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Average Partition Function for an Electron in Frisch-Lloyd Model

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Some additional justification and clarification about the divergence of the partition function of the attractive Frisch-Lloyd model are presented.

Luttinger and Friedberg have developed a path-integral method[1] to study the "partition function" and therefore the density of states for disordered systems. By using this method to Frisch-Lloyd system,[2] it was found that the partition function diverges when the δ-functions are attractive.[3),4)] But there still remain points which should be clarified.

First, it is claimed that "the Frisch-Lloyd model for attractive δ-function does not represent a stable model for a physical system" in Ref. 3). In fact, this statement is not quite correct. Since the partition function by the path-integral method is a single particle partition function, as far as we treat the electrons as Boltzmann gas, the system will be unstable.

For a "Boltzmann" electron gas system, the N-particle partition function of the model system $Z_N(\beta)$ is given by $(z(\beta))^N/N!$, where $z(\beta)$ is the single particle partition function by the path-integral method. Therefore the divergence of $z(\beta)$ implies the divergence of the free energy of the "Boltzmann" electron gas moving in the disordered model system. However, if we treat electrons as fermions, the divergence of the single particle partition function does not necessarily imply the non-existence of the free energy of the Fermi gas. In fact, if Fermi-Dirac statistics are used for the electrons moving in the Frisch-Lloyd disordered system, there is no problem with the instability of the model. It is the exclusion principle which prevents particles from going into the same state and therefore stabilizes the model system. Basically, it is a question of convergence of a certain integral. The grand partition function of a Fermi-Dirac system is given by $Q=e^{-\beta\Omega}$, and

$$\Omega=\frac{1}{\beta}\int_{-\infty}^{+\infty}g(\varepsilon)\ln(1+e^{-\beta(\varepsilon-\mu)})d\varepsilon\ ,$$

where $g(\varepsilon)$ is the single particle density of states. As $\varepsilon\to-\infty$, it is given by[3)]

$$g(\varepsilon)\sim e^{-c|\varepsilon|^{1/2}\ln|\varepsilon|}\ ,$$

and $\ln(1+e^{-\beta(\varepsilon-\mu)})\to-\beta(\varepsilon-\mu)$ for $\varepsilon<\mu$, as $\varepsilon\to-\infty$, so near the lower limit, the contribution to Ω is finite, because the integral is finite at the lower limit. This assumes $T\neq0$, but it is also true for $T=0$, because

$$\Omega\underset{\beta\to\infty}{\to}\int_{-\infty}^{\mu_0}g(\varepsilon)(\varepsilon-\mu_0)d\varepsilon\quad\text{for }T\to0$$

which also converges at the lower limit and μ_0 is a finite quantity too.[5)]

The second point is: the final result of Ref. 1) is used in Ref. 4), and it should be noted that, in order to arrive at (2·52) and (2·53) from (2·30)~(2·33) in Ref. 1), one must make perturbation approximation and low temperature approximation to calculate the Q as in (2·46) and (2·47). In order to show that the same result could be obtained without making these approximations, i.e., the divergence of the single particle partition function is not coming from these approximations, we work directly with Eqs. (2·30)~(2·33) in Ref. 1), and follow the argument of Ref. 4). According to Ref. 4), we assume that the effective potential is of the form $-\lambda\delta(x)$. We calculate the partition function $z(\beta)$ from the Green's function formula (2·30)~(2·33) directly instead of solving the effective Schrödinger equation. Therefore, we give a more rigorous justification for the conclusion of Ref. 4).

According to the formula (2·30)~(2·33) in Ref. 1), the partition function of a random system is given by

$$\frac{z(\beta)}{z_0(\beta)} \geqq e^{\langle A\rangle_\phi}\langle e^{-\phi}|0\rangle\,,$$

where

$$\langle A\rangle_\phi = \rho\int_\infty\left(1-\frac{G_\beta(0,0|\phi+v_R)}{G_\beta(0,0|\phi)}\right)dR + \frac{\partial}{\partial\mu}\ln G_\beta(0,0|\mu\phi)|_\mu=1\,.$$

The equation that governs the Green's function G_β is

$$-\frac{1}{2}\frac{d^2}{dx^2}G_\beta(x,0|\phi)-\lambda\delta(x)G_\beta(x,0|\phi) = -\frac{\partial}{\partial\beta}G_\beta(x,0|\phi).$$

