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Wim Magnus, Fons Brosens

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*Highlights (for review)

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Highlights
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* quantum canonical ensemble
* bosons and fermions
* projection operator
* Fock space
* free energy, chemical potential, occupation numbers

Occupation numbers in a quantum canonical ensemble: a projection operator approach

Wim Magnus[a,b,*], Fons Brosens[c]

[a]imec, Kapeldreef 75, B-3001 Leuven, Belgium
[b]Universiteit Antwerpen, Physics Department, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium
[c]Universiteit Antwerpen, Physics Department, Universiteitsplein 1, B-2610 Antwerpen, Belgium

Abstract

Recently, we have used a projection operator to fix the number of particles in a second quantization approach in order to deal with the canonical ensemble. Having been applied earlier to handle various problems in nuclear physics that involve fixed particle numbers, the projector formalism was extended to grant access as well to quantum-statistical averages in condensed matter physics, such as particle densities and correlation functions. In this light, the occupation numbers of the subsequent single-particle energy eigenstates are key quantities to be examined. The goal of this paper is 1) to provide a sound extension of the projector formalism directly addressing the occupation numbers as well as the chemical potential, and 2) to demonstrate how the emerging problems related to numerical instability for fermions can be resolved to obtain the canonical statistical quantities for both fermions and bosons.

Keywords: quantum statistics, canonical ensemble, fermions, bosons

1. Introduction

In a previous paper [1] we proposed a projection operator for dealing with the particle number constraint in the framework of the canonical ensemble (CE). As a result, a transparent integral representation was obtained for the partition function $Z_N(\beta)$ [1] of

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[1]The interpretation of β should be handled with care. Thermal equilibrium means that the internal energy U_N is stable in time, and β is in essence a Lagrange multiplier for imposing that stability, rather than a

N identical indistinguishable fermions or bosons:

$$Z_N(\beta) = \frac{1}{2\pi} \int_{-\pi}^{\pi} G(\beta, \theta)\, \mathrm{e}^{-\mathrm{i}N\theta}\, \mathrm{d}\theta \quad ; \quad G(\beta, \theta) = \mathsf{Tr}\left(\mathrm{e}^{-\beta\hat{H}} \mathrm{e}^{\mathrm{i}\hat{N}\theta} \right), \tag{1}$$

in which the Hamiltonian $\hat{H}$ and the number operator $\hat{N}$ are of course assumed to be compatible operators. The trace of $G(\beta, \theta)$ is to be taken over the entire Fock space and the angular integration takes care of the projection onto the N-particle subspace. Whereas the formal aspects of the corresponding projection operator have been discussed extensively in Ref. [1], it should be noted that the core of the projector technique essentially reduces to a well-known integral interpretation of the Kronecker delta,

$$\delta_{n,m} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(n-m)\theta}\, \mathrm{d}\theta, \tag{2}$$

holding for any two integers n and m. Moreover, the sharply imposed restriction to the N-particle subspace entails a major difference between the CE and the grand-canonical ensemble (GCE): whereas the latter merely fixes the expectation value of the particle number operator $\hat{N}$, the former is exclusively pointing to the particular subspace addressed by an eigenvalue N of $\hat{N}$.

In principle, the projector approach is applicable to interacting particles, but exactly solvable systems of this kind are extremely rare. Mostly, one has to rely on perturbational or variational treatments, starting from non-interacting particles with supposedly known eigenstates and energy levels. As an example, we quote various studies [2, 3, 4, 5, 6, 7] having applied the projector operator technique in a quite beneficial and successful way. Furthermore, the extension [1] of the method enabling the explicit calculation of correlation functions, paved the way towards systematic explorations in condensed matter physics. A workable and reliable algorithm yielding the particle occupation numbers (or, equivalently, the distribution functions) is paramount in this respect, while being the main subject of this paper. In order to keep the course of the theory self-contained, we briefly return to the very basics of the projector formalism.

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given quantity. The internal energy $U_N(\beta) = -\mathrm{d}(\ln(Z_N(\beta)))/\mathrm{d}\beta$ is in fact the fixed quantity. This correct interpretation of the principle of maximum entropy in thermal equilibrium was treated in Appendix A of [1].

Given a system of non-interacting bosons or fermions, the Hamiltonian $\hat{\mathsf{H}}$ and the number operator $\hat{\mathsf{N}}$ can then be expressed in terms of the single-particle energy spectrum ϵ_k, where k denotes any set of generic quantum numbers properly labeling the single-particle energies:

$$\hat{\mathsf{H}} = \sum_k \hat{n}_k \epsilon_k \quad ; \quad \hat{\mathsf{N}} = \sum_k \hat{n}_k \quad ; \quad \hat{n}_k = c_k^\dagger c_k, \tag{3}$$

where the creation and destruction operators $c_k^\dagger$ and c_k satisfy appropriate (anti)commutation relations, i.e.

$$\hat{c}_k^\dagger \hat{c}_{k'}^\dagger - \xi \hat{c}_{k'}^\dagger \hat{c}_k^\dagger = \hat{c}_k \hat{c}_{k'} - \xi \hat{c}_{k'} \hat{c}_k = 0 \; ; \; \hat{c}_k \hat{c}_{k'}^\dagger - \xi \hat{c}_{k'}^\dagger \hat{c}_k = \delta_{k,k'} \; ; \; \xi = \begin{cases} +1 & \text{for bosons,} \\ -1 & \text{for fermions.} \end{cases} \tag{4}$$

As detailed in [1], the projector formalism enables an unrestricted summation over the occupation numbers n_k entering the expression for $G(\beta, \theta)$:

$$G(\beta, \theta) = \mathsf{Tr}\left(e^{-\beta \hat{\mathsf{H}}} e^{i\hat{\mathsf{N}}\theta}\right) = \prod_k \left(\sum_{n_k} \exp\left((i\theta - \beta\epsilon_k)n_k\right)\right). \tag{5}$$

Summing n_k from 0 to ∞ for bosons and from 0 to 1 for fermions, readily gives

$$G(\beta, \theta) = \prod_k \left(1 - \xi \exp\left(i\theta - \beta\epsilon_k\right)\right)^{-\xi}. \tag{6}$$

It should be noted, however, that the geometric series [2] leading to (6) for bosons ($\xi = +1$), only converges if $|\exp(i\theta - \beta\epsilon_k)| < 1$ holds for all k. The angular integration can equivalently be expressed as a complex contour integral along a circle with radius r enclosing the origin:

$$Z_N(\beta) = \frac{1}{2\pi i} \oint_{|z|=r} \frac{\tilde{G}(\beta, z)}{z^{N+1}} \, dz \quad ; \quad \tilde{G}(\beta, z) = \prod_k \left(1 - \xi z e^{-\beta\epsilon_k}\right)^{-\xi}. \tag{7}$$

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[2] Remarkably, the common ratio of a similar geometric series appearing in the grand-canonical partition function crucially depends on the grand-canonical chemical potential $\bar{\mu}(N)$. More specifically, as convergence requires the common ratio to be smaller than 1, $\bar{\mu}(N)$ is bound to be located below ϵ_0. The latter, in turn, requires that the single-particle ground-state energy be strictly positive. In this light, it is explicitly assumed that $\epsilon_0 > 0$ until the recurrence relations for the partition function and the occupation numbers are established. Afterwards, a simple gauge transformation consisting of a constant energy shift can be performed to generalize the results to the case of arbitrary, but finite values of ϵ_0.

