Thermodynamics of Fermions in One Dimension with a δ-Function Interaction*

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The equilibrium thermodynamics of a one-dimensional fermion system with a repulsive δ-function interaction is found to be derivable from the solution of a set of coupled integral equations. The equations for the attractive case are also given.

One of the interesting problems in the one-dimensional δ-function interaction model is the thermodynamics of the fermion system. For the boson system, the solution has been given by Yang and Yang.[1] In this paper we show that a similar procedure can be applied to solve the fermion case, though in the latter it is far more difficult to find all the excited states of the system. Here the Hamiltonian of the system is

$$H=-\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^{\,2}}+2c\sum_{i>j}\delta(x_i-x_j),\quad c>0, \tag{1}$$

and we will consider the case where the wave function belongs to the symmetry $[2^M 1^{N-2M}]$ of the permutation group. The ground-state energy of such a system is given by Yang[2] in solving the following algebraic equations:

$$e^{ipL}=\prod_{\Lambda'}\left(\frac{-p+\Lambda'-ic}{-p+\Lambda'+ic}\right), \tag{2a}$$

$$\prod_{p'}\left(\frac{-p'+\Lambda-ic'}{-p'+\Lambda+ic'}\right)=-\prod_{\Lambda'}\left(\frac{-\Lambda'+\Lambda-ic}{-\Lambda'+\Lambda+ic}\right),\quad c'=\tfrac{1}{2}c, \tag{2b}$$

where L is the length of the box. In the ground state, the p's and Λ's are real numbers. In the excited states, the Λ's might be complex. As regards the distribution of such Λ's in the complex plane, we make the following assumption, leaving its justification to be discussed in later publications. We assume that the Λ's are located in strings in the complex plane, that is, the Λ in a string is of the form

$$\Lambda=\xi+i\mu\eta+O(e^{-kL}),\quad \mu=-(m-1),\ -(m-3),\ \cdots,\ (m-1), \tag{3}$$

where $\eta=\frac{1}{2}c$, $k>0$ is a certain number, and ξ is real. The integer m defines the length of the string which contains m complex numbers. Thus the two numbers ξ and m (which depends on ξ) define a string uniquely. Using the notation $C(\xi,n)$ for such a string, we obtain from (2a) and (2b)

$$e^{ipL}=\prod_{C(\xi',n)}\left(\frac{-p+\xi'-in\eta}{-p+\xi'+in\eta}\right), \tag{4a}$$

$$\prod_{p'}\left(\frac{-p'+\xi-im\eta}{-p'+\xi+im\eta}\right)=(-1)^m\prod_{C(\xi',n)}{}'\left(\frac{-\xi'+\xi-i(n-m)\eta}{-\xi+\xi+i(n-m)\eta}\right)\left[\frac{-\xi'+\xi-i(n-m+2)\eta}{-\xi'+\xi+i(n-m+2)\eta}\,\frac{-\xi'+\xi-i(n-m+4)\eta}{-\xi'+\xi+i(n-m+4)\eta}\right.$$
$$\left.\times\cdots\frac{-\xi'+\xi-i(n+m-2)\eta}{-\xi'+\xi+i(n+m-2)\eta}\right]^2\left(\frac{-\xi'+\xi-i(n+m)\eta}{-\xi'+\xi+i(n+m)\eta}\right), \tag{4b}$$

where the product Π' extends to all the strings except $C(\xi,m)$. Taking the logarithms of (4a) and (4b) we have

$$\sum_{p'}\theta\left(\frac{\xi-p'}{m}\right)=2\pi J_\xi+\sum_{C(\xi',m)}\sum_{l}a_{mnl}\,\theta\left(\frac{\xi-\xi'}{n-l}\right), \tag{5a}$$

$$pL=2\pi I_p+\sum_{C(\xi',n)}\theta\left(\frac{\xi'-p}{n}\right), \tag{5b}$$

where $\theta(p)=2\tan^{-1}(p/\eta)$, J_ξ and I_p are integers or half-integers coming from the undetermined multiple of 2π in the logarithms, and

$$a_{mnl} = \begin{cases} 1 & \text{for } l=\pm m,\ l\neq m, \\ 2 & \text{for } l=-(m-2), -(m-4), \cdots (m-2), \\ 0 & \text{otherwise.} \end{cases} \tag{6}$$

