Large deviations in rarefied quantum gases

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Abstract: *The probability of observing a large deviation (LD) in the number of particles in a region Λ in a dilute quantum gas contained in a much larger region V is shown to decay as* $\exp[-|\Lambda|\Delta F]$*, where $|\Lambda|$ is the volume of Λ and ΔF is the change in the appropriate free energy density, the same as in classical systems. However, in contrast with the classical case, where this formula holds at all temperatures and chemical potentials our proof is restricted to rarefied gases, both for the typical and observed density, at least for Bose or Fermi systems. The case of Boltzmann statistics with a bounded repulsive potential can be treated at all temperatures and densities. Fermions on a lattice in any dimension, or in the continuum in one dimension, can be treated at all densities and temperatures if the interaction is small enough (depending on density and temperature), provided one assumes periodic boundary conditions.*

1. Introduction.

We study the probability distribution of the number of particles in a box Λ for a quantum system in a region $V \supset \Lambda$ described by a grand-canonical ensemble with reciprocal temperature β and chemical potential μ. We are primarily interested in the case where the volume of V is much larger than that of Λ, $|V| >> |\Lambda|$, i.e. in properties remaining valid in the thermodynamic limit $V \to \mathbb{R}^d$ with μ, β fixed and $|\Lambda|/|V| \to 0$. The particles interact with a pair potential $v(x-y)$ so the Hamiltonian of the system is given by

1.1
$$H_V = \sum_{i=1}(-\frac{1}{2}\Delta_{x_i} - \mu) + \sum_{i<j} v(x_i - x_j), \quad x_i \in V \tag{1.1}$$

where the Laplace operator is considered with Dirichlet boundary conditions on the walls of V, which we assume for simplicity to be a cube with side length L (centered at the origin), or with periodic boundary conditions in the Fermionic case at small v considered in sec. 7. The analysis in sections 3–6 carries over to the cases of Neumann, periodic or mixed boundary conditions and for most (reasonable) shapes of the containers V and Λ. This does not imply that effects of the boundary conditions in quantum systems are well understood: it just means that in sections 3–6 we do not consider values of μ and T where phase transitions are possible. In fact the cases considered in sec. 7. make essential use of the periodicity in the boundary conditions.

The potential $v(x)$ is assumed to vanish for $|x| > D$ and to be bounded, smooth and stable. The particles will be assumed to obey either Boltzmann, Bose or Fermi statistics. Hard core interactions can also be treated, leading to results analogous to those of Sections 3–6 but the Fermionic cases in Section 7 would require new ideas in the presence of hard cores. For simplicity we do not consider this type of interaction here.

The number of particles in a region Λ which, again for the sake of simplicity, we take to be a cube of side length ℓ centered at the origin is given by $N_\Lambda(\underline{x}) = \sum_i \chi_\Lambda(x_i)$ where $\underline{x} = (x_1, \ldots)$ denotes a configuration of particles in V and χ_Λ is the indicator function of the box Λ ($\chi_\Lambda(x) = 1$ if $x \in \Lambda$ and $\chi_\Lambda(x) = 0$ otherwise). The dimension of the space will be taken $d = 3$ but our analysis holds in any dimension. The probability of finding exactly n particles in the box Λ is then given by

1.2
$$\Pi(n) = \frac{\mathrm{Tr}\,\delta_n e^{-\beta H_V}}{\mathrm{Tr}\,e^{-\beta H_V}} \tag{1.2}$$

where $\delta_n(\underline{x}) = 1$ if $N_\Lambda(\underline{x}) = n$ and 0 otherwise.

We note that formally the only difference in $\Pi(n)$ between quantum and classical systems, is the nature of the probability distribution of configurations $\underline{x}$ in V. For a classical system this is given by a Gibbs measure while for a quantum system it has to be computed via the density matrix.

The pressure P, Helmholtz free energy f and expected density ρ at temperature β^{-1} and chemical potential μ are given as usual by

1.3
$$\beta P(\beta,\mu)=\lim_{L\to\infty} L^{-d}\log\,\mathrm{Tr}\, e^{-\beta H_V},\qquad \beta f(\beta,\rho)=\inf_{\mu}\{\beta\mu\rho-\beta P(\beta,\mu)\} \tag{1.3}$$

We shall restrict our analysis to values of β,μ where the above functions are differentiable and the extremum is achieved at a single point $\mu=\mu(\beta,\rho)$ so that the expected particle density in V

1.4
$$\rho=\frac{\partial}{\partial\mu}P(\beta,\mu),\qquad \mu=\frac{\partial}{\partial\rho}f(\beta,\rho) \tag{1.4}$$

We call the region in which this differentiability holds the "no phase transitions region". This is a larger region than the region $\mathcal{A}(\mathcal{G})$ where the functions P,ρ,f have been proved by Ginibre, see the review [Gi71], to be analytic in $z=e^{\beta\mu}$: a disk in the z–plane with radius $R(\beta)>0$ (an estimate for $R(\beta)$ is quoted later, see (3.4)). The region $\mathcal{A}(\mathcal{G})$ is also a region where upper and lower bounds on the derivatives $\frac{\partial P}{\partial\rho},\frac{\partial f}{\partial\mu}$ can be established:

Let

1.5
$$\begin{aligned}\Delta F(\beta,\rho,\rho_0)&\stackrel{def}{=} f(\beta,\rho)-f(\beta,\rho_0)-\frac{\partial f(\beta,\rho)}{\partial\rho}\Big|_{\rho=\rho_0}(\rho-\rho_0)\\&=[f(\beta,\rho)-\mu(\beta,\rho_0)\rho]-[f(\beta,\rho_0)-\mu(\beta,\rho_0)\rho_0]\end{aligned}, \tag{1.5}$$

ΔF is the difference between the Helmholtz free energy at density ρ and its linear extrapolation from ρ_0 (which is positive where (1.4) holds if $\rho\neq\rho_0$). We shall prove that the probability of finding a density ρ in Λ, when the expected density in V is ρ_0, is given asymptotically by

1.6
$$\Pi(n\simeq\rho\ell^d)\sim e^{-\beta\Delta F(\beta,\rho,\rho_0)\,\ell^d} \tag{1.6}$$

for large ℓ, provided $\rho-\rho_0$ is small enough. More mathematically this is stated as follows:

Let β,μ be fixed in the analyticity region $\mathcal{A}(\mathcal{G})$ and let ρ_0 be the corresponding density (so that $\rho_0=\rho(\beta,\mu)$). If the side ℓ of the box Λ tends to infinity and, correspondingly, the container side also tends to infinity so that $L/\ell\to\infty$ then

1.7
$$\lim_{\ell\to\infty}\ell^{-d}\log\sum_{\tilde\rho\in[a,b]}\Pi(\tilde\rho\ell^d)=\max_{\tilde\rho\in[a,b]}-\beta\,\Delta F(\beta,\tilde\rho,\rho_0) \tag{1.7}$$

This holds for all statistics if the interval $[a,b]$ is contained in an interval $[-\delta_0(\beta,\mu),\delta_0(\beta,\mu)]$ centered at ρ_0 with $\delta_0(\beta,\mu)>0$ small enough (estimated in (3.4)).

In Section 5 we obtain (1.7) by proving its finite ℓ version (which contains various finite size corrections). We then prove, in 6, a similar result for Boltzmann Statistics with arbitrary (β,μ), $\beta>0$ assuming a bounded repulsive (*i.e.* positive) interaction v: this extends the validity of (1.6) far beyond the analyticity region $\mathcal{A}(\mathcal{G})$. We can also treat Bose statistics in a region somewhat larger than $\mathcal{A}(\mathcal{G})$ but still under the very restrictive assumption that $e^{\beta\mu+2\beta B}<1$ where B is the stability constant of the interaction potential v, *i.e.* $\sum_{i<j=1}^n v(x_i-x_j)>-Bn$ for all $(x_1,\ldots,x_n)$. Our method does not seem extendable to more general Bosonic systems in spite of the strong results of Park, sec. 5 of [Pa85].

A further extension in Section 7, using completely different techniques (see [GM00] for a review), deals with weakly interacting Fermi systems on a lattice: given β,ρ_0 the above theorem holds if the interaction potential is small enough (depending on density and temperature) and if *periodic boundary conditions are assumed on the container V*. The results can also be extended to continuum systems in $d = 1$. They hold for values of μ, where the method of Sec. 2-6 fails.

The above restrictions always exclude the region in β, μ where genuine quantum phase transitions may occur (like superfluidity or superconductivity). Substantial further work appears necessary to deal with this regime despite the fact that the ideal Fermi and Bose gas (no interactions) can be treated completely by other methods, see [LLS99].

2. The Ginibre representation.

The key technical ingredient in our analysis is the Ginibre representation of the quantum partition functions, [Gi71]. We describe here only that part of the formalism which we need to derive our results.

Let $\Omega = (x, \omega)$ be a Brownian path starting at x at $t = 0$ and returning to x at a later time b: this is a continuous function $t \to \omega(t) \in \mathbb{R}^d$ defined for $t \in [0, b]$. The time length b will be fixed as $b = \beta$ in the case of Boltzmann statistics but it will take the values $b = \beta, 2\beta, 3\beta, \ldots$ in the case of Bose or Fermi statistics.

Functions of Ω will be integrated with a measure $d\Omega$ which is defined as $d\Omega = dx \cdot P_{xx}(d\omega)$ in terms of the *conditional Wiener measures* $P^b_{xy}(d\omega)$ (see [Gi71] p. 343);[1]

2.1
$$\int F(\Omega) d\Omega \overset{def}{=} \sum_{j=1}^{*} \frac{(-1)^{(j-1)\sigma}}{j} \int dx \int P^{j\beta}_{xx}(d\omega) F(\Omega) \tag{2.1}$$

where, see [Gi71] p.361, the statistics are distinguished by the upper limit $*$ and the sign exponent σ as

2.2
$$\begin{cases} * = 1 & \text{Boltzmann statistics} \\ * = \infty,\ \sigma = 0 & \text{Bose statistics} \\ * = \infty,\ \sigma = +1 & \text{Fermi statistics} \end{cases} \tag{2.2}$$

and the integration is over all $x \in V$ and $\omega(t) \in V$ for all t.

For $\Omega_k = (x_k, \omega_k)$ such that ω_k has time length $j_k\beta$ we imagine that ω_k consists of j_k strings, each of time length β with the i–th string denoted by $\omega_{k,i}(t) = \omega_k(i\beta + t)$, $t \in [0, \beta]$. We can consider each bit of string of length β as a "particle" and the collection $\underline{\Omega} = (\Omega_1, \ldots, \Omega_n)$ as "trajectory configurations" or as "configurations of particles delocalized by quantum indeterminacy" The "energy" of a configuration $\underline{\Omega}$ is then defined as

2.3
$$U(\underline{\Omega}) = \frac{1}{2\beta} \sum_{(k,i) \neq (k',i')} \int_0^\beta v(\omega_{k,i}(t) - \omega_{k',i'}(t))\, dt \tag{2.3}$$

which is consistent with the intuitive delocalization interpretation above in which the "number of particles" in the configuration $\underline{\Omega}$ is simply $j_1 + \ldots + j_n$. It is convenient to introduce two notions of number of particles of $\underline{\Omega}$ inside Λ as

2.4
$$N_\Lambda(\underline{\Omega}) = \sum_{(k,i)} \chi_\Lambda(\omega_{k,i}(0)), \qquad \tilde{N}_\Lambda(\underline{\Omega}) = \beta^{-1} \sum_{(k,i)} \int_0^\beta \chi_\Lambda(\omega_{k,i}(t))\, dt \tag{2.4}$$

and note that $N_\Lambda(\underline{\Omega})$ is an integer while $\tilde{N}_\Lambda(\underline{\Omega})$ is generally not, except that $\tilde{N}_V(\underline{\Omega}) = N_V(\underline{\Omega})$ is always so.