The radius r should be chosen small enough to ensure that the contour $|z| = r$ does not enclose any of the poles of $\tilde{G}(\beta, z)$ appearing in the case of bosons. Though being a useful starting point for further investigations, the above integral representations do not generally lead to closed form expressions for Z_N or quantities derived from it. As an exception, we mention the special case of one-dimensional harmonic oscillators [3] that was solved analytically upon invoking two Euler identities [1]. Unfortunately, we overlooked the magisterial treatment of non-interacting fermions with equidistant single-particle energies by Schönhammer [8], that turns out to remain quite relevant to the present paper.

Although the projection operator approach was applied to derive generic expressions for the two- and four-point correlation functions, no detailed explicit results were reported in [1]. In section (2) we derive numerically tractable recurrence relations for both the chemical potentials and the occupation numbers, the latter being needed crucially to compute the correlation functions. In the same section we remedy the numerical instabilities that were prohibitive for extending the number of particles at will in the case of fermions [1]. In particular new results are presented addressing not only the occupation numbers but also the dependence of the chemical potential, the Helmholtz free energy, the internal energy and the entropy of the two-dimensional electron gas (2DEG) on the particle number.

2. Occupation numbers and chemical potential

Consider the occupation number $g_{k,N}(\beta)$, defined as the expectation value $\left\langle \hat{c}_k^\dagger \hat{c}_k \right\rangle_{\beta,N}$ of the N-particle system (3):

$$g_{k,N}(\beta) = -\frac{1}{\beta} \frac{1}{Z_N(\beta)} \frac{\partial Z_N(\beta)}{\partial \epsilon_k}. \qquad (8)$$

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[3] Formula (25) in [1] contains a serious misprint, and should read

$$Z_N(\beta) = \frac{1}{\prod_{k=1}^{N} \left(1 - e^{-k\beta\hbar\omega}\right)} \times \begin{cases} e^{-N\beta\hbar\omega/2} & \text{for bosons,} \\ e^{-N^2\beta\hbar\omega/2} & \text{for fermions.} \end{cases} \qquad (25)$$

Temporarily disregarding the trivial result $g_{k,N=0}(\beta) = 0$, one readily obtains from the representation (7)

$$g_{k,N}(\beta) = \frac{e^{-\beta\epsilon_k}}{Z_N(\beta)} \frac{1}{2\pi i} \oint_{|z|=r>0} \frac{\tilde{G}(\beta, z)}{1 - z\xi e^{-\beta\epsilon_k}} \frac{1}{z^N} dz. \tag{9}$$

Because of the pole of order N in the origin, the residue theorem yields

$$g_{k,N}(\beta) = \frac{1}{Z_N(\beta)} \frac{e^{-\beta\epsilon_k}}{(N-1)!} \frac{\partial^{N-1}}{\partial z^{N-1}} \frac{\tilde{G}(\beta, z)}{1 - \xi z e^{-\beta\epsilon_k}}\Bigg|_{z=0}. \tag{10}$$

Using $\frac{\partial^j}{\partial z^j} \frac{1}{1-az} = \frac{j!a^j}{(1-az)^{j+1}}$ and $\frac{\partial^n \tilde{G}(\beta,z)}{\partial z^n}\Big|_{z=0} = n!\, Z_n(\beta)$ in Leibniz' differentiation rule for function products, one ends up with

$$g_{k,N}(\beta) = \sum_{j=1}^{N} \xi^{j-1} e^{-j\beta\epsilon_k} \frac{Z_{N-j}(\beta)}{Z_N(\beta)}. \tag{11}$$

Separating the first term ($j = 1$) and substituting $j \to j-1$ into the remaining sum, one immediately recognizes a recurrence relation

$$g_{k,N}(\beta) = \left(1 + \xi g_{k,N-1}(\beta)\right) e^{-\beta\epsilon_k} \frac{Z_{N-1}(\beta)}{Z_N(\beta)}, \tag{12}$$

that was earlier obtained by Schmidt [9] and exploited by Schönhammer to treat fermionic systems ($\xi = -1$) (see Eq. (19) of [8]).

If $\epsilon_{k=0}$ had to be shifted to a positive value in order to avoid spurious poles in the complex plane, one might choose to undo the corresponding gauge transformation at this point since all complex integrations required to set up the recurrence relation are carried out.

Introducing the standard definition of the chemical potential [4] in the CE,

$$\mu_N(\beta) = F_{N+1}(\beta) - F_N(\beta) \quad \text{with} \quad Z_N(\beta) = e^{-\beta F_N(\beta)}, \tag{13}$$

and using $\sum_k g_{k,N}(\beta) = N$, one obtains

$$g_{k,N} = e^{-\beta(\epsilon_k - \mu_{N-1})} \left(1 + \xi g_{k,N-1}\right), \tag{14}$$

$$e^{-\beta\mu_{N-1}} = \frac{1}{N} \sum_k e^{-\beta\epsilon_k} \left(1 + \xi g_{k,N-1}\right), \tag{15}$$

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[4]In Eq. (12) of [8] $F_N - F_{N-1}$ was used to define μ_N, rather than Eq. (13) in the current paper.

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where the temperature parameter β (considered to be fixed for the time being) was omitted as an argument for the sake of notation's simplicity in the subsequent calculations. The initialization of the above recurrence relations is simple:

$$g_{k,0} = 0 \quad ; \quad e^{-\beta\mu_0} = \sum_k e^{-\beta\epsilon_k}. \tag{16}$$

Note that $e^{\beta\mu_{N-1}}$ is the basic numerical quantity for implementing the recurrence relations. At the end of the calculations the chemical potential itself and, hence, also the free energy can be easily obtained.

Anticipating the numerical implementation the relation to the GCE may be beneficially established at this point by comparison with the distribution function of the GCE, i.e.

$$f_k(\mu) = \frac{1}{e^{\beta(\epsilon_k - \bar{\mu}_N)} - \xi} \quad ; \quad \sum_k f_k(\bar{\mu}_N) = N, \tag{17}$$

where $\bar{\mu}_N$ (to be distinguished from μ_N) denotes the chemical potential in the GCE.

For arbitrary values of N and N' the relation between $g_{k,N-1}$ and $f_k(\bar{\mu}_{N'})$ can be further elucidated. Assuming the validity of the generic inequality, $0 \leq g_{k,N-1} \leq g_{k,N}$, recurrence relation (14) immediately implies

$$g_{k,N-1} \leq f_k(\mu_{N-1}). \tag{18}$$

Furthermore, using the identity $1 = (e^{\beta(\epsilon_k - \mu_{N-1})} - \xi) f_k(\mu_{N-1})$ to replace 1 in the factor $(1 + \xi g_{k,N-1})$ of (14), we are left with an alternative formulation of the original recurrence relation:

$$g_{k,N} = f_k(\mu_{N-1}) + \xi e^{-\beta(\epsilon_k - \mu_{N-1})} \left(g_{k,N-1} - f_k(\mu_{N-1})\right). \tag{19}$$

Combining (19) with (18) for fermions, we may infer $g_{k,N} \geq f_k(\mu_{N-1})$, thus arriving at

$$f_k(\mu_0) \leq g_{k,1} \leq \cdots \leq f_k(\mu_{N-1}) \leq g_{k,N} \leq f_k(\mu_N) \leq \cdots \quad \text{for fermions.} \tag{20}$$

For bosons ($\xi = +1$) we were unable to find a similar ladder relation, but the inequality (18) can now be replaced by a stronger one:

$$g_{k,N} \leq f_k(\mu_{N-1}) \quad \text{for bosons.} \tag{21}$$

At this point, the simultaneous treatment of bosons and fermions becomes a hindrance rather than a convenience and, hence, we treat fermions and bosons separately in the following sections.

