Thermodynamic limit of the free 1DEG on a circle

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We derive the density matrix for a one dimensional free electron gas on a circle.

CONTENTS

I. A SIMPLE DERIVATION

Consider $N = 2p + 1$ (with $p = 0, 1, 2, 3, \dots$ free polarized fermions on a circle of circumference L.

At an inverse temperature β the density matrix for one of those fermions is,

$$
\begin{aligned}
\rho_1(x, y; \beta) &= \frac{1}{L}\theta_3\left(\frac{\pi}{L}(x-y), \exp(-\beta\lambda(\frac{2\pi}{L})^2)\right) \\
&= \lim_{q\to\infty} \frac{1}{L}\sum_{n=-q}^{q} \exp(-\beta\lambda(\frac{2\pi}{L})^2 n^2) \exp(-i\frac{2\pi}{L}n(x-y)) \\
&= \lim_{q\to\infty} k_q(x, y; \beta) \quad ,
\end{aligned}
\tag{1.1}
$$

where $\lambda = \hbar^2/(2m)$ and m is the fermions mass.

The density matrix of the N fermions is,

$$
\begin{aligned}
\rho(\mathbf{x}, \mathbf{y}; \beta) &= \frac{1}{N!}\det\{\rho_1(x_i, y_j; \beta)\}_{i,j=1}^N \\
&= \lim_{q\to\infty} \frac{1}{N!}\det\{k_q(x_i, y_j; \beta)\}_{i,j=1}^N \\
&= \lim_{q\to\infty} K_q(\mathbf{x}, \mathbf{y}; \beta) \quad ,
\end{aligned}
\tag{1.2}
$$

where $\mathbf{x} = (x_1, x_2, \dots, x_N)$, $\mathbf{y} = (y_1, y_2, \dots, y_N)$, and y_i, x_j are the initial and final positions of the fermions.

Notice that because of Pauli' s principle (see appendix),

$$
K_q = 0 \quad \text{when} \quad q < p \quad . \tag{1.3}
$$

For the particular case $q = p$ there is a simple expression for K_q, namely,

$$
\begin{aligned}
K_p(\mathbf{x}, \mathbf{y}; \beta) = \frac{1}{N!}\frac{2^{N(N-1)}}{L^N}\exp(-2\beta\lambda(\frac{2\pi}{L})^2\sum_{n=1}^{p} n^2) \\
\prod_{1\le i<j\le N} \sin(\frac{\pi}{L}(x_i - x_j))\sin(\frac{\pi}{L}(y_i - y_j)) \quad .
\end{aligned}
\tag{1.4}
$$

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This expression is the exact density matrix of the ground state (when $\beta \to \infty$) of the N fermions.

For example let' s find the partition function $Z(\beta)$ of the fermion system in the thermodynamic limit. We need to calculate the trace $Z_p(\beta)$ of $K_p(\mathbf{x}, \mathbf{y}; \beta)$ and then take p to infinity.

$$\begin{aligned} Z_p(\beta) &= \int_{-L/2}^{L/2} dx_1 \cdots \int_{-L/2}^{L/2} dx_N \, K_p(\mathbf{x}, \mathbf{x}; \beta) \\ &= \exp(-2\beta\lambda(\frac{2\pi}{L})^2 \sum_{n=1}^{p} n^2) \frac{1}{N!} \frac{2^{N(N-1)}}{(2\pi)^N} I_N \quad , \end{aligned} \tag{1.5}$$

where,

$$\begin{aligned} I_N &= \int_{-\pi}^{\pi} d\theta_1 \cdots \int_{-\pi}^{\pi} d\theta_N \prod_{1 \le i < j \le N} \sin^2((\theta_i - \theta_j)/2) \\ &= N! \frac{(2\pi)^N}{2^{N(N-1)}} \quad . \end{aligned} \tag{1.6}$$

So we get,

$$Z_p(\beta) = \exp(-2\beta\lambda(\frac{2\pi}{L})^2 \sum_{n=1}^{p} n^2) \quad . \tag{1.7}$$

Or for the free energy,

$$\begin{aligned} F_p(\beta) &= 2\lambda(\frac{2\pi}{L})^2 \sum_{n=1}^{p} n^2 \\ &= \frac{\pi^2}{3} \rho^2 \lambda \frac{N^2 - 1}{N} \quad . \end{aligned} \tag{1.8}$$