[1] This is simply defined to be the measure on the paths starting at x and ending at y in a time b formally given by $P^b_{xy}(d\omega) \overset{def}{=} P_x(d\omega)\delta(\omega(b) - y)$ where $P_x(d\omega)$ is the usual Wiener distribution

The remarkable representation for the grand canonical partition function (due to Ginibre) is,

2.5 $$Z(\beta,\mu;V)\stackrel{def}{=}\operatorname{Tr}e^{-\beta H_V}=\sum_{n=0}^\infty\int_{N_V(\underline{\Omega})=n} z^n\,e^{-\beta U(\underline{\Omega})}\,\frac{d\,\underline{\Omega}}{n!} \tag{2.5}$$

where $\underline{\Omega}=(\Omega_1,\ldots,\Omega_n)$ and $z\stackrel{def}{=}e^{\beta\mu}$ defines the *activity.* (2.5) makes the quantum partition function look like the classical partition function of a gas of closed contours of length roughly $\sqrt{\beta}$ for all values of z in the Boltzmann statistics and for $ze^{2\beta B}<1$ in the Bose and Fermi case; B is a stability constant defined by $U(x_1,\ldots,x_n)\ge -Bn,\forall n$.

Remarkably, the quantum reduced density matrices also admit a natural "classical" representation in terms of the above contours but we shall not need such a representation here, see [Gi71].

3. The cluster expansion for rarefied gases.

One of the important consequences of the above classical representation of a quantum system is that it immediately allows us to take advantage of the techniques developed to study Mayer and virial expansions of classical gases. The basic remark is that it is "easy" to take the logarithm of a classical partition function. By simple algebraic considerations the logarithm is obtained as a formal power series in z and the difficult part is to show the convergence of such an expansion.

The formal power series expression of the grand canonical pressure $\beta P(\beta,\mu)$, defined in (1.3) is obtained in the form:

3.1 $$\log Z(\beta,\mu,V)=\beta P(\beta,\mu;V)=\sum_{n=0}^\infty\int_{N_V(\underline{\Omega})=n} z^n\,\Phi^T(\underline{\Omega})\,\frac{d\,\underline{\Omega}}{n!}, \tag{3.1}$$

The r.h.s. of (3.1) still looks like a partition function with $\Phi^T(\underline{\Omega})$ replacing $e^{-\beta U(\underline{\Omega})}$, see eq. (4.15) in [Gi71]. However, *unlike* the functions $e^{-\beta U(\underline{\Omega})}$, the functions $\Phi^T(\underline{\Omega})$ have the "*cluster property*" of "decay" at infinity, i.e. if $\underline{\Omega}=(\underline{\Omega}',\underline{\Omega}'')$ consists of trajectories $\underline{\Omega}'=(\Omega'_1,\ldots,\Omega'_{n'})$, $\underline{\Omega}''=(\Omega''_1,\ldots\Omega''_{n''})$ with $(\underline{\Omega}',\underline{\Omega}'')\stackrel{def}{=}(\Omega'_1,\ldots,\Omega'_{n'},\Omega''_1,\ldots\Omega''_{n''})$, then

3.2 $$|\Phi^T(\underline{\Omega}',\underline{\Omega}'')|=0\qquad\text{if } d(\underline{\Omega}',\underline{\Omega}'')>D \tag{3.2}$$

where $d(A,B)$ is the distance of two sets A,B and the trajectories are considered here as the union of the sets of points they occupy as time varies. This is an elementary property that follows from the explicit expression for the functions Φ^T in terms of "Mayer graphs", see eq. (4.3) in [Gi71] (see also [GMM71], eq. (4.2) and (4.3) at p. 176, for a similar simpler case).

The functions $\Phi^T(\underline{\Omega})$ are like the functions $e^{-\beta U(\underline{\Omega})}$ *translation invariant* in the sense that they have the same value for $\underline{\Omega}$ and for a translate of $\underline{\Omega}$ as long as the two contour configurations are inside V: this is a property that will be used to guarantee the existence of the limit as $L\to\infty$.

Furthermore trajectories that are long give a small contribution to (3.1) at small fugacities because, see eq. (4.39) in[Gi71],

3.3 $$\int_{N(\underline{\Theta})=p}|d\,\underline{\Theta}\,|\,|\Phi^T(\underline{\Omega},\underline{\Theta})|<(2^{-1}e^{-\beta w})^{q-1}R^{-(p+q-1)} \tag{3.3}$$

Here, $q=N(\underline{\Omega})$ and w is the maximum of v, $|d\,\underline{\Theta}\,|$ means that we use the Bosonic measure (which maximizes the integral) whether the system verifies Bose, Fermi or Boltzmann statistics, $N(\underline{\Theta})$ is the number of elementary trajectories composing the configuration $\underline{\Theta}$ and

3.4
$$R = R(\beta) = 2^{-1}\, e \exp -\beta\, w\; - 2\beta\, B - \beta\, l(\beta)^{-d} e^{\beta B} C \int |v(x)| dx \tag{3.4}$$

In (3.4) $l(\beta) = \sqrt{2\pi\beta}$ is the "thermal length" and $C = \sum_{j=1}^{\infty} 2^{-j} j^{-d/2}$, see [Gi71], eq. (3.16) (here we made a special choice for the parameter ξ in [Gi71], namely $\xi = 2^{-1} e^{-\beta\, w}$). Since $w < \infty$ hard cores cannot be considered. The bound in (3.3) holds uniformly in V and it can be considerably improved in the case of Boltzmann statistics, see [Gi71] eq. (3.15).

Note the asymptotic values of $R(\beta)$: $R(\infty) = 0$ always and $R(0) = 0$ if $d > 2$ while $R(0) = r_0 > 0$ if $d \le 2$.

We shall further need the following remark: suppose that the partition function defined in (2.5) is altered by inserting a factor $\varphi(\underline{\Omega})$ which has the property of factoring:

3.5
$$\varphi(\underline{\Omega}', \underline{\Omega}'') = \varphi(\underline{\Omega}')\varphi(\underline{\Omega}'') \tag{3.5}$$

for all $\underline{\Omega}', \underline{\Omega}''$ then (remarkably)

3.6
$$\begin{aligned} \log Z_\phi(\beta, \mu; V) &\stackrel{def}{=} \log \sum_{n=0}^{\infty} \int_{N_V(\underline{\Omega})=n} z^n\, \varphi(\underline{\Omega})\, \frac{d\,\underline{\Omega}}{n!} e^{-\beta U(\underline{\Omega})} = \\ &= \sum_{n=0}^{\infty} \int_{N_V(\underline{\Omega})=n} z^n\, \varphi(\underline{\Omega}) \Phi^T(\underline{\Omega})\, \frac{d\,\underline{\Omega}}{n!} \end{aligned} \tag{3.6}$$

Consequently if $|z| \max_\Omega |\varphi(\Omega)| < R$ the series in (3.6) converges uniformly in the size L of the container and the sums in the r.h.s. of (3.1) and (3.6) are therefore convergent representations of the logarithms of the partition functions (2.5) and (3.6) that define them. The bound (3.3) goes back to the theory of the Kirkwood–Salsburg equations and of the Mayer and virial expansions, see [Ru69], [Gi71].

4. Laplace transform of the probability.

Turning back to the large deviations problem it is natural to look for properties of the Laplace transform (generating function) $\Gamma(\lambda)$ of the probability distribution $\Pi(n)$, defined in (1.2)

4.1
$$\Gamma(\lambda) \stackrel{def}{=} \sum_{n=0}^{\infty} e^{\beta\lambda n} \Pi(n) \equiv \frac{\mathrm{Tr}\, e^{\beta\lambda N_\Lambda} e^{-\beta H_V}}{\mathrm{Tr}\, e^{-\beta H_V}} \tag{4.1}$$

This admits again a simple Brownian path representation:

4.2
$$\Gamma(\lambda) = \frac{\sum_{n=0}^{\infty} \int_{N_V(\underline{\Omega})=n} z^n e^{\lambda\beta N_\Lambda(\underline{\Omega})} e^{-\beta U(\underline{\Omega})} \frac{d\,\underline{\Omega}}{n!}}{\sum_{n=0}^{\infty} \int_{N_V(\underline{\Omega})=n} z^n e^{-\beta U(\underline{\Omega})} \frac{d\,\underline{\Omega}}{n!}} \tag{4.2}$$

Note that $N_\Lambda(\underline{\Omega})$ defined in (2.4) appears here. The similar expression with $N_\Lambda(\underline{\Omega})$ replaced by $\tilde N_\Lambda(\underline{\Omega})$ is a representation of the ratio:

4.3
$$\frac{\mathrm{Tr}\, e^{\beta\lambda N_\Lambda - \beta H_V}}{\mathrm{Tr}\, e^{-\beta H_V}} \tag{4.3}$$

which is related to (4.1) as we shall see, but which is interesting in its own right.

The theory of sections 2 and 3 applies to the expressions (4.1), (4.3): in fact, since the functions $\varphi(\underline{\Omega}) = e^{\lambda\beta N_\Lambda(\underline{\Omega})}$ have the factorization property (3.5), eq. (4.1) can be written as

4.4 $$\Gamma(\lambda)=\exp\,\Big(\sum_{n=0}^{\infty}\int_{\substack{\underline{\Omega}\cap\Lambda\neq\emptyset\\ N_V(\underline{\Omega})=n}} z^n\,(e^{\lambda\beta N_\Lambda(\underline{\Omega})}-1)\,\Phi^T(\underline{\Omega})\,\frac{d\,\underline{\Omega}}{n!}\Big) \tag{4.4}$$

Let now z be less than R then (*c.f.r.* (3.4)), if

4.5 $$|z|\,|e^{\beta\lambda}|<R\qquad\text{or}\qquad \lambda<\delta(\beta,\mu)=\beta^{-1}(\log R-\beta\mu) \tag{4.5}$$

the right side of (4.4) converges to a limit as $V\to\infty$. This limit of $\Gamma(\lambda)$ is uniform in V. Clearly this is a key point that holds because of the bounds (3.3) and (3.4). Furthermore the same convergence bound implies that the argument of the exponential in (4.4) can be differentiated term by term with respect to λ still yielding convergent series.

Conclusion: the generating function (4.1) is analytic in λ in a small interval $|\lambda|<\delta(\beta,\mu)$ around 0. In fact one has analyticity in a bigger region of λ which contains the infinite real semi-axis $\lambda<\delta(\beta,\mu)$.