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3. Boson occupation numbers

For bosons ($\xi = +1$), the recurrence relations (14) and (15) now become

$$g_{k,N} = e^{-\beta(\epsilon_k - \mu_{N-1})} (1 + g_{k,N-1}),\qquad(22)$$

$$e^{-\beta\mu_{N-1}} = \frac{1}{N} \sum_k e^{-\beta\epsilon_k} (1 + g_{k,N}).\qquad(23)$$

As commonly known, the GCE chemical potential that fixes the *average* number of particles rather than the actual, integer number of particles, does not exceed the single-particle ground state energy ϵ_0. Accordingly, it is quite tempting to consider ϵ_0 as well as a rigorous upper bound for any μ_N, although the formal proof turns out to be less trivial than in the GCE case (see Appendix A). The restriction $\mu_N < \epsilon_0$ ensures the numerical stability of the encoded recurrence relations (22–23), although one may have to remedy some overflow and underflow deficiencies appearing in the case of extremely low temperatures.

As an example, we treat bosonic harmonic oscillators, omitting however the vacuum energy for the sake of simplicity in the subsequent work. If desired, it can be restored at the end of the calculation. Accordingly, we consider the Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}},\qquad(24)$$

where the components of $\mathbf{k}$ are non-negative integers and the energy spectrum is given by

$$\epsilon_{\mathbf{k}} = \hbar\omega \sum_{j=1}^{D} k_j \quad ; \quad k_j = 0, 1, \cdots, \infty.\qquad(25)$$

D is the spatial dimension (1, 2 or 3 at will). In view of the rapidly growing degeneracy, it proves more natural to relabel the single-particle energy levels in terms of a shell index q, pointing to an energy shell of states that share a common energy $\tilde{\epsilon}_q$ with a dimension dependent degeneracy d_q:

$$q = 0, 1, 2, 3, \ldots \quad ; \quad \tilde{\epsilon}_q = \hbar\omega q \quad ; \quad d_q = \begin{cases} 1 & \text{if } D = 1, \\ q + 1 & \text{if } D = 2, \\ (q+1)(q+2)/2 & \text{if } D = 3. \end{cases}\qquad(26)$$

The occupation numbers $g_{\mathbf{k},N}$ having the same degeneracy as $\epsilon_{\mathbf{k}}$, $\tilde{g}_{q,N}$ denote the occupation number of any particular state in the energy shell $\tilde{\epsilon}_q$, that, in turn, determines the energy occupation probability $p_{q,N}$ of all energy levels in shell

$$p_{q,N} = \frac{1}{N} d_q \tilde{g}_{q,N}. \tag{27}$$

The recurrence relations (22–23) for $\tilde{g}_{q,N}$ become

$$\tilde{g}_{q,N} = e^{-\beta(\hbar\omega q - \mu_{N-1})} \left(1 + \tilde{g}_{q,N-1}\right) \tag{28}$$

$$e^{-\beta\mu_{N-1}} = \frac{1}{N} \sum_{q=0}^{\infty} d_q e^{-\beta \quad} \left(1 + g_{q,N-1}\right), \tag{29}$$

and are now initialized by

$$\tilde{g}_{q,N=0} = 0 \quad ; \quad \tilde{g}_{q,N=1} = e^{-\beta \quad} e^{\beta\mu_0} = e^{-\beta\hbar\omega q} \left(1 - e^{-\beta\hbar\omega}\right)^D, \tag{30}$$

where the required summation in $\mu_0(\beta) = -(1/\beta) \sum_k e^{-\beta\epsilon_k}$, as appearing in Eq. (16), was done analytically.

In one dimension ($D = 1$), one can check by induction that

$$\tilde{g}_{q,N}\big|_{1D} = \sum_{j=1}^{N} e^{-\beta\hbar\omega q j} \prod_{m=N+1-j}^{N} \left(1 - e^{-\beta\hbar\omega m}\right), \tag{31}$$

$$e^{\beta\mu_N}\big|_{1D} = 1 - e^{-\beta\hbar\omega(N+1)}, \tag{32}$$

which is useful to monitor the numerical recursion work, because it is tractable with symbolic algebra with only 2 independent parameters, namely N and the dimensionless temperature $\tau = 1/(\beta\hbar\omega)$.

For 10^3 oscillators the energy occupation numbers for the 1D case and the 3D case are shown in Fig. (1) and Fig. (2). Apparently, the profiles of the latter case attain maximum levels as a direct consequence of the non-trivial 3D degeneracy factors d_q. The evolution of the chemical potential (in units of $\hbar\omega$) as a function of the number of particles is shown in Fig. (3) for 1D, and in Fig. (4) for 3D (solid lines). For the sake of comparison, also the corresponding GCE chemical potentials are shown. As expected, the chemical potentials of the CE deviate noticeably from their GCE counterparts for relatively small numbers of bosons. The difference can be explained by the observation

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that the GCE standard variation of the particle number operator $\hat{N}$ can be neglected with respect to the expectation value of $\hat{N}$ only for sufficiently large numbers of particles, whereas the CE standard variation equals zero for all N by construction.
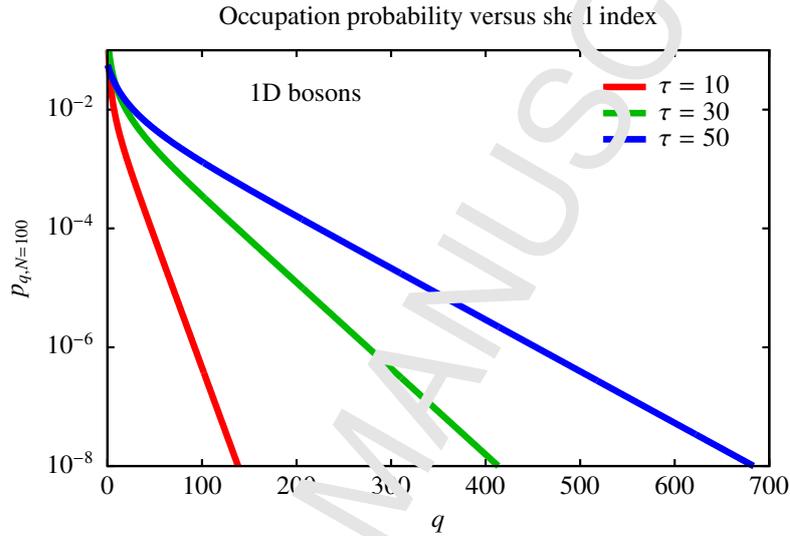
Occupation probability versus shell index

Figure 1: Probability $p_{q,N}$ of occupying energy level $\tilde{\epsilon}_q$ for 100 1D harmonic oscillators as a function of the shell index q, given three values of the dimensionless temperature $\tau = 1/(\beta\hbar\omega)$.

Furthermore, as an illustration, we have shown the temperature dependence of the chemical potential and the internal energy $U_N = \langle\hat{H}\rangle_N$ for 10, 100 and 1000 3D harmonic oscillator bosons in Fig. (5) and Fig. (6) respectively. As expected, the bosonic nature is most pronounced in the low temperature regime ($\tau < 4$), whereas the internal energy matches the classical limit, i.e. $U_N(\tau) \to 3N\hbar\omega/(\exp(-1/\tau) - 1)$ at high temperatures

