{\hbar^2}{2m} \sum_{\sigma} \int dx \left(\nabla \Psi^\dagger_{\sigma}(x) \right) \left(\nabla \Psi_{\sigma}(x) \right)$$

- In the final line $x_1 = x_2 = x$ after imposing $\int \delta(x_2 - x_1)\, dx_2$

$$= \frac{\hbar^2}{2m} \sum_{\sigma} \sum_{ij} \int dx \left(\nabla \Psi_i(kx) \right) \left(\nabla \Psi_j(kx) \right) \quad a^\dagger_{i,\sigma} a_{j,\sigma}$$

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$$= \frac{\hbar^2 k^2}{2m} \sum_{\sigma} \sum_{ij} \left[\sqrt{i(i-1)}\, \delta_{i-2,j} - (2i+1)\delta_{ij} + \sqrt{(i+1)(i+2)}\, \delta_{i+2,j} \right] a^\dagger_{i,\sigma} a_{j,\sigma}$$

$$\boxed{= \frac{-\hbar^2}{4m} k^2 \sum_{\sigma} \sum_{i} \left[\sqrt{i(i-1)}\, a^\dagger_{i-2,\sigma} a_{i,\sigma} - (2i+1)\, a^\dagger_{i,\sigma} a_{i,\sigma} + \sqrt{(i+1)(i+2)}\, a^\dagger_{i+2,\sigma} a_{i,\sigma} \right]}$$

2^{nd} quantized K.E.

PTO.

$$V_i^{(N)} = \sum_{\sigma\sigma'} \int d^3x_1 \int d^3x_2 \, \langle x_1,\sigma \,|\, V(x) \,|\, x_2,\sigma' \rangle \, \psi^\dagger_\sigma(x_1)\, \psi_{\sigma'}(x_2)$$

$$= \frac{1}{2} m\omega^2 \sum_{\sigma\sigma'} \int d^3x_1 \int d^3x_2 \; X_2^2 \; \underbrace{\langle x_1,\sigma \,|\, x_2,\sigma' \rangle}_{\delta(x_1-x_2)\,\delta_{\sigma\sigma'}} \, \psi^\dagger_\sigma(x_1)\, \psi_{\sigma'}(x_2)$$

$x_1 = x_2 = x$
$\sigma = \sigma'$
(After imposing δ functions)

$$= \frac{1}{2} m\omega^2 \sum_{\sigma} \int d^3x \; X^2 \; \psi^\dagger_\sigma(x)\, \psi_\sigma(x)$$

$$= \frac{1}{2} m\omega^2 \sum_{\sigma} \sum_{ij} \int d^3x \; \underbrace{\frac{1}{k}}_{I} k X \psi_i(kx) \; \frac{1}{k} k X \psi_j(kx) \; a^\dagger_{\sigma i}\, a_{\sigma j}$$

$$= \frac{1}{2} m\omega^2 \frac{1}{k^2} \sum_{\sigma} \sum_{ij} \int d^3x \left[\sqrt{\frac{i}{2}}\, \psi_{i-1}(kx) + \sqrt{\frac{i+1}{2}}\, \psi_{n+1}(kx) \right]$$
$$\times \left[\sqrt{\frac{j}{2}}\, \psi_{j-1}(kx) + \sqrt{\frac{j+1}{2}}\, \psi_{j+1}(kx) \right] a^\dagger_{\sigma i}\, a_{\sigma j}$$

$$= \frac{1}{4} \frac{m\omega^2}{k^2} \sum_{\sigma} \sum_{ij} \Big(\sqrt{ij}\, \delta_{ij} + \sqrt{i(j+1)}\, \delta_{i-1,j+1} + \sqrt{(i+1)(j)}\, \delta_{n+1,m-1}$$
$$+ \sqrt{(i+1)(j+1)}\, \delta_{i,j} \Big) \, a^\dagger_{\sigma i}\, a_{\sigma j}$$

$$\boxed{= \frac{1}{4} \frac{m\omega^2}{k^2} \sum_{\sigma} \sum_{j} \Big[(2j+1)\, a^\dagger_{\sigma j}\, a_{\sigma j} + \sqrt{(j+1)(j+2)}\; a^\dagger_{j+2,\sigma}\, a_{j,\sigma} + \sqrt{(j-2)j}\; a^\dagger_{j-2,\sigma}\, a_{j,\sigma} \Big]}$$

2nd quantized $V(x)$

$$U_{12}^{(N)} = U_0 I_{12}$$

$$= U_0 \sum_{\substack{\sigma_1\sigma_2\\ \sigma_3\sigma_4}} \iiiint dx_1\, dx_2\, dx_3\, dx_4 \; \langle x_1\sigma_1 ; x_2\sigma_2 \,|\, I_{12} \,|\, x_3\sigma_3 ; x_4\sigma_4 \rangle$$
$$\psi^\dagger_{\sigma_1}(x_1)\, \psi^\dagger_{\sigma_2}(x_2)\, \psi_{\sigma_3}(x_3)\, \psi_{\sigma_4}(x_4)$$