And in the thermodynamic limit,

$$f(\beta) = \lim_{p \to \infty} F_p(\beta)/N = \frac{\pi^2}{3} \rho^2 \lambda \quad . \tag{1.9}$$

As expected the free energy is independent of temperature in the thermodynamic limit. Moreover we found the expected results for the ground state energy

$$E_0 = \lambda L \int_{-k_F}^{k_F} k^2 \frac{dk}{2\pi} = \left(\frac{L}{2\pi}\right) \frac{2}{3} \lambda k_F^3 = N \left(\frac{\lambda \rho^2 \pi^2}{3}\right), \tag{1.10}$$

where the Fermi wave vector is $k_F = \pi\rho$.

But we see from equation (1.2) that in the thermodynamic limit (i.e. $p \to \infty$ and $\rho = N/L$ constant) it fails to give the exact density matrix of the fermions at finite inverse temperature β for which it is necessary to relax the constraint $q = p$ and respect the order of the two limits, first the one over q and only later the one over p.

Appendix A: A determinantal identity

Given three functions of two variables, K(x,y), L(x,y) and M(x,y) such that,

$$K(x, y) = \sum_{n=-\infty}^{\infty} L(x, n) M(n, y) \quad . \tag{A1}$$

Take the following product,

$$\begin{aligned} & K(x_1, y_{\pi 1}) K(x_2, y_{\pi 2}) \cdots K(x_n, y_{\pi n}) = \\ & \sum_{k_1, k_2, \ldots, k_n} [L(x_1, k_1) L(x_2, k_2) \cdots L(x_n, k_n)] \\ & \qquad [M(k_1, y_{\pi 1}) M(k_2, y_{\pi 2}) \cdots M(k_n, y_{\pi n})] \quad . \end{aligned} \tag{A2}$$

Summing appropriately with respect to all permutations we obtain,

$$\det\{K(x_i, y_j)\}_{i,j=1}^n = \sum_{k_1,k_2,\ldots,k_n} L(x_1, k_1)L(x_2, k_2)\cdots L(x_n, k_n)\det\{M(k_i, y_j)\}_{i,j=1}^n \quad . \tag{A3}$$

The region of summation can be decomposed in nonoverlapping regions Δ_ν characterized by the inequalities $k_{\nu 1} < k_{\nu 2} < \cdots < k_{\nu n}$, where ν is an arbitrary permutation of the set $(1, 2, \ldots, n)$ into itself.

Transforming the region Δ_ν by the change of variable $k_{\nu i} \to k_i$ $(i = 1, 2, \ldots, n)$ and collecting the resulting sums, we obtain, for the righthand side of (A3),

$$\sum_{k_1<k_2<\ldots<k_n} \sum_\nu (-)^{|\nu|} L(x_1, k_{\nu^{-1}1})L(x_2, k_{\nu^{-1}2})\cdots L(x_n, k_{\nu^{-1}n}) \det\{M(k_i, y_j)\}_{i,j=1}^n \quad , \tag{A4}$$

where the signature $(-)^{|\nu|}$ in each term appears as a consequence of rearranging the rows of $\det M$.

So we derived the following composition formula [1],

$$\det\{K(x_i, y_j)\}_{i,j=1}^n = \sum_{k_1<k_2<\ldots<k_n} \det\{L(x_i, k_j)\}_{i,j=1}^n \det\{M(k_i, y_j)\}_{i,j=1}^n \quad . \tag{A5}$$

Applied to the function k_q defined in (1.1) as,

$$k_q(\theta, \phi) = \sum_{n=-q}^{q} \mu_n e^{in\theta} e^{-in\phi} \quad , \tag{A6}$$

we see that for $q \geq (N-1)/2$,

$$\det\{k_q(\theta_i, \phi_j)\}_{i,j=1}^N = \mu_0 \prod_{n=1}^{q} |\mu_n|^2 \sum_{-q\leq k_1<k_2<\ldots<k_n\leq q} \det\{e^{ik_j\theta_i}\}_{i,j=1}^N \det\{e^{-ik_i\phi_j}\}_{i,j=1}^N \quad . \tag{A7}$$

So when $q = (N-1)/2$ the sum has only one term which is given by equation (1.4). And for $q < (N-1)/2$, $\det\{k_q\} = 0$.

[1] Which holds also after replacing the sums with integrals.