4. Fermion occupation numbers

For fermions ($\xi = -1$) the recurrence relations (14–15) obviously read

$$g_{k,N} = e^{-\beta(\epsilon_k - \mu_{N-1})}\left(1 - g_{k,N-1}\right), \tag{33}$$

$$e^{-\beta\mu_{N-1}} = \frac{1}{N}\sum_k e^{-\beta\epsilon_k}\left(1 - g_{k,N-1}\right). \tag{34}$$
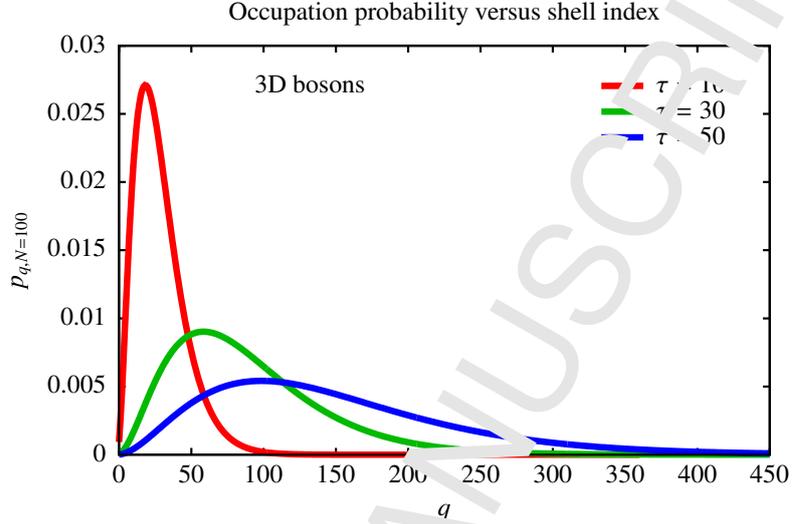
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Occupation probability versus shell index

Figure 2: Probability $p_{q,N}$ of occupying energy level $\bar{\epsilon}_q$ for 100 3D harmonic oscillators as a function of the shell index q, given three values of the dimensionless temperature $\tau = 1/(\beta\hbar\omega)$.

For the sake of convenience but without loss of generality, we may assume that k exclusively runs through non-negative integers labeling the energy eigenvalues ϵ_k in ascending order and starting at $\epsilon_0 = 0$.

The recursive solution of (33) and (34) is prone to numerical errors that propagate with k, while being proportional to $e^{-\beta(\epsilon_k - \mu_{N-1})}$. Dealing with fermions, however, we must abandon the requirement that the chemical potential be restricted to values below $\epsilon_0 = 0$, and realize that the sign of $\epsilon_k - \mu_{N-1}$ determines the magnitude of the numerical errors appearing in the recursive flow. Clearly, the error level decreases provided that $\mu_{N-1} < \epsilon_k$ for all k i.e. as long as $\mu_{N-1} < 0$. For sufficiently large N, however, the Helmholtz free energy attains a minimum, say at $N = N_{\min}$, beyond which $F_N > F_{N-1}$ and, hence, $\mu_{N-1} > 0$ holds. Phrased otherwise, once $N > N_{\min}$, the chemical potential crosses the energy spectrum and, in particular, the low energy section below μ_{N-1} causes the errors to grow exponentially. Moreover, the expression for $e^{-\beta\mu_{N-1}}$ in (34) shows that μ_{N-1} greedily accumulates the numerical errors on $g_{k,N-1}$. This explains in depth the numerical accuracy problem encountered in [1] where the recurrence relation for the partition function was directly addressed.
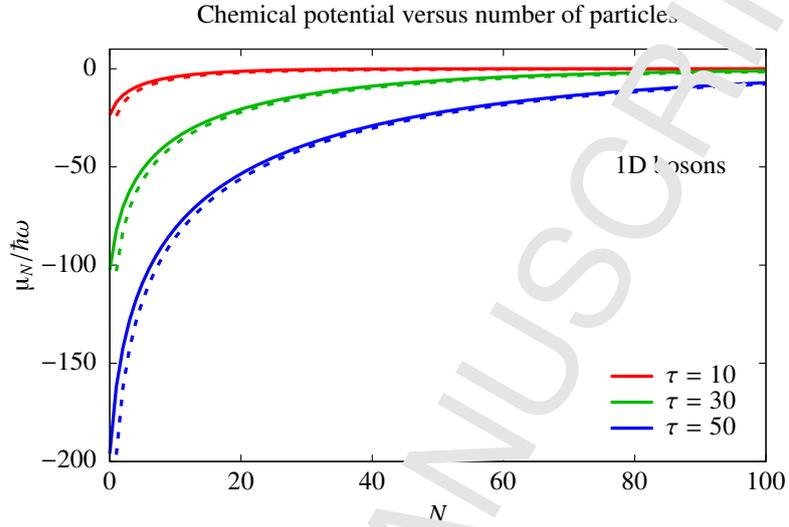
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Chemical potential versus number of particles

Figure 3: Scaled chemical potential $\mu_N/(\hbar\omega)$ for 1D bosonic harmonic oscillators as a function of the number of particles, given three values of the dimensionless temperature $\tau = 1/(\beta\hbar\omega)$. Solid and dashed curves correspond to CE and GCE results respectively.

For a typical 2DEG at room temperature and contained in a rectangle $0 \leqslant x \leqslant L_x$, $0 \leqslant y \leqslant L_y$, we found that $N_{\min} = 374$ for $L_x = L_y = 100$ nm. Bearing the latter in mind as well as the gradual deterioration of the results for $g_{k,N}$ and its cumulative effect on μ_{N-1}, to be expected when N exceeds $N_{\min}$, one may now understand why the results become totally unreliable and numerically unstable for $N > 520$ (even yielding negative values for the partition function). Being attributed loosely to the infamous sign problem for fermions [1], this issue is now clarified in greater detail by the error analysis of (33-34).

Fortunately, the narrow boundaries (20) enable detection and correction of any erroneous behavior of μ_{N-1} at an early stage if the temperature is not extremely low. (In that case a suitable Sommerfeld expansion might be appropriate.) When the inequality $g_{k,N-1} < f_k(\mu_{N-1})$ is violated for the first time at $k = 0$, the relative error on $e^{-\beta\mu_{N-1}}$ is still small. Since this happens for $N \gg 1$, we may anticipate the detrimental accumulation of numerical errors by exploiting the observation that the canonical distribution function converges to the grand-canonical one, when N grows arbitrarily large.
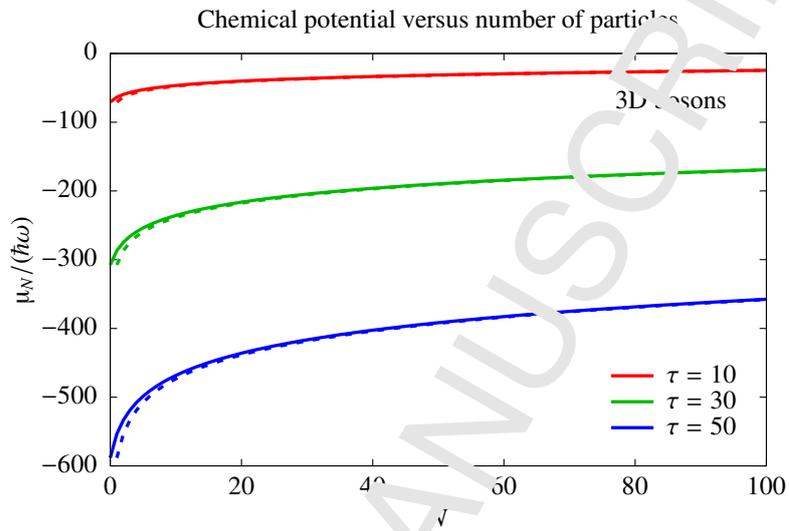
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Figure 4: Scaled chemical potential $\mu_N/(\hbar\omega)$ for 3D bosonic harmonic oscillators as a function of the number of particles, given three values of the normalized temperature $\tau = 1/(\beta\hbar\omega)$. Solid and dashed curves correspond to CE and GCE results respectively.
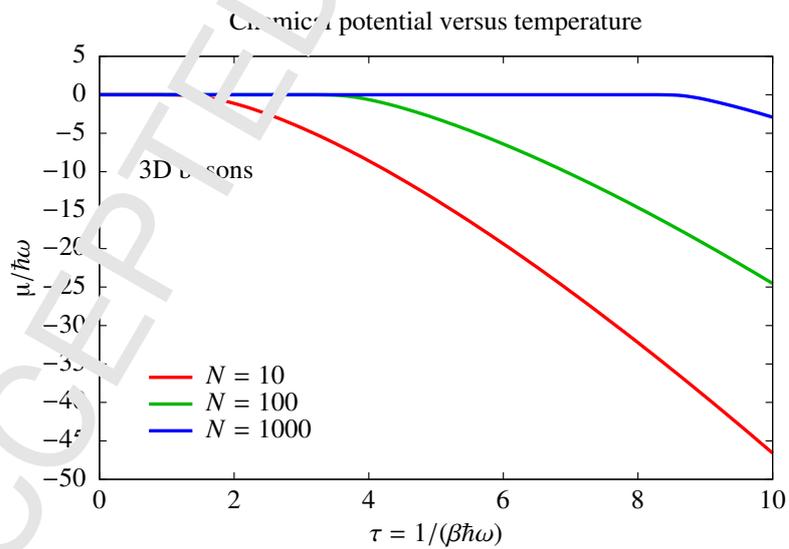