Its solution is given by

$$G_\beta(x,0|\phi)=\lambda\int_0^\beta d\beta'\,G_{\beta'}(x=0,0|\phi)\times\frac{1}{\sqrt{2\pi(\beta-\beta')}}e^{-x^2/2(\beta-\beta')}+\frac{1}{\sqrt{2\pi\beta}}e^{-x^2/2\beta}\,.$$

We may solve $G_\beta(x=0,0|\phi)$ by Laplace transform technique. The result is given by

$$G_\beta(x=0,0|\phi)=1/\sqrt{2\pi\beta} + \frac{\lambda}{2}e^{\lambda^2\beta/2}\,\mathrm{Erfc}(-\lambda\sqrt{\beta}/2 \equiv g_\phi(\beta),$$

where Erfc(x) is the complimentary error function. According to Kac formula, we obtain $\langle e^{-\phi}|0\rangle=(2\pi\beta)^{1/2}G_\beta(0,0|\phi)$. By the same procedure, we also obtain

$$G_\beta(0,0|\mu\phi)\equiv g_{\mu\phi}(\beta)=1/\sqrt{2\pi\beta}+\frac{\mu\lambda}{2}e^{(\mu\lambda)^2\beta/2}\times\mathrm{Erfc}(-\mu\lambda\sqrt{\beta}/2).$$

Hence, we find

$$\frac{\partial}{\partial\mu}\ln G_\beta(0,0|\mu\phi)|_{\mu=1} = \frac{(1+\lambda^2\beta)\left[\frac{\lambda}{2}e^{\lambda^2/2}\,\mathrm{Erfc}\left(-\lambda\frac{\sqrt{\beta}}{2}\right)\right]+\left[\frac{\lambda^2}{\sqrt{2\pi}}\sqrt{\beta}\right]}{(2\pi\beta)^{-1/2}-\frac{\lambda}{2}e^{\lambda^2\beta/2}\,\mathrm{Erfc}\left[-\lambda\frac{\sqrt{\beta}}{2}\right]}.$$

Now, we have to find $G_\beta(0,0|\phi+v_R)$. For this purpose, let us simplify the notation by defining

$$\tilde{G}(x,\beta)\equiv G_\beta(0,x|\phi+v_R),$$
$$\tilde{g}(\beta)\equiv\tilde{G}(x=0,\beta),\quad \tilde{h}(\beta)\equiv\tilde{G}(x=R,\beta).$$

The equation satisfied by $\tilde{G}(x,\beta)$ is

$$-\frac{1}{2}\frac{d^2}{dx^2}\tilde{G}-\lambda\delta(x)\tilde{G}(x,\beta) - v_0\delta(x-R)\tilde{G}(x,\beta) = -\frac{\partial}{\partial\beta}\tilde{G}(x,\beta).$$

By Fourier transform technique, we obtain

$$\tilde{G}(x,\beta)=\frac{1}{\sqrt{2\pi\beta}}e^{-(x^2/2\beta)} + \lambda\int_0^\beta\tilde{g}(\beta')\frac{1}{\sqrt{2\pi(\beta-\beta')}}\times e^{-(x^2/2(\beta-\beta'))}d\beta' + v_0\int_0^\beta\tilde{h}(\beta')\frac{1}{\sqrt{2\pi(\beta-\beta')}}\times e^{-((x-R)^2/2(\beta-B'))}d\beta'\,.$$

Setting $x=0$ and $x=R$ in the above equation, we have a pair of equations:

$$\tilde{g}(\beta)=\frac{1}{\sqrt{2\pi\beta}} + \lambda\int_0^\beta d\beta'\,\tilde{g}(\beta')\frac{1}{\sqrt{2\pi(\beta-\beta')}}$$

$$+v_0\int_0^{\beta}d\beta'\tilde{h}(\beta')\frac{e^{-(R^2/2(\beta-\beta'))}}{\sqrt{2\pi(\beta-\beta')}},$$

$$\tilde{h}(\beta)=\frac{1}{\sqrt{2\pi\beta}}e^{-(R^2/2\beta)}$$
$$+\lambda\int_0^{\beta}d\beta'\frac{\tilde{g}(\beta')}{\sqrt{2\pi(\beta-\beta')}}e^{-(R^2/2(\beta-\beta'))}$$
$$+v_0\int_0^{\beta}d\beta'\frac{\tilde{h}(\beta')}{\sqrt{2\pi(\beta-\beta')}}.$$