Now we can approach the limit $N, M, L \to \infty$ proportionally, obtaining

$$\int_{-\infty}^{\infty} \theta'\left(\frac{\xi-p}{m}\right) \rho(p)dp = 2\pi(\sigma_m + \sigma_{m,h}) + \sum_n a_{mnl} \int_{-\infty}^{\infty} \theta'\left(\frac{\xi-\xi'}{n-l}\right) \sigma_n(\xi')d\xi', \tag{7a}$$

$$1 = 2\pi(\rho+\rho_h) - \sum_n \int_{-\infty}^{\infty} \theta'\left(\frac{p-\xi'}{n}\right) \sigma_n(\xi')d\xi', \tag{7b}$$

where

$$\begin{aligned} &N\sigma_m d\xi = \text{the number of } \xi\text{'s for strings } C(\xi'm) \text{ in the interval } [\xi, \xi+d\xi], \\ &N\sigma_{m,h} d\xi = \text{the number of "holes" for the above } \xi\text{'s in the interval } [\xi, \xi+d\xi], \text{ etc.,} \end{aligned} \tag{8}$$

and

$$E/L = \int_{-\infty}^{\infty} p^2\rho(p)dp, \quad N/L = \int_{-\infty}^{\infty} \rho dp, \tag{9a}$$

$$M/L = \sum_n \int_{-\infty}^{\infty} n\sigma_n(\xi)d\xi. \tag{9b}$$

From (7a) and (7b) one can easily obtain

$$1/2\pi = \rho + \rho_h - \tfrac{1}{2}\int_{-\infty}^{\infty} G_1(p-k)\rho dk + \tfrac{1}{2}\int_{-\infty}^{\infty} G_0(p-k)\sigma_{1,h}dk, \tag{10a}$$

$$\sigma_n + \sigma_{n,h} = \tfrac{1}{2}\int_{-\infty}^{\infty} G_0(p-k)(\sigma_{n+1,h} + \sigma_{n-1,h})dk, \quad n \geq 2, \tag{10b}$$

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} G_0(p-k)(\sigma_{n+1,h} - \sigma_{n,h}) = 0, \tag{10c}$$

$$\frac{N-2M}{L} = \lim_{n\to\infty} \int_{-\infty}^{\infty} \sigma_{n,h}dk, \tag{10d}$$

where $\sigma_{0,h} = \rho$ and

$$G_n(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{e^{-i\omega k}e^{-n\eta|\omega|}}{ch\eta\omega}\, d\omega. \tag{11}$$

One can now minimize the free energy $(E-TS)/L$ to obtain the equilibrium distribution ρ's and σ_m's. If one writes

$$\rho_h/\rho = \exp[\epsilon(p)/T], \quad \sigma_{m,h}/\sigma_m = \exp[\sigma_m(k)/T] \tag{12}$$

and makes the variation

$$\delta((E-TS)/L) = 0 \tag{13}$$

subject to the conditions

$$\delta(N/L) = 0, \quad \delta((N-2M)/L) = 0, \tag{14}$$

one obtains the following:

$$A = p^2 - \epsilon - \tfrac{1}{2}T\int_{-\infty}^{\infty} G_1(p-k)\ln(1+e^{-\epsilon/T})dk - \tfrac{1}{2}T\int_{-\infty}^{\infty} G_0(p-k)\ln(1+e^{\varphi_1/T})dk, \tag{15a}$$

$$\varphi_1 = \tfrac{1}{2}T\int_{-\infty}^{\infty} G_0(p-k)[\ln(1+e^{\varphi_1/T}) - \ln(1+e^{-\epsilon/T})]dk, \tag{15b}$$

$$\varphi_n = \tfrac{1}{2}T\int_{-\infty}^{\infty} G_0(p-k)\{\ln[1+\exp(\varphi_{n+1}/T)] + \ln[1+\exp(\varphi_{n-1}/T)]\}dk, \quad n \geq 2, \tag{15c}$$

$$B = \lim_{n\to\infty} \tfrac{1}{2}T\int_{-\infty}^{\infty} G_0(p-k)\{\ln[1+\exp(\varphi_{n+1}/T)] - \ln[1+\exp(\varphi_n/T)]\}dk, \tag{15d}$$

where A and B are the Lagrange multipliers for the conditions (14), respectively. B can be seen as magnetic field. Once ϵ and the φ_n's are obtained, one has

$$\rho=-(1/2\pi)(1+e^{\epsilon/T})^{-1}\partial\epsilon/\partial A, \tag{16a}$$

$$\sigma_{m,h}=-(1/2\pi)[1+\exp(-\varphi_m/T)]^{-1}\partial\sigma_{m}/\partial A. \tag{16b}$$