Figure 5: Scaled chemical potential $\mu_N/(\hbar\omega)$ for 3D bosonic harmonic oscillators as a function of the normalized temperature $\tau = 1/(\beta\hbar\omega)$, given three values of N, the number of particles.
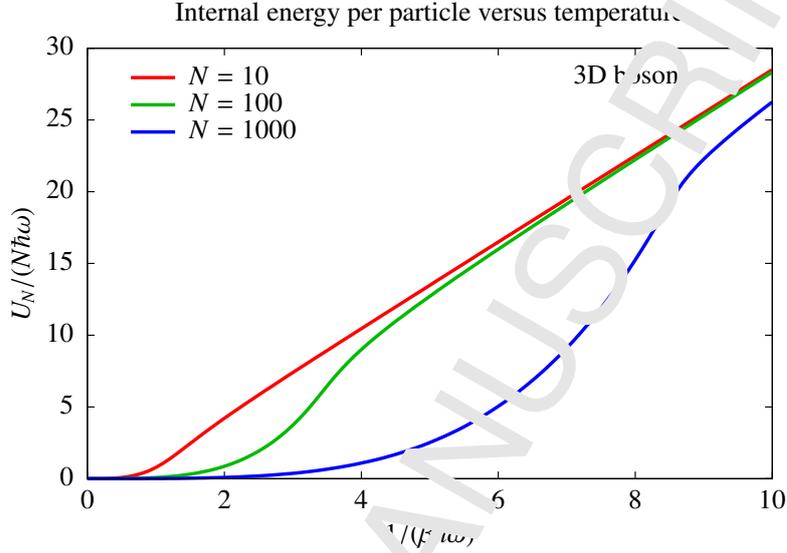
Figure 6: Scaled internal energy $U/(N\hbar\omega)$ for 3D bosonic harmonic oscillators as a function of the normalized temperature $\tau = 1/(\beta\hbar\omega)$, given three values of N, the number of particles.

Full knowledge of $f(\bar{\mu})$, though, would require us to solve the transcendental equation $\sum_k f_k(\bar{\mu}(N)) = N$ for $\bar{\mu} = \bar{\mu}(N)$, the grand-canonical chemical potential compatible with N particles. However, a first order Taylor expansion

$$f_k(\mu) = f_k(\bar{\mu}) + (\mu - \bar{\mu}) \left. \frac{\mathrm{d}f_k(\mu)}{\mathrm{d}\mu} \right|_{\mu=\bar{\mu}} + O\left((\mu - \bar{\mu})^2\right)$$

$$\rightarrow f_k(\mu) \approx f_k(\bar{\mu}) + \beta (\mu - \bar{\mu}) \, e^{\beta(\epsilon_k - \bar{\mu})} \left(f_k(\bar{\mu})\right)^2 \tag{35}$$

provides a sufficiently accurate approximation in most circumstances.

Let N_c be the lowest value of N for which the preceding occupation number $g_{k=0,N_c-1}$ erroneously exceeds $f_{k=0}(\bar{\mu}(N_c - 1))$ in the course of the recursion. Imposing the sum rule $\sum_k f_k(\mu_{N_c-1}) = N_c - 1$ in (35) then gives the correction

$$\beta\mu_{N_c-1} = \beta\bar{\mu}(N_c - 1) + \frac{N_c - 1 - \sum_k f_k(\bar{\mu}(N_c - 1))}{\sum_k e^{\beta(\epsilon_k - \bar{\mu}(N_c-1))} \left(f_k(\bar{\mu}(N_c - 1))\right)^2}. \tag{36}$$

For $N > N_c$, the recursion (33) of course becomes increasingly inaccurate, but since this is a regime of slowly varying μ_N with N, we keep using (35), with $\tilde{\mu}$ and μ being

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replaced respectively by μ_{N-1} and μ_N. Summing over k one thus finds

$$N > N_c \;:\; \beta\mu_N = \beta\mu_{N-1} + \frac{1}{\sum_k e^{\beta(\epsilon_k - \mu_{N-1})} \left(f_k(\mu_{N-1})\right)^2} \tag{37}$$

At any stage of the calculation one easily monitors the quality of the approach by checking whether $\sum_k g_k(\mu_N) = N$ remains valid. In case of failure however, we have no alternative approach available so far, and we are left with the fermion sign problem remaining unresolved for that particular case.

In order to test the procedure, we first apply it to a two dimensional (2D) electron gas for which Schönhammer [8] has developed an alternative approach by linearizing its energy spectrum. Comparison with our approach (see below) shows an excellent agreement.

5. Two-dimensional electron gas – linearized energy spectrum

Consider again a 2D electron gas in a rectangle $0 \leqslant x \leqslant L_x$, $0 \leqslant y \leqslant L_y$, with periodic boundary conditions imposed on the single-electron wave functions. Before linearization, the energy spectrum ($\cdot$) is expressed in terms of 2D wave vectors $k_{x,y} = 2\pi n_{x,y}/L_{x,y}$ as

$$\epsilon_k \to \epsilon_{n_x,n} = \frac{\hbar^2}{2m_e}\left[\left(\frac{2\pi n_x}{L_x}\right)^2 + \left(\frac{2\pi n_y}{L_y}\right)^2\right] \quad;\quad n_x, n_y = 0, \pm 1, \pm 2, \ldots \tag{38}$$

where m_e denotes the electron effective mass. Since we are dealing with fermions ($\xi = -1$), the recurrence relations (14–15) obviously read

$$g_{k,N} = e^{-\beta(\epsilon_k - \mu_{N-1})}\left(1 - g_{k,N-1}\right) \quad;\quad e^{\beta\mu_N} = \frac{N+1}{\sum_k e^{-\beta\epsilon_k}\left(1 - g_{k,N}\right)}. \tag{39}$$

While being valid for fermions with an arbitrary single-particle spectrum, the recurrence relation (39) turns out to coincide [5] with the one obtained by Schönhammer in Eq. (19) of Ref. [8], when applied to fermions with a linear energy spectrum. Focusing on the latter, we note that the density of states in 2D wave vector space equals $L_x L_y/(2\pi)^2$. On average, a circle with radius K thus encloses $n_K = \pi K^2 L_x L_y/(2\pi)^2$

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[5]Schönhammer adopts the definition $\mu_N = F_N - F_{N-1}$, whereas we use $\mu_N = F_{N+1} - F_N$.