We define for each Λ, $|\Lambda|=l^d$,

4.6 $$\begin{aligned}\beta P_\ell(\beta,\mu;\lambda)&=\ell^{-d}\sum_{n=0}^{\infty}\int_{\substack{\underline{\Omega}\cap\Lambda\neq\emptyset\\ N_V(\underline{\Omega})=n}} z^n(e^{\lambda\beta N_\Lambda(\underline{\Omega})}-1)\,\Phi^T(\underline{\Omega})\frac{d\,\underline{\Omega}}{n!}\\ \rho_\ell(\beta,\mu;\lambda)&=\ell^{-d}\sum_{n=0}^{\infty}\int_{\substack{\underline{\Omega}\cap\Lambda\neq\emptyset\\ N_V(\underline{\Omega})=n}} z^n\,e^{\lambda\beta N_\Lambda(\underline{\Omega})}N_\Lambda(\underline{\Omega})\,\Phi^T(\underline{\Omega})\frac{d\,\underline{\Omega}}{n!}=\partial_\lambda P_\ell(\beta,\mu;\lambda)\end{aligned} \tag{4.6}$$

The convergence bounds in (3.3) and the translation invariance of the Φ^T functions then imply that the above expressions have limits as $\ell\to\infty$ provided that the size of the container V is also such that $L/\ell\to\infty$. (Indeed the integrals over $\underline{\Omega}$ in (4.6) can be written as the difference between integrals over completely arbitrary configurations $\underline{\Omega}$ except for the restriction that they contain one point (*e.g.* x_1) inside Λ and integrals over configurations that intersect the boundary. The latter contribute a quantity of $o(\ell^d)$ in the expression for P and $o(1)$ in the expression for the density).[2] The limits of βP_l and ρ_l are given by

4.7 $$\begin{aligned}\beta(P(\beta,\mu+\lambda)-P(\beta,\mu))&=\sum_{n=0}^{\infty}\int^{*}_{N(\underline{\Omega})=n} z^n(e^{\lambda\beta n}-1)\,\Phi^T(\underline{\Omega})\,\frac{d\,\underline{\Omega}}{n!}\\ \rho(\beta,\mu+\lambda)&=\sum_{n=1}^{\infty}\int^{*}_{N(\underline{\Omega})=n} z^n e^{\lambda\beta n}n\,\Phi^T(\underline{\Omega})\frac{d\,\underline{\Omega}}{n!}=\partial_\lambda P(\beta,\mu+\lambda)\end{aligned} \tag{4.7}$$

where the $*$ over the integral means that the point $x_1=\omega_{1,1}(0)$ is not integrated over; it can be fixed at the origin.

The approach to the limits is uniform in the parameters β,μ in any closed region contained in the analyticity domain $\mathcal{A}(\mathcal{G})$. One could also evaluate the finite ℓ corrections and show that if $L/\ell\ge 2$ (say) then their sizes are of order ℓ^{-1} and in fact consist of two terms of respective orders L^{-1} and ℓ^{-1} (*i.e.* quantities of the order of "surface/volume" coming from boundary effects due to the boundaries of V and of Λ respectively): however one would have to enter into the details of Ginibre's work, so that we just note that (3.3) and translation invariance imply that the corrections go to zero as $\ell\to\infty$.

5. Large deviations in the analyticity region (4.5).

Given the above information, obtained from [Gi71], the derivation of the large deviations results follows the standard path set up in the classical theory of [MS67].

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[2] In fact a closer analysis would reveal that such terms can be estimated to have size $O(\ell^{d-1})$ and $O(\ell^{-1})$, *i.e.* that they are boundary terms, see [Gi71] proof of lemma 2.2, p.366.

For β and $\mu=\mu_0$ we call, *c.f.r.* (4.5), $\rho_\ell=\rho_\ell(\beta,\mu_0;0)$ and denote the grand canonical averages at chemical potential μ by $\langle\cdot\rangle_\mu$. We estimate the probability Π that $N_\Lambda > (\rho_\ell+a)\ell^d$, for some small $a>0$, by

5.1
$$\Pi(N_\Lambda>(\rho_\ell+a)\ell^d)\le\langle e^{\lambda\beta\,(N_\Lambda-(\rho_\ell+a)\ell^d)}\rangle_{\mu_0}=e^{\beta\,\left(P_\ell(\beta,\mu_0;\lambda)-P_\ell(\beta,\mu_0;0)-\lambda\,(\rho_\ell+a)\right)\ell^d} \tag{5.1}$$

for all $\lambda\ge 0$. The limit of the coefficient of ℓ^d in the r.h.s. of (5.1) is, by (4.7), $\beta\left((P(\beta,\mu_0+\lambda)-P(\beta,\mu_0)-\partial_\mu P(\beta,\mu_0)\lambda-\lambda a\right)$, which holds for all $\lambda\ge 0$. Minimizing over λ we get (by definition of free energy), that *if a is small enough* $\Pi(N_\Lambda>(\rho_\ell+a)\ell^d)\le e^{-\beta a^2\ell^d/2\chi_++o(\ell^d)}$ where χ_+ is the minimum compressibility (*i.e.* of the second derivative of P with respect to μ) in the interval $[\mu_0-\delta,\mu_0+\delta]$. This is within the radius of convergence of our expansion, provided the value $\lambda\sim a/\chi(0)$, where the minimum is achieved, is such that $|\lambda|<\delta(\mu_0,\beta)$, *i.e.* $|a|<\delta_0(\beta,\mu_0)\overset{def}{=}\chi_+\delta(\beta,\mu_0)$ so that the above estimates on the Laplace transform hold.
The case $a<0$ can be treated in a similar manner. Hence setting $|a|<\delta_0(\beta,\mu)$ we get

(I) *Large deviation property 1:*

5.2
$$\Pi(|N_\Lambda-\rho\ell^d|>a\ell^d)\le e^{-\beta a^2\ell^d/2\chi_++o(\ell^d)} \tag{5.2}$$

for $a\in(0,\delta_0(\beta,\mu_0))$.

The relation (5.2) gives an upper bound on arbitrarily large fluctuations which, since the number of possible values of N between $-a\ell^d$ and $a\ell^d$ is "only" $2a\ell^d$ and the total probability is 1 implies that inside any density interval of size $|a|\le\delta_0(\beta,\mu_0)$ centered at ρ_0 there must be at least one value of N whose probability is $\ge O(\ell^{-d})$. We write this result as

(II) *Large deviation property 2:*

5.3
$$\Pi(N_\Lambda\overset{a}{\sim}\rho_0\ell^d)\ge O(a^{-1}\ell^{-d}) \tag{5.3}$$

where $N\overset{\varepsilon}{\sim}\rho\ell^d$ denotes the event $|N-\rho_0\ell^d|<\varepsilon\ell^d$.

This shows that the numbers $\sim\rho_0\ell^d$ have a "high probability", and is our second "large deviations" result.

We now consider a density value ρ_0+a corresponding to a chemical potential $\mu_0+\lambda_a$, with $a\in(0,\delta_0(\mu_0,\beta))$, and note that the same argument can be applied to the probability distribution generated by replacing $e^{-\beta H_V}$ in (1.2) by $e^{-\beta\lambda_a N_\Lambda/2}e^{-\beta H_V}e^{-\beta\lambda_a N_\Lambda/2}$. Calling $\tilde\Pi(N_\Lambda)$ this distribution we therefore conclude that

5.4
$$\tilde\Pi(N_\Lambda\overset{\varepsilon}{\sim}(\rho_0+a)\ell^d)\ge O(\varepsilon^{-1}\ell^{-d})e^{o(\ell^d)} \tag{5.4}$$

Therefore, with the notation introduced after (5.3),

5.5
$$\begin{aligned}\Pi(N_\Lambda\overset{\varepsilon}{\sim}(\rho_0+a)\ell^d)=&\;\frac{\sum_{N_\Lambda\overset{\varepsilon}{\sim}(\rho_0+a)\ell^d}\operatorname{Tr}e^{-\beta H_V}e^{\beta\lambda_a\,N_\Lambda}}{\operatorname{Tr}e^{-\beta H_V}e^{\beta\lambda_a\,N_\Lambda}}\cdot\\ &\cdot\,e^{-\lambda_a\beta(\rho_0+a)\ell^d}\,\frac{\operatorname{Tr}e^{-\beta H_V}e^{\beta\lambda_a\,N_\Lambda}}{\operatorname{Tr}e^{-\beta H_V}}\,e^{O(\varepsilon\ell^d)}=\\ =&\;\tilde\Pi(N_\Lambda\overset{\varepsilon}{\sim}(\rho_0+a)\ell^d)e^{-\lambda_a\beta(\rho_0+a)\ell^d}\,\frac{\operatorname{Tr}e^{-\beta H_V}e^{\beta\lambda_a\,N_\Lambda}}{\operatorname{Tr}e^{-\beta H_V}}\,e^{O(\varepsilon\ell^d)}\end{aligned} \tag{5.5}$$

where we have multiplied and divided by $\operatorname{Tr}e^{-\beta H_V}e^{\beta\lambda_a\,N_\Lambda}$ and introduced in the first tern in the l.h.s. $e^{\beta\lambda_a\,N_\Lambda}$ compensating it by $e^{-\lambda_a\beta(\rho_0+a)\ell^d}e^{O(\ell^d)}$ which is possible because of the restriction $N_\Lambda\overset{\varepsilon}{\sim}(\rho_0+a)\ell^d$ in the sum.

The first term is between 1 and $O(\varepsilon^{-1}\lambda^{-d}e^{-O(\varepsilon\ell^d)})$ by (5.4) and the last ratio can be written, again as done above and in the previous section, as

5.6
$$\exp\Big(\sum_{n=0}^{\infty}\int_{N(\underline{\Omega})=n} z^{N(\underline{\Omega})}\,(e^{\beta\lambda_a N_\Lambda(\underline{\Omega})}-1)\,\frac{d\,\underline{\Omega}}{n!}\Big) \tag{5.6}$$

where the integrals over $\underline{\Omega}$ can be divided into regions with $\underline{\Omega}$ entirely outside the box Λ, which cancel because $N_\Lambda(\underline{\Omega})\equiv 0$, and into those partly inside and partly outside, which contribute a quantity of $o(\ell^d)$,[3] and those entirely inside Λ, which by the analysis in sec. 4 give $\ell^d\,\beta\,(P(\beta,\mu_0+\lambda_a)-P(\beta,\mu_0))=o(\ell^d)$.

Hence we see that

(III) *Large deviations property 3:*

5.7
$$\begin{aligned}\Pi(N_\Lambda \overset{\varepsilon}{\sim} (\rho_0+a)\ell^d) &= e^{\ell^d\,\beta\,\left(-\lambda_a(\rho_0+a)+P(\beta,\mu_0+\lambda_a)-P(\mu_0)\right)}\,O(\varepsilon^{-1}\ell^{-d}e^{O(\varepsilon\ell^d)}) = \\ &= e^{-\beta\ell^d\,\left(f(\beta,\rho_0+a)-f(\rho_0)-\partial_\rho f(\beta,\rho_0)\,a\right)}\,O(\varepsilon^{-1}\ell^{-d}e^{O(\varepsilon\,\ell^d)})\end{aligned} \tag{5.7}$$

having used the relations $\beta P(\beta,\mu_0)=\beta\mu_0\rho_0-\beta f(\beta,\rho_0)$ if $\mu_0=\partial_\rho\,f(\beta,\rho_0)$ (see [Ru69], eq. (4.17)).

The smoothness of the functions f,P has been tacitly used in the above discussion. This allows us to take advantage of the arbitrariness of ε (which we could even choose to be an inverse power of ℓ with a small exponent) and to interchange limits and maximizations so that (5.7) implies the result stated in sec. 1. Indeed we deduce that in the interval $[\rho_0+a,\rho_0+b]\ell^d$ there is a value of N whose probability multiplied by $e^{\Delta F(\beta,\rho_0+a)\ell^d}$ is $\ge O(e^{(b-a)O(\ell^d)}\ell^{-d})$ times the exponential in (5.7) and a,b are arbitrary in $(0,\delta_0(\beta,\mu_0))$. This is the main result claimed in Sec. 1.

6. Beyond the analyticity region.

A completely different method can be used to study systems satisfying Boltzmann statistics at *arbitrary chemical potential* or Bose gases *in the region* $e^{\beta\mu+2\beta B}<1$. The method does not apply to Fermi systems. We illustrate it in the bounded positive interaction case: more general cases can presumably be treated along similar lines but we shall not attempt to do so here.