The free energy F and the pressure P are then given by

$$\frac{F}{L}=A\frac{N}{L}-\frac{T}{2\pi}\int_{-\infty}^{\infty}\ln(1+e^{-\epsilon/T})dk-B\left(\frac{N-2M}{L}\right), \tag{17a}$$

$$P=(T/2\pi)\int_{-\infty}^{\infty}\ln(1+e^{-\epsilon/T})dk. \tag{17b}$$

Other thermodyanmic quantities can be obtained readily.

One can easily show that in (15a)-(17b) the limit $c\to 0$ gives the result for a free-fermion gas, and the limit $c\to\infty$ gives the result for a free-fermion system where each single-particle energy level can only be occupied by either a spin-up or a spin-down particle. As $T\to 0$, (10a) and (10b) also go back to the equations of Yang.[2] Details of the exact solution of (15a)-(15d) will be published later.

One can obtain the fugacity and virial expansion by writing in (15a) and (15b)

$$\exp(-\epsilon/T)=\sum_{n=1}^{\infty}a_n(k,T)z^n,\quad \exp(\varphi_\nu/T)=\sum_{n=0}^{\infty}b_n^{(\nu)}z^n,\quad z=e^{A/T}, \tag{18}$$

and solve for a_n. In the case $B=0$, the pressure P is

$$P=\frac{(\pi T)^{1/2}}{2\pi}\left\{2z+z^2\left[2^{1/2}+2^{-1/2}\int_{-\infty}^{\infty}\frac{\eta}{\pi(\eta^2+p^2)}\exp\left(\frac{-2p^2}{T}\right)dp\right]+\cdots\right\}. \tag{19}$$

This agrees with the result obtained directly by the standard method. Higher-order terms in the virial expansion can be obtained systematically also.

We have also obtained the thermodyanmics of the repulsive fermion-boson mixture, of fermions in the attractive case, and of fermions with higher spins in both the repulsive and attractive cases. For attractive fermions of spin $\frac{1}{2}$ we obtain

$$2(p^2-\eta^2)-\epsilon+T\int_{-\infty}^{\infty}K_2\ln(1+e^{-\epsilon/T})dk+T\int_{-\infty}^{\infty}K_1\ln(1+e^{-\psi/T})dk=2A,$$

$$p^2-\psi+T\int_{-\infty}^{\infty}K_1\ln(1+e^{-\epsilon/T})dk+\tfrac{1}{2}T\int_{-\infty}^{\infty}G_1\ln(1+e^{-\psi/T})dk-\tfrac{1}{2}T\int_{-\infty}^{\infty}G_0\ln(1+e^{\varphi_1/T})dk=A,$$

$$\tfrac{1}{2}T\int_{-\infty}^{\infty}G_0\ln[1+\exp(\varphi_{\nu+1}/T)]\,dk+\tfrac{1}{2}T\int_{-\infty}^{\infty}G_0\ln[1+\exp(\varphi_{\nu-1}/T)]\,dk-\varphi_\nu=0,\quad \nu\geq 1,$$

$$\lim_{\nu\to\infty}\tfrac{1}{2}T\int_{-\infty}^{\infty}G_0\{\ln[1+\exp(\varphi_\nu/T)]-\ln[1+\exp(\sigma_{\nu-1}/T)]\}\,dk=B, \tag{20}$$

where $\varphi_0=\psi$, $K_n(x)=(2\pi)^{-1}2n\eta(n^2\eta^2+x^2)^{-1}$, and

$$\sigma_{\nu,h}=(2\pi)^{-1}[1+\exp(-\varphi_\nu/T)]^{-1}\partial\varphi/\partial A,\quad \rho=-(2\pi)^{-1}(1+e^{\epsilon/T})^{-1}\partial\epsilon/\partial A. \tag{21}$$