states, the single-particle energy on the edge of the circle thus being $\epsilon_K \quad \hbar^2 K \quad (2m_e) = 2\pi\hbar^2 n_K/(m_e L_x L_y)$. For sufficiently large wave vectors, the single particle energies can therefore be replaced by a linearized spectrum

$$\tilde{\epsilon}_n = n\Delta \quad ; \quad \Delta = \frac{2\pi\hbar^2}{m_e L_x L_y} \quad ; \quad n = 0, 1, 2, \cdots, \tag{40}$$

resulting in the following recurrence relation, replacing (39)

$$g_{n,N}^{\text{lin}} = e^{-\beta\left(n\Delta - \mu_{N-1}^{\text{lin}}\right)} \left(1 - g_{n,N-1}^{\text{lin}}\right) \tag{41}$$

$$e^{\beta\mu_N^{\text{lin}}} = \frac{N+1}{\sum_{n=0}^{\infty} e^{-\beta n\Delta}\left(1 - g_{n,N}^{\text{lin}}\right)} \tag{42}$$

Clearly, the mere introduction of the linearized spectrum does not offer any improvement on the numerical accuracy. The latter goal may be reached most easily by implementing the analytical results obtained by Schönhammer [8]. Although it is tempting to translate his formulas literally, some care is required because he considers a spectrum $\epsilon_i = i\Delta$, $i = 1, 2, \cdots$. Of course, a gauge transformation relates both approaches, but applying it in detail to all intermediate relations and quantities is not a trivial task. Instead, a careful recalculation adopting the notation of (40) and following the approach we proposed in Sec. 4 of [1], yields the following results for the CE partition function Z_N^{lin}, the free energy F_N^{lin}, the internal energy U_N^{lin} and the chemical potential μ_N^{lin},

$$Z_N^{\text{lin}} = e^{-\beta N(N-1)\Delta/2} \prod_{n=1}^{N} \frac{1}{1 - e^{-\beta n\Delta}}, \tag{43}$$

$$F_N^{\text{lin}} = \frac{1}{2}N(N-1)\Delta + \frac{1}{\beta}\sum_{n=1}^{N} \ln\left(1 - e^{-n\beta\Delta}\right), \tag{44}$$

$$U_N^{\text{lin}} = \left(\frac{1}{2}N(N-1) + \sum_{n=1}^{N} \frac{n}{e^{n\beta\Delta} - 1}\right)\Delta, \tag{45}$$

$$\mu_N^{\text{lin}} = N\Delta + \frac{1}{\beta}\ln\left(1 - e^{-\beta(N+1)\Delta}\right). \tag{46}$$

The analytical expression for μ_N^{lin} given by Eq. (46) not only replaces the numerical iteration outlined in (41) and (42), but also enables the conversion of (41) into a recurrence

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relation connecting subsequent level numbers n for any **fixed** particle number N:

$$g_{0,N}^{\text{lin}} = 1 - e^{-\beta N \Delta}, \tag{47}$$

$$g_{n+1,N}^{\text{lin}} = 1 - e^{-\beta N \Delta} - \frac{e^{\beta \Delta (n+1)} - 1}{e^{\beta N \Delta}} g_{n,N}^{\text{lin}}, \tag{48}$$

$$\leftrightarrow \quad g_{n,N}^{\text{lin}} = \frac{e^{\beta N \Delta}}{e^{\beta \Delta (n+1)} - 1} \left(1 - e^{-\beta N \Delta} - g_{n+1,N}^{\text{lin}} \right). \tag{49}$$

as was already established by Schönhammer [8]. In order to remain fully self-contained, we (re)derive these equations in the spirit of the projector approach in Appendix B. Subtle differences in the intermediate results as compared to, for instance, Eqs. (15, 20) and (21) in [8] are due to the different energy scale (ground state energy $\epsilon_0 = 0$ in the present approach, but $\epsilon_0 = \Delta$ in [8]), and the above mentioned difference in the definition of the chemical potential.

The recurrence relation (48) is numerically accurate and stable as long as $e^{\beta N \Delta} > e^{\beta \Delta (n+1)} - 1$, i.e., $n < \ln \left(e^{\beta N \Delta} + 1 \right) / (\beta \Delta) - 1$. However, even if n is too large to fulfill this condition, numerical convergence based on Eq. (49) can still be achieved, provided one finds a valuable *initial* value of $g_{n,N}^{\text{lin}}$, compatible with sufficiently large n. The latter shouldn't be too difficult, since $\lim_{n \to \infty} g_{n,N}^{\text{lin}} = 0$. Suppose that $g_{n_c+1,N}^{\text{lin}}$ in (49) is negligible for some large enough n_c. Then $g_{n_c,N}^{\text{lin}}$ should satisfy $g_{n_c,N}^{\text{lin}} \ll 1$, i.e., $e^{\beta \Delta (N - n_c - 1)} \ll 1$ which makes it capable of initializing (49). In practice, we required this condition to be satisfied in double precision Fortran up to machine accuracy, but a less severe treatment should not harm, since the numerical error in (49) is self-correcting. The main purpose of the present section being the corroboration of our results by those obtained by Schönhammer for the linearized energy spectrum, we refer to [8] for a more detailed investigation of the latter.

6. Two-dimensional electron gas – quadratic energy spectrum

Finally, we revisit the ordinary 2DEG, characterized by the quadratic dispersion relation (23), and apply the numerical algorithm, iterating on the recursion relations (33 – 34) for $N \leq N_c$ and avoiding the numerical instability issues for $N > N_c$, as outlined in Eqs. (35 – 37). As an illustration, we show the chemical potential as a function of N in Fig. (7) for $T = 77$ K and $T = 300$ K. The figure also indicates the critical particle

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number N_c beyond which the Taylor expansion based algorithm star. corre. ting the fermionic occupation numbers that are found to violate the inec. ıalı, $0 \leqslant \tilde{g}_{q,N} \leqslant 1$. The precise value of N_c not only depends on T and the parame. s that specify the single-electron dispersion relation (L_x and L_y in the present ase) b. t also on the tolerance used to estimate the numerical errors on the occupation n. mber. The values of N_c reported in Fig. (7) correspond to a tolerance of 10^{-10}. I addı, Fig. (7) clearly illustrates that the asymptotic, linear dependence on N i. attained. ooner at relatively low temperatures. The latter may be expected from the close. form expression – Eq. (32) in [1] – that is available for the GCE chemica. potenı. in the thermodynamic limit, i.e. when $L_x, L_y, N \to \infty$ while the areal elect. concentration $n_S = N/(L_x L_y)$ remains finite:

$$\bar{\mu}_{TL} = \frac{1}{\beta} \ln \left(\exp \left(\frac{2\pi^2 n_S}{m_e} - 1 \right) \right). \tag{50}$$

Finally, the occupation numbers are plotte. versus the shell energy $\tilde{\epsilon}_q$ in Fig. (8) for different values of N. Using the shen energy $\tilde{\epsilon}_q$ as the independent variable instead of the very shell index q, we may straightforwardly analyze the profile of the CE occupation numbers in compa. ison w. h the Fermi-Dirac distribution that would govern a GCE approach. It turns out. at. or the adopted parameter set, the CE distribution function profile is predominantly exponential up to $N = 500$, while the deviation from a Fermi-Dirac distribution ν. mes negligible for $N > 3000$.

7. Concluding re. arks

Not or y the pa. ition function and its derived quantities, but also the boson and fermion u. cu. atio. numbers (distribution functions) can be extracted from a workable set of coupled recurrence relations that are straightforwardly derived in the framework of the projec. on operator approach. Except for the special case of one-dimensional. armonic oscillators, analytical solutions of the recurrence relations are rare, if not un. vailable, and a numerical treatment turns out to be paramount for most applications, specially in condensed matter physics and related areas.