The method is very similar to the one used in classical statistical mechanics by [La72], [Ol88]. This entails comparing $\Gamma(\lambda)$ in (4.1) with the partition function $Z(\beta,\mu+\lambda;\Lambda)$ obtained by replacing H_V in the right side of (4.1) with H_Λ. More precisely we want to prove that $|\Lambda|^{-1}\log\Gamma(\lambda)\to|\Lambda|^{-1}\log Z(\beta,\mu+\lambda;\Lambda)=P(\beta,\mu+\lambda)$ which would give us directly the desired result. For a classical system this is done by first noting that $\Gamma(\lambda)$ is (for $L-l>D$) nothing else than $\int Z(\beta,\mu+\lambda;\Lambda|\eta)d\nu(\eta)$. Here η is the configuration of particles outside Λ, $d\nu(\eta)$ is the induced Gibbs measure and $Z(\beta,\mu+\lambda;\Lambda|\eta)$ is the partition function (or normalization factor) for the grand canonical ensemble with chemical potential $\mu+\lambda$, in a box Λ with boundary conditions η. The proof of the LD formula is then basically a version of the proof of equivalence of ensembles, [Ru69].

To carry out a similar analysis for the quantum Boltzmann and Bose case it is necessary to use trajectories $\underline{\Omega}$ instead of configurations. One simply considers probabilities of events happening in a fictitious *gas of closed paths*: the probability of a configuration $\underline{\Omega}=(\Omega_1,\ldots,\Omega_n)$ of this gas is,

6.1
$$z^n e^{-\beta U(\underline{\Omega})}d\,\underline{\Omega}/Z(\beta,\mu,V) \tag{6.1}$$

[3] Once more a closer analysis shows that such terms can be estimated to have size $O(\ell^{d-1})$, *i.e.* that they are boundary terms.

with the notation of the previous sections. We can now write $\underline{\Omega} = (\underline{\Omega}_\Lambda, \underline{\Omega}_{ext})$ in which the contours in $\underline{\Omega}_\Lambda$ are totally or partially inside Λ and those in $\underline{\Omega}_{ext}$ *do not have any points inside* Λ. Then the probability distribution in (6.1) induces conditional probabilities $W_\Lambda(\underline{\Omega}_\Lambda | \underline{\Omega}_{ext})$ verifying the appropriate "*DLR equations*"

6.2
$$W_\Lambda(\underline{\Omega} \mid \underline{\Omega}_{ext}) = \frac{z^n e^{\beta U(\underline{\Omega} \mid \underline{\Omega}_{ext})} \, d\underline{\Omega}/n!}{\tilde{Z}(\beta, \mu; \Lambda | \underline{\Omega}_{ext})} \tag{6.2}$$

where $\tilde{Z}$ is the appropriate normalization. (Fermions cannot be treated in this way because the integration $d\underline{\Omega}$ is *not positive*).

The main estimate on which the analysis will rely is that, in analogy to the classical case, the contribution to the partition function from trajectories which cross $\partial\Lambda$ is proportional to $\partial\Lambda$. More precisely there exists a function $\vartheta(\beta, z)$ such that

6.3
$$\frac{1}{|\partial\Lambda|} \log \sum_m \widetilde{\int}_{N_V(\underline{\Omega})=m, \Omega_1 \cap \partial\Lambda \neq \emptyset} z^m e^{-\beta U(\underline{\Omega} \mid \underline{\Omega}')} d\underline{\Omega}/m! < \vartheta(\beta, z) < \infty \tag{6.3}$$

for all $\Lambda \subseteq V$ and for all configurations $\underline{\Omega}'$; the tilde over the integral means that the contours in $\underline{\Omega}$ must all intersect Λ. This is an estimate that can be proved without restrictions in the case of a Boltzmann statistics; however in the case of bosons it can only be proved under the condition $ze^{2\beta B} < 1$; for a proof see [Gi71] proof of lemma 2.2, p.366.[4]

The probability $\Pi(N)$ that $N_\Lambda(\underline{\Omega}) = N$ can be estimated by considering the probability of the same event conditioned on the presence of an external configuration $\underline{\Omega}_{ext}$: if the resulting estimate coincides with (1.6) up to a correction by a factor $e^{O(\ell^{d-1})}$ *independently* of $\underline{\Omega}_{ext}$ the proof of (1.7) will be achieved.

(IV) *Large deviation property 4:*

Suppose that the interaction potential v is positive and bounded. Let β, μ_0 be in the region $e^{\beta\mu_0 + 2\beta B} < 1$ in the Bose case or arbitrary in the Boltzmann case. We also assume that there is no phase transition at β, μ_0. Let ρ_0 be the corresponding density (so that $\rho_0 = \rho(\beta, \mu_0)$), i.e. $\frac{\partial P(\beta,\mu)}{\partial\mu}$, is continuous at μ_0. If the side ℓ of the box Λ tends to infinity and, correspondingly, the container side L also tends to infinity so that $L/\ell \to \infty$, then

6.4
$$\lim_{\ell \to \infty} \ell^{-d} \log \sum_{\tilde{\rho} \in [a,b]} \Pi(\tilde{\rho}\ell^d) = \max_{\tilde{\rho} \in [a,b]} -\beta \, \Delta F(\beta, \tilde{\rho}, \rho_0) \tag{6.4}$$

This holds for the Bose system provided the interval $[a, b]$ is contained in an interval $(0, \rho_{max}(\beta))$ where $\rho_{max}(\beta)$ is the maximal density that can be achieved as the chemical potential varies compatibly with the restriction $e^{\beta\mu_0 + 2\beta B} < 1$. (There is no such restriction in the Boltzmann case).

The assumption of boundedness on the potential does not allow hard cores. However the technique below also applies to the hard core case with a tail which is not necessarily repulsive: to avoid technicalities we do not discuss this case. Eliminating completely all

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[4] In an unpublished note by Lupini and one of us, (GG), this region was slightly extended to cover cases with $ze^{2\beta B} > 1$ in systems with hard core interactions. This made use of the fact that hard cores force the Brownian paths Ω to be "quite extended" (*i.e.* $O(a)$ if a is the core radius) while they have average size $O(\sqrt{\beta})$: therefore they have a low probability if β is small. Hence one can take $ze^{2\beta B} > 1$ (by $O(e^{a^2/\beta})$ provided β is small enough. The analysis could be extended to cover also such cases which, however, are conceptually not really different from the case considered here.

restrictions, *i.e.* assuming just stability or possibly superstability of the potential, seems to require new ideas.

To prove (6.4) we fix the configuration $\underline{\Omega}_{ext}$ outside Λ and we look first for a lower bound for $\Pi_(n)$. This is obtained by remarking that if $\underline{\Omega}\subset\Lambda$ then for configurations $\underline{\Omega}$ in which all trajectories are at least a distance D from $\partial\Lambda$, $|U(\underline{\Omega}\mid\underline{\Omega}_{ext})|=0$.

Hence, if Λ_D is the region in the interior of Λ separated from the boundary of $\partial\Lambda$ by a corridor of width D, the numerator of the fraction (obtained from (6.2)) expressing $\Pi(n)$ can be bounded below by $\big(\int_{\underline{\Omega}\subset\Lambda_D,n_\Lambda(\Omega)=n} e^{\beta\mu_0 n}e^{-U(\underline{\Omega})}d\underline{\Omega}/n!\big)$ which is $e^{\beta\mu_0 n}$ times the *canonical* partition function Q^D_n for the system with Dirichlet boundary conditions (*i.e.* vanishing boundary conditions) on $\partial\Lambda_D$ and no external particles outside the box Λ_D.

The denominator in (6.2) is bounded above by $Z^0_\Lambda(\mu_0,\beta)e^{\vartheta(\mu_0,\beta)|\partial\Lambda|}$ where Z^0_Λ is the grand canonical partition function for the system with Dirichlet boundary conditions on $\partial\Lambda$ and no external particles outside the box Λ; the second factor bounds the contributions to the integral from the contours of $\underline{\Omega}$ that cross the boundary *via* the bound (6.3). Hence

6.5 $$\Pi_\Lambda(N)\ge\frac{e^{\beta\mu_0 N}Q^D_N}{Z^0_\Lambda(\mu_0,\beta)}e^{-\vartheta(\mu_0,\beta)\,|\partial\Lambda|}\tag{6.5}$$

Likewise Z^0_Λ gives a lower bound to the denominator of (6.2) while an upper bound on the numerator is

6.6 $$\Big(\sum_{k=0}^{N}\int_{N_\Lambda(\underline{\Omega})=N-k} e^{\beta\mu_0(N-k)}\,e^{-\beta U(\underline{\Omega})}\Big)e^{\vartheta(\beta,\mu_0)|\partial\Lambda|}\tag{6.6}$$

and again we recognize that the integral gives the canonical partition function for $N-k$ particles in $\partial\Lambda$ with Dirichlet (and no outside particles) boundary condition multiplied by $e^{\beta\mu_0(N-k)}$. Therefore

$$\begin{aligned}\Pi_{\Lambda,N}&\le e^{\vartheta|\partial\Lambda|}\,N\max_{k\le N}\frac{e^{\beta\mu_0(N-k)}Q_{N-k}(\beta)}{Z^0_{\Lambda_D}(\beta,\mu_0)}=\\ &=e^{\vartheta|\partial\Lambda|}\,N\max_{0<\delta<\rho}\frac{e^{(\beta\mu_0(\rho-\delta)-\beta f(\beta,\rho-\delta))|\Lambda|}}{e^{(\beta\mu_0\rho_0-\beta f(\beta,\rho_0))\,|\Lambda|}}\,e^{o(|\Lambda|)}\end{aligned}\tag{6.7}$$

where we have used the fact that the canonical thermodynamic limit (with Dirichlet boundary conditions) is uniform in the density in any closed interval contained in $(0,\rho_{cp})$, see [Ru69], and furthermore that the maxima in (6.7) are certainly achieved, uniformly in the volume, for $k>\eta|\Lambda|$ for some $\eta>0$.

In fact the maximum of the r.h.s. of (6.7) is achieved precisely at $\delta=0$ by the convexity properties of the free energy because

6.8 $$\frac{e^{(\beta\mu_0(\rho-\delta)-\beta f(\beta,\rho-\delta))\,|\Lambda|}}{e^{(\beta(\mu_0\rho_0-\beta f(\beta,\rho_0))\,|\Lambda|}}=e^{-\beta(f(\beta,\rho-\delta)-f(\beta,\rho_0)-\partial_\rho f(\beta,\rho_0)(\rho-\delta-\rho_0))\,|\Lambda|}\tag{6.8}$$

Where we have used the relation between grand canonical pressure and canonical free energy. We have assumed above that there are no phase transitions in the sense that for each chemical potential considered there is just one density possible. In particular this means that $\rho=\frac{\partial P(\beta,\mu)}{\partial\mu}$ and $\mu=\frac{\partial f(\beta,\rho)}{\partial\rho}$ and therefore (6.7), (6.8) and (6.5) imply (6.4). Existence of phase transitions affect the argument and the results in the same way as they do in classical statistical mechanics and we do not discuss the details.

The above method is purely probabilistic and it relies on two properties: (1) the measure $d\mathbf{\Omega}$ is positive and (2) inequality (6.3). Therefore it applies also to the Bose gas case whenever (6.3) can be checked. The inequality (6.3) does not hold if $ze^{2\beta B} > 1$ so that new ideas seem necessary to treat the Bose statistics case in spite of the important results of [Pa85] which, by relying on Ginibre's representation of the Gibbs distributions, provide a proof of boundary conditions independence.

