Physics 726: Assignment 4

(to be submitted by Thursday, February 25, 2016)

A collection of interacting spinless fermions, confined to an infinite square well of width L, is described by the Hamiltonian

$$\hat{H} = \int_0^L dx\, \hat{\psi}^\dagger(x) T(x) \hat{\psi}(x) + \frac{1}{2}\int_0^L dx \int_0^L dy\, \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y) V(x,y) \hat{\psi}(y)\hat{\psi}(x).$$

Here, $T(x) = -(\hbar^2/2m)\partial^2/\partial x^2$ inside the well and $T = \infty$ outside; $V(x,y) = (\kappa/2)(x-y)^2$ represents a Hooke's law potential—either attractive ($\kappa > 0$) or repulsive ($\kappa < 0$)—between the particles.

From undergraduate quantum mechanics, we know that the one-body term has eigenfunctions

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\!\left(\frac{n\pi x}{L}\right)$$

that satisfy $T\phi_n = h^2 n^2/8mL^2 \phi_n \equiv \varepsilon_n \phi_n$. As we showed in Assignment 3, an expansion of the field operators in these one-body modes,

$$\hat{\psi}(x) = \sum_{n=1}^{\infty} \phi_n(x) c_n \quad \text{and} \quad \hat{\psi}^\dagger(x) = \sum_{n=1}^{\infty} \phi_n^*(x) c_n^\dagger,$$

leads to an alternative expression of the Hamiltonian

$$\hat{H} = \sum_n \varepsilon_n c_n^\dagger c_n + \sum_{k,l,m,n} V_{k,l,m,n} c_k^\dagger c_l^\dagger c_m c_n,$$

which is the sum of a diagonal, occupation-number term and an off-diagonal term that describes two-body scattering events of amplitude

$$\begin{aligned} V_{k,l,m,n} &= \frac{1}{2}\int_0^L dx \int_0^L dy\, \phi_k^*(x)\phi_l^*(y)\frac{1}{2}\kappa(x-y)^2 \phi_m(y)\phi_n(x) \\ &= \frac{\kappa}{L^2}\int_0^L dx\, \sin\!\left(\frac{k\pi x}{L}\right)\sin\!\left(\frac{n\pi x}{L}\right)\int_0^L dy\, \sin\!\left(\frac{l\pi y}{L}\right)(x^2 - 2xy + y^2)\sin\!\left(\frac{m\pi y}{L}\right). \end{aligned}$$

1. Start by considering the interaction matrix elements $V_{k,l,m,n}$.

   (a) Demonstrate that $V_{k,l,m,n} = V_{l,k,n,m}$ whenever the interaction potential obeys the coordinate-exchange symmetry $V(x,y) = V(y,x)$.

   (b) Show that the *direct* ($k = n$, $l = m$) contribution is

   $$V_{n,m,m,n} = V_{m,n,n,m} = \frac{\kappa L^2}{24}\left[1 - \frac{3}{\pi^2}\left(\frac{1}{m^2} + \frac{1}{n^2}\right)\right].$$

   (c) Show that the *exchange* ($k = m$, $l = n$) contribution is

   $$V_{m,n,m,n} = V_{n,m,n,m} = -\frac{32\kappa L^2}{\pi^4}\frac{m^2 n^2}{(m^2 - n^2)^4}$$

   when $m + n$ is odd, and $V_{m,n,m,n} = 0$ otherwise.

2. In the absence of interactions, the ground state of the N-fermions-in-a-box system is $|F^{(N)}\rangle = c_N^\dagger \cdots c_2^\dagger c_1^\dagger |\text{vac}\rangle$. The corresponding ground-state energy is

   $$E_0 = \sum_n \varepsilon_n \langle F^{(N)}| c_n^\dagger c_n |F^{(N)}\rangle = \sum_{n=1}^{N} \varepsilon_n.$$

   Suppose that the Hooke's law force acting between the particles can be treated as a weak perturbation around this non-interacting limit.

(a) Prove that the first-order energy shift is

$$\Delta E = \sum_{k,l,m,n} V_{k,l,m,n} \langle F^{(N)}|c_k^\dagger c_l^\dagger c_m c_n|F^{(N)}\rangle = \sum_{1\le m<n\le N} 2(V_{m,n,n,m} - V_{m,n,m,n}).$$

(b) What is the estimated ground-state energy $E_0 + \Delta E$ of the two-particle system?

(c) What is the estimated ground-state energy when the box contains three particles?

(d) The unperturbed energy E_0 and the first-order energy shift ΔE each scale in a characteristic way with the number of particles. For instance,

$$E_0 = \sum_{n=1}^{N} \varepsilon_n = \frac{\hbar^2 N(1+N)(1+2N)}{48mL^2} = \frac{\hbar^2 N^3}{24mL^2} + O(N^2),$$

so that the energy per particle

$$\frac{E_0}{N} \sim \frac{\hbar^2 \rho^2}{24m}$$

is a quadratic function of the particle density $\rho = N/L$. Perform the comparable analysis for ΔE.

(e) Give a physical picture of what it means for perturbation theory to break down at very large, negative values of the spring constant κ. *Hint:* try to justify a transition comparable to Wigner crystallization.