The solution of these equations can be obtained by Laplace transformation as follows:

$$\tilde{g}(\beta)=g(\beta)+\mathcal{L}^{-1}\left\{\frac{v_0e^{-\sqrt{2s}|R|}\tilde{h}(s)}{\sqrt{2s}-1}\right\}$$

and

$$\tilde{h}(s)=(2\sqrt{\pi s}\,e^{-\sqrt{2s}|R|})/(2s-\sqrt{2s}\,v_0-\sqrt{2s}\,\lambda+\lambda v_0-\lambda v_0e^{-\sqrt{2s}|R|}).$$

As a result, the integral

$$\int_{-\infty}^{+\infty}dR\left(1-\frac{G_\beta(0,0|\phi+v_R)}{G_\beta(0,0|\phi)}\right)$$

can be written as

$$\frac{1}{\lambda g(\beta)}\mathcal{L}^{-1}\left\{\frac{1}{\sqrt{2s}-\lambda}\times\ln\left[\frac{(\sqrt{2s}-\lambda)(\sqrt{2s}-v_0)}{\sqrt{2s}(\sqrt{2s}-\lambda-v_0)}\right]\right\}.$$

Now, let us use the following theorems:

THOREM I:

If $f(s)=\mathcal{L}(F(t))$, then

$$2^{n/2}\pi^{1/2}s^{1/2(n-1)}f(\sqrt{s})\underset{\mathcal{L}^{-1}}{\overset{\mathcal{L}}{\rightleftarrows}}t^{-1/2(n+1)}\times\int_0^{\infty}due^{-u^2/4t}\,\mathrm{He}_n\left(u\frac{1}{\sqrt{2t}}\right)F(u),$$

where He_n is Hermite polynomial which is defined as

$$\mathrm{He}_n(x)=n!\sum_{m=0}^{n/2}\frac{(-1)^m x^{n-2m}}{m!(n-2m)!}.$$

THEOREM II:

If $f(s)=\mathcal{L}(F(t))$, then $f(2s)\underset{\mathcal{L}^{-1}}{\overset{\mathcal{L}}{\rightleftarrows}}1/2F(t/2)$ and saddle point approximation, we can obtain

$$\int_{-\infty}^{+\infty}dR\left(1-\frac{{}^{G}V_R+\phi}{G_\phi}\right)\simeq\frac{2}{\lambda\sqrt{\pi}}\ln\left(\frac{\lambda-v_0}{\gamma\lambda v_0}\right)-\frac{1}{\lambda}\ln(\lambda\beta)+\frac{e^{\beta(\lambda v_0+v_0^2/2)}}{\beta\lambda^2v_0}.$$

For β large, we have

$$-\langle A\rangle_\phi=-\frac{2\rho}{\lambda\sqrt{\pi}}\ln\left(\frac{\lambda-v_0}{\gamma\lambda v_0}\right)+\frac{\rho}{\lambda}\ln(\lambda\beta)-\frac{\rho}{\beta\lambda^2v_0}e^{\beta(\lambda v_0+v_0^2/2)}-\beta\lambda^2.$$

Therefore

$$I(\beta)\geqq e^{-\langle A\rangle_\phi\langle e^{-\phi}|0\rangle_\beta}=\sqrt{2\pi\beta}\exp\left\{-\beta\frac{\lambda^2}{2}+\frac{\rho}{\lambda}\ln(\lambda\beta)-\frac{\rho}{\beta\lambda^2v_0}e^{\beta(\lambda v_0+(v_0/2))}-\frac{2}{\lambda\sqrt{\pi}}\ln\left(\frac{\lambda-v_0}{\gamma\lambda v_0}\right)\right\}.$$

If we try to maximize the exponent of the above equation, we find that there is no best self-consistent vale of λ except $\lambda=\infty$. We therefore reach the same conclusion as before,[3),4)] that the single particle partition function diverges for the attractive Frisch-Lloyd random system.

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3) J. M. Luttinger, Phys. Rev. **B13** (1976), 4555.
4) Chin-Yuan Lu, J. of Phys. **C12** (1979), 3687.
5) private communication with J. M. Luttinger.