7. Beyond the small activity region for weakly interacting fermions on a lattice.

In this section we discuss Fermionic lattice systems. Using the methods developed for the study of ground states in Fermionic systems allows one to deal with arbitrary μ_0 and β at small coupling, thus enlarging the region in which LD relations can be obtained, at least if one assumes periodic boundary conditions, i.e. regarding V as a torus. (This is certainly *very restrictive* but we note that periodicity of boundary conditions is an assumption under which most of the existing results on fermions have been derived.)

Results can be obtained for all μ_0 (*i.e.* also positive μ_0 which is not possible with the previous method). *In the continuum case, however, similar results can be derived only in one-dimension or if an ultraviolet cut-off is imposed on* $\vec{k}$. We shall fix *a priori* μ_0, β, with $\beta > 0$, and *then* discuss the large deviations for v small enough (depending on the choice of β, μ_0).

One can wonder how is it that the low temperature techniques that, even for lattice systems, have been proved useful only in 1-dimensional cases (meeting serious, so far insurmountable, difficulties in higher dimension) can be of help here in an arbitrary dimension. However the low temperature techniques were devised to treat the case $\beta = +\infty$, *i.e.* ground states. We would encounter the same difficulties in their application to large deviations theory if we tried to employ them for the purpose of analyzing LD at zero temperature. Applying them at $\beta^{-1} > 0$ and at weak interaction is, however, not difficult at least for lattice systems.

We consider a d-dimensional square box of even integer side L with periodic boundary conditions, and $\vec{x} = (n_1, ..., n_d)$, with $n_i = -L/2, \ldots, L/2$. The Hamiltonian is similar to (1.1) with the Laplace operator replaced by the discrete Laplace operator. If there is no interaction all properties of the system can be obtained through the free *Schwinger function*, also called *propagator*,

7.1
$$g(\underline{x}) = \frac{1}{\beta|V|} \sum_{k_0, \vec{k}} \frac{e^{ik_0(x_0+0^-)+i\vec{k}\vec{x}}}{-ik_0 + E(\vec{k}) - \mu_0} \tag{7.1}$$

where $x_0 \in (-\beta, \beta)$ and $k_0 = \frac{2\pi}{\beta}(m + \frac{1}{2})$, $m = 0, \pm 1, \ldots$, and $k_i = \frac{2\pi n_i}{L}$, $n_i = 0, \pm 1, \ldots$, $\pm L/2$, $\vec{k} = (k_1, .., k_d)$, L being the length of the side of V and $E(\vec{k}) = \sum_{i=1}^d (1 - \cos k_i)$. The symbol $x_0 + 0^-$ means that the value is the limit from the left.

The "propagator", see for instance Sec. 2 in [BG90] or [BGPS92], is defined in terms of the creation and annihilation operators for fermions $a^\pm_{\underline{x}}$ and of the free Hamiltonian $T = \sum -(\frac{1}{2}\Delta_{\underline{x}_i} - \mu_0) = \int_V a^+_{\underline{x}}(-\frac{1}{2}\Delta_{\underline{x}} - \mu_0)a^-_{\underline{x}}\, d\underline{x}$ as

7.2
$$\begin{aligned} g_+(\underline{\xi}, t) =&\mathrm{Tr}\, e^{-(\beta-t)T} a^-_{\underline{x}} e^{-tT} a^+_{\underline{x}'} / \mathrm{Tr}\, e^{-\beta T} \\ g_-(\underline{\xi}, t) =&\mathrm{Tr}\, e^{-(\beta-t)T} a^+_{\underline{x}} e^{-tT} a^-_{\underline{x}'} / \mathrm{Tr}\, e^{-\beta T} \end{aligned} \tag{7.2}$$

if $\underline{\xi} = \underline{x} - \underline{x}'$, $t > 0$, which are combined to form a single function:

7.3
$$g(\underline{\xi}, t) = \begin{cases} g_+(\underline{\xi}, t) & \text{if } \beta > t > 0 \\ -g_-(-\underline{\xi}, -t) & \text{if } -\beta < t \le 0 \end{cases} \tag{7.3}$$

And (7.1) is a well known Fourier representation of the function in (7.3), having replaced the temperature parameter t with x_0 for uniformity of notation. Note that the function

$g(\underline{x}, t)$ has to be regarded as a function of t which is defined and periodic, although not continuous, in $[-\beta, \beta]$ (and of $\underline{x}$ defined and periodic in $[-L, L]^d$): this is important to keep in mind when studying Fourier transforms.

Note that $k_i \le 2\pi$ while k_0 is unbounded: this unboundedness of the sum is an *ultraviolet problem* "in the temperature direction" and restricting to a lattice has the advantage that no ultraviolet problem is present in the "spatial direction". The ultraviolet problem in the temperature direction is somewhat trivial: it is however essential to have no cut-off in the k_0 values. Such cut–offs violate "reflection positivity", *i.e.* the resulting system is no longer Hamiltonian and the physical interpretation becomes unclear.

We define the "distance on the periodic box V" as $d_L(x_i) = \frac{L}{\pi}\sin(\frac{\pi x_i}{L})$ and $d_\beta(x_0) = \frac{\beta}{\pi}\sin(\frac{\pi x_0}{\beta})$ and $\underline{d}_{\beta,L}(\underline{x}) = (d_L(x_1), ..., d_L(x_d), d_\beta(x_0))$. This becomes the ordinary distance in the limit $L \to \infty$.

In the following we shall sometimes write $\sum_{\vec{x}}$ as $\int d\vec{x}$.

For all positive integers α there exists a constant C_α, independent of $\beta, |V|, \mu_0$ such that

7.4
$$|g(\underline{x} - \underline{y})| \le \nu^{-1}\,\frac{C_\alpha}{1 + \nu^\alpha |\underline{d}_{\beta,L}(\underline{x} - \underline{y})|^\alpha} \tag{7.4}$$

where $\nu^{-1} = 1 + 1/\max\{-\mu_0, \beta^{-1}\}$.

In fact let $h(t)$ a C^∞ function which is 1 for $t > 2$ and 0 for $t < 1$; we can decompose the propagator g into its ultraviolet and infrared parts g_u, g_i; we write

7.5
$$\begin{aligned} & g(\underline{x} - \underline{y}) \equiv g_u(\underline{x} - \underline{y}) + g_i(\underline{x} - \underline{y}) \stackrel{def}{=} \\ & \stackrel{def}{=} \frac{1}{\beta|V|}\sum_{k_0,\vec{k}} h(k_0^2)\frac{e^{ik_0(x_0+0^-)+i\vec{k}\vec{x}}}{-ik_0 + E(\vec{k}) - \mu_0} + \frac{1}{\beta|V|}\sum_{k_0,\vec{k}}(1 - h(k_0^2))\frac{e^{ik_0x_0+i\vec{k}\vec{x}}}{-ik_0 + E(\vec{k}) - \mu_0} \end{aligned} \tag{7.5}$$

and we estimate them separately.
(1) First we check that the bound (7.4) holds for $g_i(\underline{x})$; if $n_0, n_1, ..., n_d$ are positive integers then

7.6
$$|(d_L(x_1)^n_1 ... d_L(x_i)^{n_d} d_\beta(x_0)^{n_0}) \cdot g_i(\underline{x})| \le \frac{1}{\beta|V|}\sum_{k_0,\vec{k}} |\partial_{k_1}^{n_1} ... \partial_{k_0}^{n_0} \hat{g}_i(\underline{k})| \tag{7.6}$$

where $\partial_{k_i}, \partial_{k_0}$ denotes the discrete derivative on the lattice of the wave numbers k. Noting that the denominator in (7.1) is greater than $\max\{-\mu_0, \beta^{-1}\}$, one obtains for $g_i(\underline{x} - \underline{y})$ the bound (7.4) because the sum over k_0 is finite and that over $\vec{k}$ tends to an integral over the Brillouin zone which is also finite.
(2) The next relation that we need is that, for all α there is a constant C_α such that

7.7
$$|g_u(\underline{x} - \underline{y})| \le \frac{C_\alpha}{1 + \nu^\alpha\, |\underline{d}_{\beta,L}(\underline{x} - \underline{y})|^\alpha} \tag{7.7}$$

The "only" problem in checking (7.7) is that the sum over k_0 is unbounded and the summand is $O(k_0^{-1})$ so that the sum is improperly convergent if $n_0 = 0$: indeed using (7.6) we see that if $|n_0| \ge 1$ the discrete derivative is applied either to the denominator (and gives a quantity bounded by $O(k_0^{-2})$) or it is applied to $(1 - h(k_0^2))$, and $\partial_{k_0} h(k_0^2)$ has compact support.
Therefore we have to check that the lack of convergence only causes a discontinuity of the function g_u at the origin and $\pm\beta$ and it does not affect the large distance behavior.

The non smoothness is just a discontinuity hence it does not affect the size of g_u at the origin. A direct check that $g_u(\underline{x})$ is bounded is obtained by rewriting g_u as

7.8

$$\begin{aligned}&\frac{1}{\beta V}\sum_{\underline{k}} h(k_0^2)\,\frac{e^{ik_0x_0+\vec k\cdot\vec x}(E(\vec k)-\mu_0)}{(-ik_0+E(\vec k)-\mu_0)(-ik_0)}+\delta_{\vec x,\vec 0}\,\frac{1}{\beta}\,\sum_{k_0}(h(k_0^2)-1)\,\frac{e^{ik_0x_0}}{-ik_0}+\\&+\frac{1}{2}\delta_{\underline{x},\underline{0}}-\chi(x_0)\delta_{\vec x,\vec 0}\stackrel{def}{=}\overline{g}(\vec x,x_0)-\chi(x_0)\delta_{\vec x,\vec 0}\end{aligned}\tag{7.8}$$

where $\chi(x_0)=1$ if $x_0\ge 0$ and $\chi(x_0)=0$ otherwise; furthermore $\delta_{\vec x,\vec y}$ denotes the Kronecker delta on the lattice points and we use that (recall that g,g_u,g_i are periodic, although not continuous, functions of x_0 in $[-\beta,\beta]$).

7.9

$$\beta^{-1}\sum_{k_0=(m+\frac{1}{2})2\pi/\beta}\frac{e^{ik_0(x_0+0^-)}}{-ik_0}=-\frac{1}{2}\mathrm{sign}(x_0)=\frac{1}{2}-\chi(x_0)\ .\tag{7.9}$$

The function $\overline{g}$ is defined by the r.h.s. of (7.8); the first two sums in (7.8) are absolutely convergent (the second is a finite sum); hence g_u is finite near $x_0=0$. Furthermore the Fourier transform $\hat{\overline{g}}(\underline{k})$ of $\overline{g}$ is such that its "L_1–norm" $(\beta V)^{-1}\sum_{k_0,\underline{k}}|\hat{\overline{g}}(\underline{k})|$ is uniformly bounded in V because (if $k_0=\pi\beta^{-1}n$ with n integer)

7.10

$$\begin{aligned}&|\hat{\overline{g}}(\underline{k})|\le\frac{2d+|\mu_0|}{k_0^2}\chi(|k_0|>1)+\frac{\chi(|k_0|<1)}{2\pi\beta^{-1}}+\frac{\beta}{2}\delta_{k_0,0}\qquad\Rightarrow\\&(\beta V)^{-1}\sum_{k_0,\underline{k}}|\hat{\overline{g}}(\underline{k})|\le c\,(1+|\mu_0|)\beta\end{aligned}\tag{7.10}$$

for a suitable constant c. Note that instead the Fourier transform of g *has a logarithmically divergent* L_1–norm in the above sense because of the last term in (7.8).