Two body operator

$$= U_0 \sum_{\sigma\sigma'} \iint dx\, dx' \; \psi^\dagger_\sigma(x)\, \psi^\dagger_{\sigma'}(x')\, \psi_\sigma(x)\, \psi_{\sigma'}(x')$$

$$= U_0 \sum_{\sigma\sigma'} \sum_{ijmn} \iint dx\, dx' \; \psi_i(kx)\, \psi_j(kx')\, \psi_m(kx)\, \psi_n(kx')$$

$$= U_0 \sum_{\sigma\sigma'} \sum_{ijmn} \delta_{im}\, \delta_{jn}\, a^\dagger_{i\sigma}\, a^\dagger_{j\sigma'}\, a_{m\sigma}\, a_{n\sigma'}$$

$$= \boxed{U_0 \sum_{\sigma\sigma'} \sum_{ij} a^\dagger_{i\sigma}\, a^\dagger_{j\sigma'}\, a_{i\sigma}\, a_{j\sigma'}}$$ 2^{nd} quantized U

Now, from KE & $U(x)$ we will take the $a^\dagger_{i\sigma} a_{i\sigma}$ (i.e. from the non-interacting terms)

$$\sum_\sigma \sum_i \left[\frac{m\omega^2}{4k^2}(2i+1) + \frac{k^2\hbar^2}{4m}(2i+1) \right] a^\dagger_{i\sigma} a_{i\sigma}$$

$$= \sum_\sigma \sum_i \left\{ \left[\frac{1}{4} m\omega^2 \frac{\hbar}{m\omega} + \frac{\hbar^2}{4m} \frac{m\omega}{\hbar} \right] (2i+1)\, \underbrace{a^\dagger_{i\sigma} a_{i\sigma}} \right.$$

This is the number operator

$$= \frac{\hbar\omega}{2} \sum_\sigma \sum_i \left(i + \frac{1}{2}\right) N_{i,\sigma} \underset{i\to n}{=} E_n \left(n + \frac{1}{2}\right)$$

$$E_n = \sum_\sigma \sum_n \frac{\hbar\omega}{2} N_{n,\sigma}$$

b Given,

$$|\Psi_g^{HF}\rangle = \prod_m^{\frac{N}{2}-1} a^\dagger_{m+}\, a^\dagger_{m-} |0\rangle$$

$$\& \quad \langle \Psi_g^{HF} | \underbrace{a^\dagger_{n\sigma} a_{n\sigma}}_{\text{Number operator.}} | \Psi_g^{HF} \rangle = \Theta\left(\frac{N}{2} - 1 - n\right)$$

- From the KE $+ U(x)$, the non-interacting terms will be the ones to contribute to the ground state of HF due to orthogonality.

$$E_{kin} + E_{V(x)} = \frac{\hbar\omega}{4} \sum_{n\sigma} \left(n + \frac{1}{2}\right) \langle \Psi_g^{HF} | a^\dagger_{n\sigma} a_{n\sigma} | \Psi_g^{HF} \rangle$$

$$= \frac{\hbar\omega}{4} \sum_n \left(n + \frac{1}{2}\right) \Theta\left(\frac{N}{2} - 1 - n\right) \overbrace{2\left(\frac{N}{2} - 1\right)}^{\sum_\sigma}$$

$$= \frac{\hbar\omega}{2} \sum_{n=0}^{\frac{N}{2}-1} \left(n + \frac{1}{2}\right) \left(\frac{N}{2} - 1\right) = \frac{\hbar\omega}{2} \underbrace{\left(\frac{1}{32}(N-10)(N-2)N\right)}_{\text{Wolfram alpha of Sum.}}$$

Interaction potential:

$$U_0 \langle \Psi_g^{HF} | \sum_{\sigma\sigma'} \sum_{ij} a^\dagger_{i\sigma} a^\dagger_{j\sigma'} a_{i\sigma} a_{j\sigma'} | \Psi_g^{HF} \rangle$$

$$= U_0 \sum_{\sigma\sigma'} \sum_{ij} \langle \Psi_g^{HF} | a^\dagger_{i\sigma} \left(\delta_{ij} \delta_{\sigma\sigma'} - a_{i\sigma} a^\dagger_{j\sigma'} \right) a_{j\sigma'} | \Psi_g^{HF} \rangle$$

$$= U_0 \sum_{\sigma\sigma'} \sum_{ij} \langle \Psi_g^{HF} | a^\dagger_{i\sigma} a_{i\sigma} - a^\dagger_{i\sigma} a_{i\sigma} a^\dagger_{j\sigma'} a_{j\sigma'} | \Psi_g^{HF} \rangle$$

$$= U_0 \left(\sum_{\sigma} \sum_{i} \langle \Psi_g^{HF} | a^\dagger_{i\sigma} a_{i\sigma} | \Psi_g^{HF} \rangle - \sum_{\sigma\sigma'} \sum_{ij} \langle \Psi_g^{HF} | a^\dagger_{i\sigma} a_{i\sigma} a^\dagger_{j\sigma'} a_{j\sigma'} | \Psi_g^{HF} \rangle \right)$$

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$$= U_0 \left[\sum_i 2\, \Theta\left(\frac{N}{2} - 1 - n\right) - \sum_{ij} 4\, \Theta\left(\frac{N}{2} - 1 - i\right) \Theta\left(\frac{N}{2} - 1 - j\right) \right]$$

$$= U_0 \left[2 \left(\frac{N}{2} - 1\right) - 4 \left(\frac{N}{2} - 1\right)^2 \right]$$