. or bosons, one may accidentally have to deal with some minor over/underflow related issues, but the numerical stability of the iterative solutions is generally guaranteed
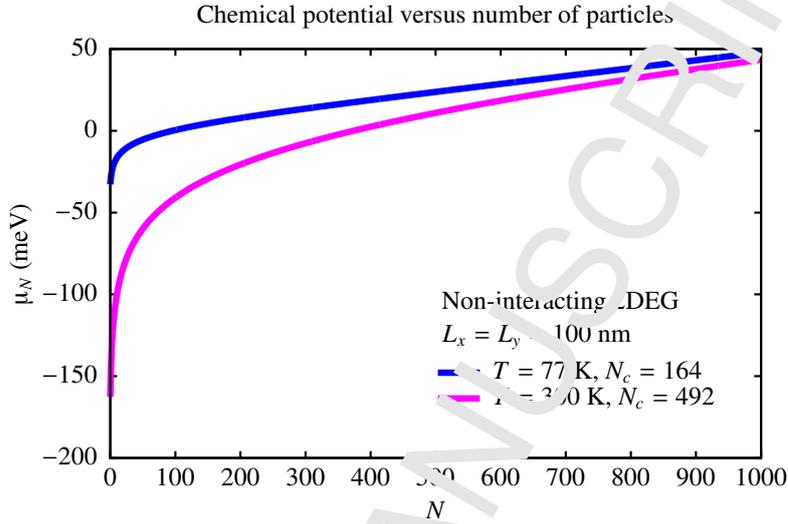
Chemical potential versus number of particles

Figure 7: Chemical potential μ_N of a 2DEG at $T = 77$ K and at $T = 300$ K as a function of the number of particles N. N_c denotes the critical particle number that marks the cross-over between CE and GCE.

thanks to the self-correcting nature of the recurrence relations.

For fermions, the numerical errors in the occupation numbers are found to grow rapidly beyond a critical value of the number of particles, as a direct consequence of the well-known sign problem. However, the proximity of the grand-canonical distribution function in that case was exploited to construct a simple algorithm remedying the unstable steps in the regime of large particle numbers. Moreover, a clear criterion assessing the validity of this alternative algorithm has been established for practical purposes.

As a final remark, we mention two possible applications of the formalism in the domain of condensed matter physics, both requiring an accurate evaluation of the occupation numbers. First, we quote the calculation of the electron density in the inversion layer of modern, nano-scaled field-effect transistors. Including the occupation numbers as a key ingredient, the electron density emerges from an iterative, self-consistent solution of Poisson's and Schrödinger's equations. Traditionally, the GCE yielding the occupation numbers in the form of familiar Fermi-Dirac distribution functions is adopted to this end. However, in the so-called sub-threshold regime that characterizes the transition of a transistor from its off-state to its on-state, the number of electrons is extremely
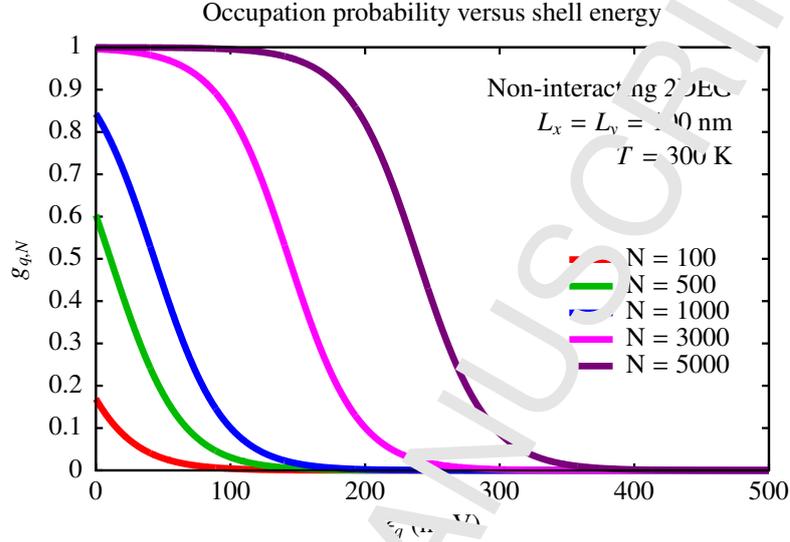
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Figure 8: Electron occupation number (distribution function) versus the single-electron energy with shell index q calculated for $T = 300$ K and for five values of N.

small, thus making the predictions of the GCE rather questionable if not erroneous. Secondly, the formation of Cooper pairs in a superconducting ring confining by construction a sharply defined number of electrons calls for a CE treatment. Nevertheless, conventional BCS theory and, particularly, the Bogoliubov transform applied to the decoupled quartic terms of the BCS Hamiltonian violates the particle number conservation. A suitable modification of the old BCS theory is thus required to conform it with CE terms.

Appendix A. Chemical potential of bosons – upper limit

This section demonstrates that, for any number of bosons, the chemical potential cannot exceed the single-particle ground-state energy ϵ_0, i.e. $\mu_N(\beta) < \epsilon_0$ for all N. Equivalently, using the identity

$$e^{\beta \mu_N(\beta)} = \frac{Z_N(\beta)}{Z_{N+1}(\beta)}, \tag{A.1}$$

we must prove that

$$Z_{N+1}(\beta) > e^{-\beta \epsilon_0} Z_N(\beta). \tag{A.2}$$

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To this end, we first introduce some auxiliary quantities:

$$u = \mathrm{e}^{-\beta\epsilon_0},$$

$$x_j = Z_1(j\beta) - \mathrm{e}^{-j\beta\epsilon_0} = Z_1(j\beta) - u^j,$$

$$\Delta_j = Z_j(\beta) - \mathrm{e}^{-\beta\epsilon_0}Z_{j-1}(\beta) = Z_j(\beta) - uZ_{j-1}(\beta), \qquad j = 1, 2, 3, \ldots$$

$$\Delta_0 = 1. \tag{A.3}$$

Note that, due to $Z_1(j\beta) > \mathrm{e}^{-j\beta\epsilon_0}$ for all positive integer values of j, each x_j is a strictly positive number. With the above notation, it remains to be demonstrated that $\Delta_N > 0$ for $N \geqslant 1$.

First, we invoke mathematical induction to prove the identity

$$Z_N(\beta) = \sum_{l=0}^{N} u^l \Delta_{N-l}, \qquad N = 0, 1, 2, \ldots \tag{A.4}$$

The latter trivially holds for $N = 0$ and $N = 1$ as can be seen by direct application of (A.3). Indeed, assuming that (A.4) holds for all particle numbers up to $N > 1$, its validity for $N + 1$ boson directly follows from

$$Z_{N+1}(\beta) = \Delta_{N+1} + uZ_N(\beta) = \Delta_{N+1} + u\left(\sum_{l=0}^{N} u^l \Delta_{N-l}\right)$$

$$= \Delta_{N+1} + \sum_{l=0}^{N} u^{l+1}\Delta_{N-l} = \Delta_{N+1} + \sum_{j=1}^{N+1} u^j \Delta_{N+1-j} = \sum_{l=0}^{N+1} u^l \Delta_{N+1-l}. \tag{A.5}$$