After the above remarks on the nature of the infrared and ultraviolet propagators we can go back to the problem of interest to us here. We study the Laplace transforms considered in 4, (4.3), and write

7.11

$$\begin{aligned}&\mathrm{Tr}e^{-\beta(H_V-\mu_0N)}e^{\beta\lambda N_\Lambda}=\\&=\sum_{n=0}^{\infty}\frac{1}{n!}(\beta\lambda)^n\sum_{\vec y_1}\ldots..\sum_{\vec y_n}\chi_\Lambda(\vec y_1)\ldots\chi_\Lambda(\vec y_n)\mathrm{Tr}[e^{-\beta(H_V-\mu_0N)}\rho(\vec y_1)\ldots.\rho(\vec y_n)]\end{aligned}\tag{7.11}$$

where $\rho(\vec x)=\psi^+_{\vec x}\psi^-_{\vec x}$. Note that since the fermions are on a lattice and in a finite container the series over n is a finite sum, by Pauli's principle.

It is well known that the partition function trace for a Fermionic Hamiltonian can be written in terms of *Grassman's variables* $\eta^+_{\underline{x}}\equiv\eta^+_{\vec x,x_0}$, $\eta^-_{\underline{x}}=\eta^-_{\vec x,x_0}$; in particular, if H_0 is the kinetic energy (with the discrete Laplacian)

7.12

$$\frac{\mathrm{Tr}[e^{-\beta(H_V-\mu_0N)}\rho(\vec y_1)\ldots.\rho(\vec y_n)]}{\mathrm{Tr}\,e^{-\beta(H_V-\mu_0N)}}=\frac{\int P(d\eta)e^{-U(\eta)}\eta^+_{\vec y_1,0}\eta^-_{\vec y_1,0}\ldots\eta^+_{\vec y_n,0}\eta^-_{\vec y_n,0}}{\int P(d\eta)e^{-U(\eta)}}\tag{7.12}$$

where $U(\eta)=\varepsilon\int d\underline{x}\,d\underline{y}v(\vec x-\vec y)\delta(x_0-y_0)\eta^+_{\underline{x}}\eta^-_{\underline{x}}\eta^+_{\underline{y}}\eta^-_{\underline{y}}$, $\int d\underline{x}=\sum_{\vec x}\int_0^\beta dx_0$. The "integral" $\int P(d\eta)\cdot$ is defined on monomials of Grassman variables (and extended to general functions by linearity) by the anticommutative Wick rule with propagator (7.1). Then we can write by (7.11),(7.12)

7.13

$$\langle e^{\lambda\beta\,N_\Lambda}\rangle_{\mu_0}=\frac{\int P(d\eta)e^{-U(\eta)}e^{\beta\lambda N_\Lambda(\eta)}}{\int P(d\eta)e^{-U(\eta)}}\tag{7.13}$$

where $N_\Lambda(\eta) = \sum_{\vec x} \chi_\Lambda(\vec x)\eta^+_{\vec x,0}\eta^-_{\vec x,0}$.

Remark: had we considered instead of the ratio in (4.3) the quantity

7.14
$$\frac{\mathrm{Tr}\, e^{-\beta(H_V-\mu_0 N+\lambda N_\Lambda)}}{\mathrm{Tr}\, e^{-\beta(H_V-\mu_0 N)}} = \frac{\int P(d\eta)e^{-U(\eta)}\, e^{\lambda\beta \hat N_\Lambda(\eta)}}{\int P(d\eta)e^{-U(\eta)}} \tag{7.14}$$

where $\hat N_\Lambda = \beta^{-1}\int dx_0 \sum_{\vec x}\chi_\Lambda(x)\eta^+_{\underline x}\eta^-_{\underline x}$ we would have obtained a different quantity but estimates for it can be obtained in a way similar to the ones we explain below: this is related to the discussion following (2.4).

In terms of Grassmanian integrals the logarithm of the Laplace transform of the probability (4.1) divided by $\beta|\Lambda|$ is given by

7.15
$$\frac{1}{\beta|\Lambda|}\log\langle e^{\lambda\beta\, N_\Lambda}\rangle_{\mu_0} = \frac{1}{\beta|\Lambda|}\log\frac{\int P(d\eta)e^{-U(\eta)}\, e^{\beta\lambda N_\Lambda}}{\int P(d\eta)e^{-U(\eta)}} \tag{7.15}$$

For a system of fermions on a cubic d-dimensional lattice with Hamiltonian (1.1), in which the Laplace operator is replaced by the discrete Laplace operator, then we can proceed to developing a *cluster expansion at small interaction* and proceed to studying the large deviations probabilities following the same strategy of Sec. 4, 5 above.

In fact by the definition of *truncated expectation*

7.16
$$\log\int P(d\eta)\, e^{\varepsilon A(\eta)} \equiv \mathcal{E}^T(e^{\varepsilon A}) \stackrel{def}{=} \sum_{n=0}^\infty \frac{\varepsilon^n}{n!}\mathcal{E}^T(A;n) \tag{7.16}$$

where $\mathcal{E}^T(A;n) = \mathcal{E}^T(A_1,A_2,\ldots,A_n)|_{A_i=A}$ with $\mathcal{E}(\cdot,\cdot,\ldots)$ is a suitably defined multilinear function of its n arguments, we can rewrite (7.15) as

7.17
$$\frac{1}{\beta|\Lambda|}\mathcal{E}^T(e^{-U}(e^{\lambda\beta N_\Lambda}-1)) \tag{7.17}$$

having exploited that Grassmanian variables anticommute (so that even monomials in Grassmanian fields commute, *unlike the Fermionic fields that generate them*). More explicitly we develop the exponential in powers and obtain

7.18
$$\frac{1}{\beta|\Lambda|}[\sum_{n=0}^\infty \frac{1}{n!}\mathcal{E}^T(-U+\int d\,\underline x\; \chi_\Lambda(\vec x)\, \eta^+_{\vec x,0}\eta^-_{\vec x,0};n) - \frac{1}{n!}\sum_{n=0}^\infty \mathcal{E}^T(-U;n)] \tag{7.18}$$

As usual one can represent the Grassmanian expressions

7.19
$$\begin{aligned} U(\eta) &= \int d\,\underline x\, d\underline y v(\vec x-\vec y)\delta(x_0-y_0)\eta^+_{\underline x}\eta^-_{\underline x}\eta^+_{\underline y}\eta^-_{\underline y}\\ N_\Lambda(\eta) &= \beta\,\lambda\int \chi_\Lambda(\vec y)\delta(y^0)\eta^+_{\underline y}\eta^-_{\underline y}\; d\underline y \end{aligned} \tag{7.19}$$

by the diagrams or "*graph elements*" in Fig.1.

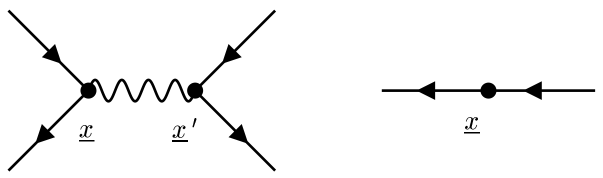

Fig.1: The lines "entering (exiting) a point" $\underline{x}$ represent the Grassmanian fields $\psi^+_{\underline{x}}$ (respectively $\psi^-_{\underline{x}}$); the wavy line connecting the dots marked $\underline{x}, \underline{x}'$ represents $v(\vec{x} - \vec{x}')\delta(x^0 - x^{0\prime})$ while the dot in the second diagram represents $\chi_\Lambda(\vec{x})\delta(x_0)$.

We can call the pair $P = (\underline{x}, \underline{x}')$ or the single point $Q = \underline{x}$ in Fig.1 a *cluster*. If

7.20
$$\begin{aligned} &dP = d\underline{x}\, d\underline{x}',\ dQ = d\underline{x},\ V(P) = v(\vec{x} - \vec{x}')\delta(x^0 - x'^0),\\ &\chi_\Lambda(Q) = \chi_\Lambda(\vec{x})\delta(x^0),\ \eta(P) = \eta^+_{\underline{x}}\eta^-_{\underline{x}}\eta^+_{\underline{x}'}\eta^-_{\underline{x}'},\ \eta(Q) = \eta^+_{\underline{x}}\eta^-_{\underline{x}} \end{aligned} \tag{7.20}$$

and if we set, as above, $\int d\underline{x}\, \cdot \stackrel{def}{=} \int_0^\beta dx^0\, d\vec{x}\, \cdot \stackrel{def}{=} \int_0^\beta dx^0 \sum_{\vec{x}} \cdot$ the (7.18) takes the form

7.21
$$\sum_{\substack{n_1, n_2\\ n_2 \ge 1}} \int (\prod_{i=1}^{n_1} V(P_i)\, dP_i) \cdot (\prod_{j=1}^{n_2} \chi_\Lambda(Q_j)\, dQ_j) \cdot \mathcal{E}^T\big((\prod_{i=1}^{n_1} \eta(P_i))\, (\prod_{j=1}^{n_2} \eta(Q_j)); n_1 + n_2\big) \tag{7.21}$$

simply by the multilinearity of the truncated expectations, see [Le87], [BGPS94]. The sum over n_2 starts from $n_2 = 1$ because the terms with $n_2 = 0$ cancel because for $\lambda = 0$ (7.17) vanishes.

We now imagine to join or "*contract*" ("Wick's contraction") pairs of lines associated with clusters (defined above) and with matching orientations in such a way that the collection of lines thus obtained, including the wavy lines, form a *tree graph* connecting all points of the clusters. The geometric object so built is called a "spanning tree" and contains $2(n_1 + n_2 - 1)$ solid lines and n_1 wavy lines. In the graph there will be, therefore, $2m \stackrel{def}{=} 4n_1 + 2n_2 - 2(n_1 + n_2 - 1) = 2(n_1 + 1)$ lines left "uncontracted".

A remarkable algebraic expression for the truncated Fermionic expectations $\mathcal{E}^T$ in (7.21) can be developed ("Lesniewsky's expansion") as

7.22
$$\sum_{T = spanning\ tree} \int dr_T(\underline{t})\, (\prod_{l \in T} g(\xi_l)) \cdot (\det G^T(\underline{t})) \tag{7.22}$$

where:
(i) $\xi_l = \underline{x} - \underline{y}$ if the line $l \in T$ joins $\underline{x}$ and $\underline{y}$,
(ii) $\underline{t}$ is a family of $2m$ "interpolation parameters in $[0, 1]$,
(iii) $r_T(\underline{t})d\underline{t}$ is a probability measure on the interpolation parameters whose structure is inessential but for the fact that $\int r_T(\underline{t})d\underline{t} = 1$,
(iv) G^T is a $m \times m$ matrix obtained by considering the m points $\underline{\tilde{x}}_1, \ldots, \underline{\tilde{x}}_m$ or $\underline{\tilde{y}}_1, \ldots, \underline{\tilde{y}}_m$ into which enter, respectively exit, uncontracted lines and setting $G^T_{ij} = t_{ij} \cdot g(\underline{\tilde{x}}_i - \underline{\tilde{y}}_j)$ with t_{ij} functions of the interpolation parameters such that $t_{i,i'} = \underline{u}_i \cdot \underline{u}_{i'}$ for a suitably defined unit vectors $\underline{u}_i \in R^m$. The latter property of the unit vectors is the only property that concerns us here.

