Linear hydrodynamics and bosonization (continued) and current operator

Exercises 2 is the repetition from the last exercise of Series 1.

Exercise 1: Lagrangian and Hamilton functions revisited (1 points) In Exercise 1 of Series 1, we have derived the equation of motion for density fluctuations in a 1D gas of length L, containing N spinless fermions:

$$\partial_t^2 \rho_k(t) + k^2 c^2 \rho_k(t) = 0. \tag{1}$$

Here $\rho_k(t) = \int \mathrm{d}x e^{ikx} \delta\rho(x,t)$ is the Fourier transform of the density fluctuations. If we wish to quantize this description, the equation of motion is not a convenient starting point. Instead, we would like to start from the Lagrangian. To derive it, we note that the equation of motion must follow from a certain Lagrangian $\mathcal{L}$, combined with the Euler-Lagrange equation, which is given by:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}}{\partial\left(\partial_t \rho_k(t)\right)}\right) - \frac{\partial \mathcal{L}}{\partial \rho_k(t)} = 0. \tag{2}$$

In this exercise we will show that we can rewrite $\mathcal{L}$ in the canonical form of the harmonic oscillator:

$$\mathcal{L} = \frac{1}{2L}\sum_k \left[m\left(\partial_t \phi_k(t)\right)^2 - m\omega_k^2 \phi_k^2(t)\right], \tag{3}$$

a form that is easily quantized.

(a) Show, by means of reverse engineering, that the Lagrangian that gives rise to the equation of motion Eq. (2) can be written as:

$$\mathcal{L} = \frac{1}{2}\sum_k \frac{1}{f(k)}\left[m\left(\partial_t \rho_k(t)\right)^2 - mk^2c^2\rho_k^2(t)\right]. \tag{4}$$

Here $f(k)$ is a function that is used to fulfill the requirement that the Lagrangian has the correct dimension. Otherwise we are free to choose it, since its form does not affect the equation of motion.

(b) What is the dimension of a Lagrangian? What does this mean for the form of $f(k)$? Comparing Eq. (3) and Eq. (4), what is the relation between $\rho_k(t)$ and $\phi_k(t)$?

Exercise 2: One-Body Potential and Orthogonality Catastrophe (3 points) In the same way, we can add a one-body scattering potential

$$U = \int \mathrm{d}x U(x)\rho(x). \tag{5}$$

(a) Show that the Hamiltonian remains unchanged (up to a shift in energy) if we complete the square, i.e. change the boson modes by $\phi_k \to \phi_k + \Delta\phi_k$ with $\Delta\phi_k = U_{-k}|k|/\sqrt{L}m\omega_k^2$. The new ground state function is thus $\Phi(\{\phi_k\})) = \Psi(\{\phi_k + \Delta\phi_k\})$.

(b) Show that the overlap between the old and new ground states is

$$\langle\Phi|\Psi\rangle = \exp\left(-\sum_{k>0}\frac{|U_k|^2}{\hbar m c^3 k}\right). \tag{6}$$

Observe that $k = n\pi/L$, and that the sum in the exponent diverges in the thermodynamic limit $L \to \infty$ (while keeping $\rho_0 = N/L$ constant). For a large but finite number of particles N, we have thus $\langle\Phi|\Psi\rangle \sim N^{-\alpha}$ with some exponent $\alpha > 0$ that depends directly on the potential U. The

overlap is effectively zero, which is known as the "Orthogonality Catastrophe", and has been first investigated by P. W. Anderson in 1967 [Phys. Rev. Lett. **18**, 1049 (1967)]. It is a "catastrophe" because if $U(x)$ is abruptely (nonadiabatically) switched on at some time, there is no hope of finding the new ground state Φ by doing perturbation theory around the original ground state Ψ, because perturbation theory always produces a finite overlap between initial and finite states. This observation has stimulated a huge progress in the development of nonperturbative techniques, and most of the modern techniques we know (among them bosonization) have been applied and tested on the orthogonality catastrophe.

(c) (new) Anderson found the Orthogonality Catastrophe for a 3-dimensional metal, calculating explicitly overlap integrals between Slater determinants. Your calculation here was for a 1-dimensional system using a hydrodynamic approach. Look at Eq. (6) and give a simple technical argument why this hydrodynamic approach does not reproduce the Orthogonality Catastrophe in dimensions larger than 1. Try then to give a physical argument why the simple hydrodynamic calculation is insufficient. [Hints: (i) Observe that the divergence of the sum is due to particle-hole excitations with vanishing energy (since $k \to 0$). (ii) In fact, the hydrodynamic result is not complete even in 1 dimension because we have neglected the $2k_F$ backscattering across the Fermi surface. (iii) To which type of density fluctuations correspond the ϕ_k in higher dimensions?]