Next, we assume that $N \geqslant 2$ and expand the sum $S_N \equiv \sum_{l=1}^{N} x_l \, \Delta_{N-l}$ using the definition of x_l:

$$S_N = \sum_{l=1}^{N} Z_1(l\beta) \, \Delta_{N-l} - \sum_{l=1}^{N} u^l \, \Delta_{N-l} = Z_1(N\beta) + \sum_{l=1}^{N-1} Z_1(l\beta) \, \Delta_{N-l} - \sum_{l=1}^{N} u^l \, \Delta_{N-l}, \quad (A.6)$$

where we have isolated the term with $l = N$ in the first sum of the right-hand side. Replacing all Δ_{N-l} in the second sum by their defining expression for $l < N$, and using (A.4) to identify the third sum as $-uZ_{N-1}(\beta)$ upon the substitution $l \to l + 1$, we obtain

$$S_N = Z_1(N\beta) + \sum_{l=1}^{N-1} Z_1(l\beta) \, Z_{N-l}(\beta) - u\sum_{l=1}^{N-1} Z_1(l\beta) \, Z_{N-1-l}(\beta) - uZ_{N-1}(\beta)$$

$$= \sum_{l=1}^{N-1} Z_1(l\beta) \, Z_{N-l}(\beta) - u\sum_{l=1}^{N-1} Z_1(l\beta) \, Z_{N-1-l}(\beta) - uZ_{N-1}(\beta). \tag{A.7}$$

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Finally, exploiting the recurrence relations for $Z_N(\beta)$ and $Z_{N-1}(\beta)$ discussed in [1] and references therein, we arrive at

$$S_N = NZ_N(\beta) - u(N-1)Z_{N-1}(\beta) - uZ_{N-1}(\beta) = N\left(Z_N(\beta) - uZ_{N-1}(\beta)\right) = N\Delta_N, \quad \text{(A.8)}$$

or

$$\Delta_N = \frac{1}{N}\sum_{l=1}^{N} x_l\,\Delta_{N-l}. \quad \text{(A.9)}$$

Whereas being derived for $N \geqslant 2$, the above result trivially holds for $N = 1$, as can be seen by direct calculation. Moreover, because of $\Delta_1 > 0$, we may initiate mathematical induction under the assumption $\Delta_{N-l} > 0$ for $l < N$. Since all x_l appearing in the right-hand side of (A.9) are also strictly positive, we conclude that Δ_N must be strictly positive as well, provided that $N \geqslant 1$.

Appendix B. Fermion occupation number for a linear energy spectrum

Inserting a linear energy spectrum $\epsilon_n = n\Delta$, $n = 0, 1, 2, \cdots$ into Eq. (7), we obtain the generating function for fermions ($\xi = -1$) as

$$G(\beta, z) = \prod_{k=0}^{\infty}\left(1 + ze^{-\beta k\Delta}\right). \quad \text{(B.1)}$$

From (7) the corresponding partition function becomes

$$Z_N^{\text{lin}} = \frac{1}{2\pi i}\oint_{|z|>0}\frac{1}{z^{N+1}}\prod_{k=0}^{\infty}\left(1 + ze^{-\beta k\Delta}\right)dz, \quad \text{(B.2)}$$

while the occupation number of level n is derived from (9):

$$g_{n,N}^{\text{lin}} = \frac{e^{-n\beta\Delta}}{Z_N^{\text{lin}}}\frac{1}{2\pi i}\oint_{|z|>0}\frac{1}{z^N}\prod_{k\geqslant 0,\neq n}^{\infty}\left(1 + ze^{-\beta k\Delta}\right)dz, \quad \text{(B.3)}$$

Consider first the ground state occupation $g_{0,N}^{\text{lin}}$. A substitution $k = j + 1$ followed by a substitution $ze^{-\beta\Delta} = w$ gives

$$g_{0,N}^{\text{lin}} = \frac{e^{-i(N-1)\beta\Delta}}{Z_N^{\text{lin}}}\frac{1}{2\pi i}\oint_{|w|>0}\frac{1}{w^N}\prod_{j=0}^{\infty}\left(1 + we^{-j\beta\Delta}\right)dw. \quad \text{(B.4)}$$

Replacing j by k and w by z, and inspecting Eq. (B.2), one immediately recognizes Z_{N-1}^{lin} in the right-hand side of (B.4) such that $g_{0,N}^{\text{lin}} = e^{-\beta(N-1)\Delta} Z_{N-1}^{\text{lin}}/Z_N^{\text{lin}}$. Using (43), one readily obtains

$$g_{0,N}^{\text{lin}} = 1 - e^{-\beta N\Delta}, \tag{B.5}$$

which is equivalent to the expression for $\langle n_1 \rangle_N$ reported in Eq. (16) of [8]. Next, focusing on $n > 0$, we separate the factor $1 + z$ corresponding to $k = 0$ from the infinite product in the integral representation of $g_{n+1,N}^{\text{lin}}$ to obtain

$$g_{n+1,N}^{\text{lin}} = \frac{e^{-n\beta\Delta}}{Z_N^{\text{lin}}} \frac{1}{2\pi\mathrm{i}} \oint_{|z|>0} \left(\frac{1}{z^N} + \frac{1}{z^{N-1}} \right) \prod_{k=1,\neq n+1}^{\infty} \left(1 + ze^{-k\beta\Delta}\right) \mathrm{d}z. \tag{B.6}$$

As for the case $n = 0$, we first make the substitutions $k = j + 1$, $w = ze^{-\beta\Delta}$, and rename them back again into k and z respectively, to find

$$g_{n+1,N}^{\text{lin}} = \frac{e^{-n\beta\Delta}}{Z_N^{\text{lin}}} \frac{1}{2\pi\mathrm{i}} \oint_{|z|>0} \left(\frac{e^{-\beta(N-1)\Delta}}{z^N} + \frac{e^{-\beta(N-2)\Delta}}{z^{N-1}} \right) \prod_{k=0,\neq n}^{\infty} \left(1 + ze^{-k\beta\Delta}\right) \mathrm{d}z. \tag{B.7}$$

The contributions to the above integral corresponding respectively to the fractions $e^{-\beta(N-1)\Delta}/z^N$ and $e^{-\beta(N-2)\Delta}/z^{N-1}$ are proportional to $g_{n,N}^{\text{lin}}$ and $g_{n,N-1}^{\text{lin}}$, as can be derived from Eq. (B.3). Hence, we obtain:

$$g_{n+1,N}^{\text{lin}} = e^{-\beta N\Delta} g_{n,N}^{\text{lin}} + e^{-\beta(N-1)\Delta} g_{n,N-1}^{\text{lin}} \frac{Z_{N-1}^{\text{lin}}}{Z_N^{\text{lin}}}. \tag{B.8}$$

Using $Z_{N-1}^{\text{lin}}/Z_N^{\text{lin}} = \left(1 - e^{-\beta N\Delta}\right) e^{\beta(N-1)\Delta}$ one rediscovers the recurrence relation Eq. (18) of [8]:

$$g_{n+1,N}^{\text{lin}} = e^{-\beta N\Delta} g_{n,N}^{\text{lin}} + \left(1 - e^{-\beta N\Delta}\right) g_{n,N-1}^{\text{lin}}. \tag{B.9}$$

As such, the above recurrence relation is not particularly useful, with both the energy level index and the particle number N appearing as incremental integers. However, the application of (41) eliminating $g_{n,N-1}^{\text{lin}} = 1 - g_{n,N}^{\text{lin}} e^{\beta(n\Delta - \mu_{N-1}^{\text{lin}})}$ and the use of (46) finally yields a recurrence relation in n only, the value of N remaining fixed,

$$g_{n+1,N}^{\text{lin}} = 1 - e^{-\beta N\Delta} - e^{-\beta N\Delta} \left(e^{\beta\Delta(n+1)} - 1\right) g_{n,N}^{\text{lin}}, \tag{B.10}$$

which is easily reversed from increasing to decreasing energy level index n:

$$g_{n,N}^{\text{lin}} = \frac{e^{\beta N\Delta}}{e^{\beta\Delta(n+1)} - 1} \left(1 - e^{-\beta N\Delta} - g_{n+1,N}^{\text{lin}}\right). \tag{B.11}$$

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