The above formula is very convenient because of the Gramm–Hadamard inequality[5] which applies precisely to matrices that have the form of G^T and bounds their determinant (for all $\underline{t}$) in terms of the m–th power of the L_1–norm of the integrand in (7.1):

7.23
$$|\det G^T(\underline{t})| \le c_1^m \tag{7.23}$$

[5] This inequality concerns matrices having the form $M_{i,j} = (u_i \cdot v_j)_H$ where u_i, v_j are unit vectors in a Hilbert space H and $(u \cdot v)_H$ denotes the scalar product in H and it states that the determinant of M is bounded by 1 in absolute value. It has, essentially, the simple geometric meaning that the volume of a parallelepiped with sides of length 1 cannot exceed 1. An immediate consequence, that we employ here, is that matrices $M_{i,j} = (u_i \cdot v_j)_H\, (U_i \cdot V_j)_K$ with u_i, v_j unit vectors in a Hilbert space H and U_i, V_j unit vectors in a Hilbert space K also have determinant bounded by 1 (one just applies the previous inequality in the Hilbert space $H \times K$).

provided the norm is finite. However, as remarked in connection with (7.9), (7.10) there is no cut–off on the momentum k_0 and the norm diverges ("logarithmically"). Here we hit a problem which is serious because apparently the best estimate that we can find for this determinant using just the boundedness of the matrix elements is like (7.23) but with an extra $m!$, which would be a disaster.

Suppose, *temporarily,* that the propagator $g(\underline{x}-\underline{y})$ is replaced by $g_i(\underline{x}-\underline{y})$ (*i.e.* we impose an *ultraviolet cut-off* to the model) so that the inequality (7.23) holds: then we can quickly develop a proof of a LD result. In fact, assuming (7.23) valid with some constant c_1, we can bound the n_1, n_2 term of the series (7.21) by

7.24 $$\frac{|\lambda|^{n_2}}{n_1! n_2!}\Big(\int \frac{d\,\underline{x}}{\nu}\frac{C_\alpha}{1+\nu^\alpha|\underline{d}_{\beta,L}(\underline{x})|^\alpha}\Big)^{n_1+n_2-1}\cdot\Big(\sum_{\vec{x}} v(\vec{x})\Big)^{n_1}\cdot c_1^{n_1+1}\nu^{-1}\chi_\Lambda(\vec{y}_1)\delta(y_1) \qquad (7.24)$$

if we do not perform the integral over the center $\underline{y}_1$ of the cluster Q_1 which certainly exists because $n_2 \geq 1$: this expresses the cancellation in (7.18) between the terms arising from the first truncated expectation when one considers only the contributions from $-U$ out of the 2^n that are generated by expanding the sums in the first expectation (*i.e.* the terms corresponding to $n_2 = 0$).

We see that the difference (7.18) can be given the form

7.25 $$\sum_{\substack{n1,n2\geq 0\\ n_2\geq 1}} \lambda^{n_2}\int W(X,Y)\chi_\Lambda(Y)\,dX\,dY \qquad (7.25)$$

where $W(X,Y)$ is a translation invariant function expressible (as shown implicitly above) as a sum of a large number of tree graphs connecting the points in $Y\cup X$ with $X = (\underline{x}_1,\ldots,\underline{x}_{n_1}), Y = (\underline{y}_1,\ldots,\underline{y}_{n_2})$. Furthermore if one fixes the point $\underline{y}_1 \in Y$, say, the integral over the remaining points $X, Y^{(1)} = Y/\underline{y}_1$ is bounded, for a suitable choice of c_2, by

7.26 $$\int |W(X,\underline{y}_1,Y^{(1)})|\,dX\,dY^{(1)} \leq \varepsilon^{n_1-1}c_2^{n_1+n_2} \qquad (7.26)$$

having used Cayley's tree–counting formula to take into account of the sum over the spanning trees and having set $\varepsilon = \sum_{\vec{x}}|v(\vec{x})|$. We shall show in Appendix A1 that (7.26) holds as well without imposing an ultraviolet cut–off.

Hence we can write the difference in (7.18) with the notations of 4, see (4.7), as

7.27 $$\beta(P_\ell(\beta,\mu_0;\lambda) - P_\ell(\beta,\mu_0) = \ell^{-d}\sum_{\substack{n1,n_2\geq 0\\ n_2\geq 1}}\lambda^{n_2}\int W(X,Y)\,\chi_\Lambda(Y)dXdY \qquad (7.27)$$

which has the same structural properties as the first of (4.7) and we can therefore proceed in the same way as in 4, 5, with (7.26) playing the role of (3.3), to derive for a system of fermions on a lattice:

(V) Large deviation property 5:

Let β, μ_0 be fixed arbitrarily and let ρ_0 be the corresponding density (so that $\rho_0 = \rho(\beta,\mu_0)$). Suppose that the $\sum_{\vec{x}}|v(\vec{x})| = \varepsilon$ is small enough, depending on β,μ_0. If the side ℓ of the box Λ tends to infinity and, correspondingly, the container side also tends to infinity so that $L/\ell \to \infty$ then

7.28 $$\lim_{\ell\to\infty}\ell^{-d}\log\sum_{\rho\in[a,b]}\Pi(\rho\ell^d) = \max_{\rho\in[a,b]} -\beta\,\Delta F(\beta,\rho,\rho_0) \qquad (7.28)$$

This holds if the interval $[a,b]$ is contained in an interval $[-\delta_0(\beta,\mu_0),\,\delta_0(\beta,\mu_0)]$ centered at ρ_0 with $\delta_0(\beta,\mu_0)=c_2^{-1}\nu^{(d+2)}>0$ small enough.

We note that we can replace $v(\underline{x})$ by $|v(\underline{x})|$ in the bounds above: hence repulsivity of the potential is not necessary and has not been mentioned in the statement above. This reflects an essential difference between lattice and continuum systems, see concluding remark (7).

To conclude the proof we refer to Appendix A1 where we prove (7.25). The inequality (7.26) is studied in [BGPS94]: sec. 3 of that reference is in fact dedicated to a detailed analysis of the ultraviolet problem in a case which is more involved than the present one. See appendix A1 below.

8. Conclusions.

(1) In the cases of Boltzmann statistics with arbitrary β,μ_0 or in the case of Bose statistics with $ze^{2\beta B}<1$ the Ginibre representation allows us to regard the quantum gas as a classical gas of contours, at least for the purposes of computing the partition function or the probability distribution of the number of particles in a given region. This is so because the integration measure over the trajectories is with a positive definite measure $d\mathbf{\Omega}$. Hence we can apply the arguments used in the general derivation of the large deviations formulae from the theory of the equivalence of ensembles of [La72] as done in the classical case in [Ol88]. The applicability of such methods found an early application in the work of Ginibre, see [Gi72] p. 362. Naturally we called the results "weaker" because we did not get the "total" control on the free energy and the accurate treatment of the finite size effects that (3.3) and (3.6) allow us to derive, but the extra generality is nevertheless remarkable.

(2) The above analysis admits a straightforward extension to electron–phonon systems because of the remarks in [GGV70], see also [Gi71], p. 420.

(3) We have also implicitly obtained that the asymptotic behavior of (4.3) (when $\ell\to\infty$, $L\to\infty$ and $\Lambda/\ell\to\infty$) is the *same to leading order* as that of the r.h.s. of (4.1), in the analyticity regions considered.

(4) The results for Fermi systems, aside from being restricted to lattice systems, considered in sec. 7 cover in the fernionic case a rather different region of the (β,μ_0)–plane, compared to the ones derived in sec. 4. They are valid at any fixed β,ρ (or at any β,μ_0) provided the coupling is small enough. Thus sec. 7 provides a stronger connection with the results for free fermions in [LLS99] which are implied by our results in the interval of density $(-\delta(\beta,\mu_0),\delta(\beta,\mu_0))$ in which the latter hold.

(5) It may seem that the obstacle to deriving a LD relation in the case of the Bose or Fermi statistics and in the region where genuinely quantum phase transitions can occur is related to the problem of showing boundary condition independence of the main extensive thermodynamic quantities. However this problem has been solved in many cases: in some cases, indeed, the technical estimates of its solution imply, see [Ro70] and [Gi71] p. 365, our equations (3.4) and (6.3), which have been the basis of our results in the first six sections of this paper; but in other cases, and we think of the paper [Pa85], boundary conditions independence can be proved for very general interactions (*e.g.* bosons with just superstable, if $d<4$, or superstable and repulsive interactions, if $d\geq 4$): but the result does not imply (6.3) and therefore it seems that LD needs more than just boundary condition independence. Perhaps (6.3) has to be replaced by estimates that involve all particles coherently, as in [Pa85], rather than single ones as it is essentially the case in the proofs of (6.3) (which depend on the finite size of the individual closed brownian paths).

(6) The results in sec. 7 are valid for small interactions: how small depends on β and μ_0. The only case in which a similar result can be found for a continuum system is the

$d=1$ case. If we consider a 1–dimensional continuum system we can proceed in the same way after replacing sums over $\vec{x}$ with integrals and using that the kinetic energy grows quadratically at ∞ so that the integral replacing the sum in (7.4) is still convergent: this is peculiar to $d=1$ so that the result does not extend to higher dimension *unlike the lattice case.* Of course if an ultraviolet cut–off is imposed on $\vec{k}$ the above analysis carries over to higher dimension: since ultraviolet cut–offs on the spatial momenta $\vec{k}$ *preserve reflection positivity* the result has some interest because it expresses properties of systems which are still Hamiltonian in spite of a "strange" form of the kinetic energy for large $\vec{k}^2$.

(7) The key bound (7.26) has been rederived here (see Appendix) but it is implicit in the analysis in [BGPS94], Sec. 3, where the more complex problem of the ultraviolet stability in one dimensional Fermionic systems has been treated in detail. We have not simply referred to [BGPS94] for the sake of completeness (the result is somewhat hidden there as the concern was about different topics). It would be interesting to prove that the inequality (7.23) holds in spite of the fact that the L_1 norm of the Fourier transform of g is infinite; or, alternatively, to show that it does not hold so that the proof that we reproduce in Appendix A1 for (7.25), (7.26), *independent of* the validity of the bound (7.23), is in a sense optimal.

Acknowledgements: We are indebted to H.T. Yau and H. Spohn for several discussions and examinations of alternative methods.

A1. Appendix: Proof of (7.25), (7.26).

We shall represent the Grassmanian fields η in (7.13) as $\overline{\eta}^{\pm}+\psi^{\pm}$ where $\overline{\eta}$ has propagator $\overline{g}(\underline{x}-\underline{y})$ as defined in (7.8) while ψ has propagator, see (7.8), $-\chi(x_0)\delta_{\vec{x},\vec{0}}$.

The Grassmanian integrals in (7.13) will be written as double integrals: for instance the numerator in (7.13) will be written

A1.1
$$\int P(d\overline{\eta})\int P(d\psi)e^{-U(\overline{\eta}+\psi)+\beta\lambda N_\Lambda(\overline{\eta}+\psi)} \tag{A1.1}$$

The difference with the corresponding treatment in [BGPS94] is that we use the simplicity of the propagator of ψ to perform explicitly the integration over ψ. The integration over ψ in (A1.1) can be performed via the formula (7.16) and we replace (7.17) by

A1.2
$$\frac{1}{\beta|\Lambda|}\Big[\mathcal{E}^T_{\overline{\eta}}\left(\mathcal{E}^T_\psi(e^{-U(\overline{\eta}+\psi)+\beta\lambda N_\Lambda(\overline{\eta}+\psi)})\right)-\mathcal{E}^T_{\overline{\eta}}\left(\mathcal{E}^T_\psi(e^{-U(\overline{\eta}+\psi)})\right)\Big] \tag{A1.2}$$

The evaluation of $\mathcal{E}^T_\psi(e^{-U(\overline{\eta}+\psi)+\beta\lambda N_\Lambda(\overline{\eta}+\psi)})$ is similar to that of $\mathcal{E}^T(e^{-U(\eta)+\beta\lambda N_\Lambda(\eta)})$ in (7.18) through (7.19) above. The $\mathcal{E}^T_\psi$ will be a function expressed as a sum of Grassmanian monomials in the fields $\overline{\eta}$: each such monomial will arise as a "value" of a suitable graph according to a (classical) procedure that we proceed to describe.