Motivation for Exercise 3. The quantum mechanical (QM) description is more complete than the classical one. There must, therefore, be "backward compatibility": Any classical result can be (in principle) derived from quantum mechanics. In particular, classical quantities like energy E, density of particles n, coordinate $\vec{r}$, momentum $\vec{p}$, velocity $\vec{v}$, charge current $\vec{j}$, etc. must be equal to the expectation value of corresponding QM operators:

$$E = \mathrm{Tr}[\hat{\rho}\hat{H}], \quad n = \mathrm{Tr}[\hat{\rho}\hat{n}], \quad \vec{r} = \mathrm{Tr}[\hat{\rho}\hat{\vec{r}}], \quad \vec{p} = \mathrm{Tr}[\hat{\rho}\hat{\vec{p}}], \quad \vec{v} = \mathrm{Tr}[\hat{\rho}\hat{\vec{v}}], \quad \vec{j} = \mathrm{Tr}[\hat{\rho}\hat{\vec{j}}], \tag{7}$$

where $\hat{\rho}$ is the density matrix. This means, if we have invented, for instance, an operator $\hat{\vec{v}}$ such that $\mathrm{Tr}[\hat{\rho}\hat{\vec{v}}] = \vec{v}$, then we claim that this must be the correct QM operator corresponding to the classical speed.[1]

It turns out that for the velocity the good definition of the QM operator is the time derivative of the coordinate, given through the Heisenberg equation by $\hat{\vec{v}} \equiv \frac{\mathrm{d}}{\mathrm{d}t}\hat{\vec{r}} = \frac{i}{\hbar}[\hat{H}, \hat{\vec{r}}]$.

Let $|\psi\rangle$ be the wave function of a single spinless electron, and let $|\vec{r}\rangle$ be the Dirac notation for the position basis (i.e. $\hat{\vec{r}}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle$). Then the wavefunction is expressed by $\psi(\vec{r}) = \langle\vec{r}|\psi\rangle$. A general operator[2] $\hat{A}$ is usually not diagonal in the position basis, and matrix elements over the position basis depend on two coordinates: $\langle\vec{r}|\hat{A}|\vec{r}'\rangle = A(\vec{r},\vec{r}')$. If the electron has a spin 1/2 (as they usually do) we must complete the position basis by the spin basis and write $|\vec{r},s\rangle$ with $s = \uparrow,\downarrow$, and we have $\psi(\vec{r},s) = \langle\vec{r},s|\psi\rangle$, and $\langle\vec{r},s|\hat{A}|\vec{r}',s'\rangle = A(\vec{r},s;\vec{r}',s')$. If we know the latter quantities, the QM average of $\hat{A}$ is calculated through $A = \langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_{s,s'=\uparrow,\downarrow}\int \mathrm{d}r\mathrm{d}r'\psi^*(\vec{r},s)A(\vec{r},s;\vec{r}',s')\psi(\vec{r}',s')$. It is often useful to represent those operators then as 2×2 matrices for the spin projections s,s', and the wave function as a spinor $\psi(\vec{r}) = \binom{\psi(\vec{r},\uparrow)}{\psi(\vec{r},\downarrow)}$. For instance, the matrix elements of the Hamiltonian of a free electron becomes a diagonal matrix

$$H(\vec{r},\vec{r}') = \begin{pmatrix} -\delta(\vec{r}-\vec{r}')\frac{-\hbar^2\nabla^2_{\vec{r}'}}{2m} & 0 \\ 0 & -\delta(\vec{r}-\vec{r}')\frac{-\hbar^2\nabla^2_{\vec{r}'}}{2m} \end{pmatrix} \tag{8}$$

[1] One may ask why do we think that only one such operator exists and what are we going to do in case we find two. Luckily none of us has ever been confronted to this situation yet.

[2] Meaning here an operator acting on a one particle wave function – not to be mixed up with the creation and annihilation operators acting on second-quantization vector states. From the mathematical point of view these two operators are different; in particular, they act in different spaces. However, there is a one-to-one correspondence between them, so in every-day's life we switch, e.g., from $\hat{H} = \sum_{i=1}^{N}\frac{\hat{p}_i^2}{2m}$ to $\hat{H} = \sum_{\vec{p}}\frac{p_i^2}{2m}\hat{a}^\dagger_{\vec{p}}\hat{a}_{\vec{p}}$ and back without mentioning that we are switching between "usual" (i.e., first quantization) operators and their second-quantization analogs.

Exercise 3: Current operator (6 points) In the first 3 problems, the calculation is done in the first quantization.

1. Show that (in the first quantization)

$$\text{for} \quad \hat{H} = \frac{\hat{p}^2}{2m} \quad \text{we have} \quad \hat{\vec{v}} = \frac{\hat{\vec{p}}}{m}. \tag{9}$$

2. Calculate $\hat{\vec{v}}$ for

$$\text{for} \quad \hat{H} = \frac{\hat{p}^2}{2m}\sigma_0 + a(\sigma_1 \hat{p}_y - \sigma_2 \hat{p}_x), \quad a = \text{const}, \tag{10}$$

where we have used the matrix notation for the spin projections $s, s' = \uparrow, \downarrow$, and

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{11}$$

Check that $\hat{\vec{v}} = \frac{\hat{\vec{p}}}{m}$.

3. Show that a charge current operator defined by $\hat{\vec{j}} = \frac{ie}{\hbar}[\hat{H}, \hat{\vec{r}}]$, obeys the charge conservation law $e\frac{\partial \hat{n}}{\partial t} + \operatorname{div} \hat{\vec{j}} = 0$. where $\hat{n}$ is the particle number operator and $e\hat{n}$ the charge density.

4. Rewrite $\hat{\vec{p}}$, $\hat{\vec{v}}$ and $\hat{\vec{j}}$ in the second quantized form.