The energy and free energy are found from the following equations:

$$\tau=-(2\pi)^{-1}(1+e^{\psi/T})^{-1}\partial\psi/\partial A,\quad (N-2M)/L=\lim_{\nu\to\infty}\int_{-\infty}^{\infty}\sigma_{\nu,h}dp,\quad E/L=\int_{-\infty}^{\infty}p^2\tau dp+2\int_{-\infty}^{\infty}(p^2-\eta^2)\rho dp,$$

$$N/L=\int_{-\infty}^{\infty}\tau dp+2\int_{-\infty}^{\infty}\rho dp,\quad \frac{F}{L}=A\frac{N}{L}-\frac{T}{\pi}\int_{-\infty}^{\infty}\ln(1+e^{-\epsilon/T})dk-\frac{T}{2\pi}\int_{-\infty}^{\infty}\ln(1+e^{-\psi/T})dk-B\left(\frac{N-2M}{L}\right). \tag{22}$$

For a fermion-boson mixture[3] with M_1 fermions of species 1, M_2 fermions of species 2, and M_b

bosons, we obtain

$$A = p^2 - \epsilon - \tfrac{1}{2}T\int_{-\infty}^{\infty} G_1 \ln(1+e^{-\epsilon/T})dk - \tfrac{1}{2}T\int_{-\infty}^{\infty} G_1 \ln(1+e^{-\psi/T})dk - \tfrac{1}{2}T\int_{-\infty}^{\infty} G_0 \ln[1+\exp(\varphi_1/T)]\,dk,$$

$$C = -\psi + A - p^2 + \epsilon,$$

$$\varphi_1 = \tfrac{1}{2}T\int_{-\infty}^{\infty} G_0\{\ln[1+\exp(\varphi_2/T)] - \ln(1+e^{-\epsilon/T}) - \ln(1+e^{-\psi/T})\}\,dk,$$

$$\varphi_n = \tfrac{1}{2}T\int_{-\infty}^{\infty} G_0\{\ln[1+\exp(\varphi_{n+1}/T)] + \ln[1+\exp(\varphi_{n-1}/T)]\}\,dk, \quad n \geq 2,$$

$$B = \lim_{n\to\infty} \tfrac{1}{2}T\int_{-\infty}^{\infty} G_0\{\ln[1+\exp(\varphi_{n+1}/T)] - \ln[1+\exp(\varphi_n/T)]\}\,dk, \tag{23}$$

with

$$\rho = -(2\pi)^{-1}(1+e^{\epsilon/T})^{-1}\partial\epsilon/\partial A, \quad \tau = -(2\pi)^{-1}(1+e^{\psi/T})^{-1}\partial\psi/\partial A, \quad \sigma_{n,h} = -(2\pi)^{-1}[1+\exp(\varphi_n/T)]^{-1}\partial\varphi_n/\partial A;$$

and

$$E/L = \int_{-\infty}^{\infty} p^2\rho(p)dp, \quad N/L = (M_1+M_2+M_b)/L = \int_{-\infty}^{\infty}\rho dp, \tag{24}$$

$$M_b/L = \int_{-\infty}^{\infty}\tau dp, \quad (M_1-M_2)/L = \lim_{n\to\infty}\int_{-\infty}^{\infty}\sigma_{n,h}dp,$$

$$\frac{F}{L} = A\frac{N}{L} + C\frac{M_b}{L} - \frac{T}{2\pi}\int_{-\infty}^{\infty}\ln(1+e^{-\epsilon/T})dk - B\left(\frac{M_1-M_2}{L}\right). \tag{25}$$

All the details will be published elsewhere.

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Strain-Induced Inhomogeneity of the Surface Potential on Freshly Cleaved Semiconductor Surfaces*

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Photoelectric emission and work-function measurements on GaSb have shown that the surface potential, and therefore the band bending and work function, of freshly cleaved surfaces present variations of up to 0.5 eV over macroscopic distances along the surface. These properties vary over a period of several days at room temperature in the sense that band bending increases and inhomogeneities disappear, suggesting annealing of cleavage-induced strains or defects. The electron affinity and ionization energy of freshly cleaved surfaces are well defined: They do not present spatial or temporal variation. Related observations were made on InP and GaAs.

Cleavage in ultrahigh vacuum[1] is a classical method for preparing clean and well-defined semiconductor surfaces. It has the advantage of being simple and of producing unquestionably clean surfaces with unchanged doping and stoichiometry of the material in their vicinity. Such surfaces also produce excellent low-energy electron-diffraction patterns which, however, often