Since U and N_Λ depend upon $\overline{\eta}+\psi$ we develop the monomials in U and N_Λ obtaining a sum of 20 monomials in ψ with coefficients that depend on $\overline{\eta}$ (16 from U and 4 from N_Λ): each of such terms can be represented graphically by a graph like those in Fig. 1 in 7 in which one or more of the solid lines is replaced by a dashed line (hence we get 16 different graphs from the first and 4 different ones from the second): the dashed lines represent the Grassmanian fields ψ while the solid lines represent the fields $\overline{\eta}$.

For instance a graph with 3 solid lines and one dashed line will represent $\overline{\eta}^+_x\overline{\eta}^-_x\overline{\eta}^+_{x'}\psi^-_{x'}$ if in Fig. 1 above a dashed line has replaced the solid line entering x'.

Keeping the notation introduced in 7 we can say that while in the approach attempted in §7 we had just two types of clusters (denoted P or Q) we now have 20 different types of *clusters* symbolically represented by "*graphs elements*" like those in Fig. 1 but with one or more solid lines replaced by dashed ones. The different types of graphs elements will be labeled with a label $j = 1, 2, \ldots, 16, 17, \ldots, 20$: the last 4 will be the ones generated by the second graph element in Fig. 1 (*i.e.* by the graph element with two lines only).

The truncated expectation $\mathcal{E}^T_\psi$ is computed according to the usual rules: namely we must form all possible graphs γ with $n = \sum_{j=1}^{20} n_j$ clusters, of which n_j are of type j, in which the dashed lines are pairwise contracted or "paired" to form oriented dashed lines connecting nodes of graph elements *so that no dashed line is left out "unpaired" and the graph obtained is a connected graph* γ. The wavy lines present in the first 16 graph elements must taken into account in checking whether or not a graph is connected.

The "value" of a graph will be a monomial in the Grassmanian variables $\overline{\eta}$ rather than just a number as it was the case in 7.

Consider a graph γ formed from n_j clusters $P_{j,i}$, $i = 1, \ldots, n_j$, of type $j = 1, \ldots, 16$ or $Q_{j,i}$, $i = 1, \ldots, nj$ of type $j = 17, \ldots$, with a total of $2n_{dash}$ of dashed lines. Then γ will represent a monomial in the fields $\overline{\eta}$ that we denote $\pi_\gamma(PQ)$ and which is the product of the fields $\overline{\eta}$ associated with the solid lines (all of which remain "unpaired" because pairing only concerns the dashed lines, *i.e.* the fields ψ) of the clusters.

Since the propagator of a pair of fields $\psi^-_{\vec{x}}, \psi^+_{\vec{x}'}$ is $-\delta_{\vec{x}-\vec{x}'}\chi(x_0 - x'_0)$ a factor $(-1)^{n_{dash}}$ has to be added *together with all the Kronecker deltas and all the* $\chi(\cdot - \cdot)$ *functions expressing that the various* $x_0 - x'_0$ *differences must have a definite sign.*

We call $\Delta(\gamma)$ the value of the product of such quantities: it has value $0, \pm 1$ and we denote P_j, Q_j the collection of the nodes of the clusters $P_{j,i}$ or $Q_{j,i}$ respectively. In conclusion the value of the graph γ can be written as

A1.3
$$\int \Big(\prod_{j=1}^{16} \big(\prod_{i=1}^{n_j} V(P_{j,i})\big) \frac{dP_j}{n_j!} \Big) \cdot \Big(\prod_{j=17}^{20} \big(\prod_{i=1}^{n_j} \lambda\chi_\Lambda(Q_{j,i})\big) \frac{dQ_j}{n_j!} \Big) \pi_\gamma(PQ)\, \Delta(\gamma) \tag{A1.3}$$

The key remark is that the graph γ *cannot contain any closed loop other than the ones formed by contracting lines that exit from the same graph element (giving rise to what are usually called "tadpoles") because the* χ *functions in the propagator of* ψ *force the* x_0*'s of the various nodes of the* 20 *graph types to be in increasing order in the direction of the arrows drawn on the dashed lines that are contracted.*

Note in fact that only the graph elements corresponding to the first 16 types contain fields computed at exactly equal times (a necessary condition for the possibility of loops).

Therefore the number of graphs γ which are all trees is not bigger than $(\sum_{j=1}^{20} n_j)!$ and we can use $(\sum_{j=1}^{20} n_j)!/\prod_j n_j! < 20^{\sum_j n_j}$ in estimating the number of different monomials that we can get in the construction. The number of graphs which are not trees because of tadpoles is not much bigger (being bounded by $6^n n!$).

In this way we express $\mathcal{E}^T_\psi(e^{-U(\overline{\eta}+\psi)+\beta\lambda N_\Lambda(\overline{\eta}+\psi)}) = \log \mathcal{E}_\psi(e^{-U(\overline{\eta}+\psi)+\beta\lambda N_\Lambda(\overline{\eta}+\psi)})$ as a sum of monomials in the fields that we can "*clusters*" and which can be represented graphically in a way similar to the one used in Fig.1, Sec. 7, to represent the monomials in $-U(\eta) + \beta\lambda N_\Lambda(\eta)$; namely as in the following figure Fig.2

and analytically as

A1.4
$$\begin{aligned}&\lambda^p \int V(\underline{x}_1, \ldots, \underline{x}_n, \underline{x}'_1, \ldots, \underline{x}'_n, \underline{z}_1, \ldots, \underline{z}_p) \big(\prod_{i=1}^p \chi_\Lambda(\underline{z}_i)\big) \cdot \\ &\cdot \overline{\eta}_{\underline{x}_1} \cdots \overline{\eta}_{\underline{x}_n} \cdots \overline{\eta}_{\underline{x}'_1} \cdots \overline{\eta}_{\underline{x}'_n} \big(\prod_{i=1}^n d\underline{x}_i\big)\big(\prod_{i=1}^p d\underline{z}_i\big)\end{aligned} \tag{A1.4}$$

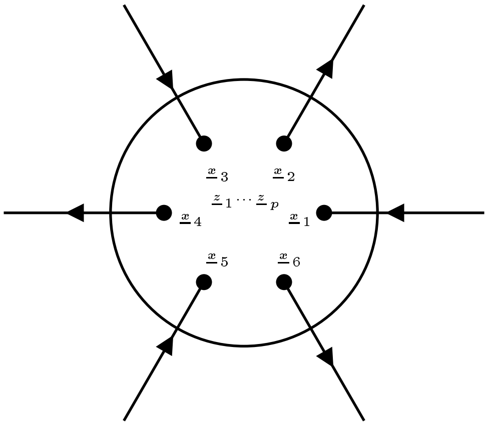

Fig.2: Illustration of a contribution to $\mathcal{E}^T_\psi$ in (A1.2) from a cluster generated by collecting all graphs γ which have 6 external lines and contain p graph elements of type > 16 with nodes at $\underline{z}_1, \ldots, \underline{z}_p$. These are graphs that contribute with a monomial of the form $\overline{\eta}^+_{\underline{x}_1}\overline{\eta}^+_{\underline{x}_3}\overline{\eta}^+_{\underline{x}_5}\overline{\eta}^-_{\underline{x}_2}\overline{\eta}^-_{\underline{x}_4}\overline{\eta}^-_{\underline{x}_6}$.

The V function is obtained by collecting and summing contributions from graphs γ which lead to a monomial of the degree $2n$ in the $\overline{\eta}$ fields and contain p graph elements with only two lines. Such contributions will admit, if $p \geq 1$, the bound

A1.5
$$\int |V(\underline{x}_1, \ldots, \underline{x}_n, \underline{x}'_1, \ldots, \underline{x}'_n, \underline{z}_1, \ldots, \underline{z}_p)|\, d\underline{x}\, d\underline{x}'\, d\underline{z}_2 \ldots d\underline{z}_p < c_2^{n+p} \qquad (A1.5)$$

Note that the kernel V may contain some delta functions (or Kronecker deltas) as it happens already in the corresponding representation for $-U$ and $\lambda\beta N_\Lambda$ described after (7.12).

We do not discuss further details because the technique has been used many times in the literature and in particular in [BGPS94]. The validity of the bound in (A1.5) is an immediate consequence of the fact that all the graphs that contribute to V are connected. This means that in the graph value one can associate a factor $v(\vec{x} - \vec{x}')\delta_{x_0 - x'_0}$ to each wavy line that connects $\underline{x}$ and $\underline{x}'$ or a factor $\delta_{\vec{x},\vec{x}'}$ (while no decay is present in the $x_0 - x'_0$) if the points are linked by a dashed line. *The lack of decay in the x_0 variables is not a problem because the x_0's vary in a finite interval* $[0, \beta]$. The combinatorics requires some care and the analysis is based on the remark following (A1.4) and is also discussed in [BGPS94], for instance.

We can now proceed to the integrations over the $\overline{\eta}$ fields.

The procedure is the same as the one above. A minor difference is that we have now *infinitely many graph elements*: namely all the ones of the form illustrated in Fig.1 and in (A1.4). This is not really a big difference because we have the bound (A1.5) which will allow us to control the proliferation of graph elements.

This time we can get, however, graphs with loops and we cannot control their number unless we are willing to obtain bounds that grow factorially with the size of the graph. To avoid the appearance of factorials we must collect many graphs together; or we must compute the expectations by using Lesniewsky's formula to avoid getting combinatorially large contribution.

The idea is that this time the propagator $\overline{g}$ of the fields $\overline{\eta}$, that we have to integrate, has a finite L_1 norm, as pointed out in the comment to (7.10), so that we can apply the formula (7.23).

Furthermore the second truncated expectation appearing in (A1.2) will not contain any term with $p > 0$ (of course), but it will otherwise coincide with the expression of the first expectation. So that the difference of the two will be given simply by the sum of the terms with $p > 0$. And combining (A1.4) with (7.23) one gets an expression like (7.25) and the bound (7.26) with the symbols $\underline{x}_1, \ldots$ and $\underline{z}_1, \ldots$ taking the place of the X and Y respectively.

Logically we avoided proving the estimate (7.23) for the full η integration, and we still do not know whether such an estimate is really valid. This has been done by performing *exactly* the (relatively) simple integral over the component ψ of the Grassmanian field $\eta = \overline{\eta} + \psi$ which is responsible for the summability problem described in the comments to (7.23). In this way it becomes clear that the logarithmic divergence of the L_1 norm of the Fourier transform of the propagator cannot really cause problems in the estimates that we need for the purposes of proving (7.26) and the LD relation 5 of 7.

It is worth stressing that the problem that we studied in this appendix (originally solved in [BGPS94]) is usually considered "irrelevant" in most of the literature: in condensed matter Physics it is very common to find that the infrared problems are directly attacked by *assuming that the propagator contains an ultraviolet cut–off* both on the $\vec{k}$ and the k_0 components.[5] This is done even in works in which the authors are aware that a cut–off on k_0 is very difficult to interpret because it breaks the reflection positivity of the theory, *i.e.* makes it "non Hamiltonian".

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[5] In the present context this means taking as propagator the g_i in (7.5) which of course allows to derive the (7.23) with no effort and save the analysis of this appendix.

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