Justification of c–Number Substitutions in Bosonic Hamiltonians

Elliott H. Lieb
Robert Seiringer
Jakob Yngvason

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One of the key developments in the theory of the Bose gas, especially the theory of the low density gases currently at the forefront of experiment, is Bogoliubov’s 1947 analysis [1] of the many-body Hamiltonian by means of a $c$-number substitution for the most relevant operators in the problem, the zero-momentum mode operators, namely $a_0 \to z, a_0^* \to z^*$. Naturally, the appropriate value of $z$ has to be determined by some sort of consistency or variational principle, which might be complicated, but the concern, expressed by many authors over the years, is whether this sort of substitution is legitimate, i.e., error free. We address this latter problem here and show, by a simple but rigorous analysis, that it is so under very general circumstances.

The rigorous justification for this substitution, as far as calculating the pressure is concerned, was done in a classic paper of Ginibre [2] in 1968, but it does not seem to have percolated into the general theory community. In textbooks it is often said, for instance, that it is tied to the imputed ‘fact’ that the expectation value of the number operator $a_0^*a_0$ is of order $V = \text{volume}$. (This was the argument in [1]). That is, Bose-Einstein condensation (BEC) justifies the substitution. As Ginibre pointed out, however, BEC has nothing to do with it. The $z$ substitution still gives the right answer even if $n_0$ is small (but it is a useful calculational tool only if $n_0$ is macroscopic). Thus, despite [2] and the thorough review of these matters in [3], there is some confusion in the literature and clarification could be useful.

In this short note we do three things. 1.) We show how Ginibre’s result can be easily obtained in a few simple lines. While he used coherent states, he did not use the Berezin-Lieb inequality [4–6], derived later, which efficiently gives upper bounds. This inequality gives explicit error bounds which, typically, are only order one compared to the total free energy or pressure times volume, which are order $N = \text{particle number}$.

2.) This allows us to go beyond [2] and make $c$-number substitutions for many $k$-modes at once, provided the number of modes is lower order than $N$.

3.) We show how the optimum value of $z$ yields, in fact, the expectation value $\langle n_0 \rangle$ in the true state when a gauge breaking term is added to the Hamiltonian. More precisely, in the thermodynamic limit (TL) the $|z|^2$ that maximizes the partition function equals the true amount of condensation in the presence of a gauge-symmetry breaking term — a point that had previously been elusive.

While we work here at positive temperature $k_B T = 1/\beta$, our methods also work for the ground state (and are even simpler in that case). To keep this note short and, hopefully, readable, we will be a bit sketchy in places but there is no difficulty filling in the details.

The use of coherent states [10, 11] to give accurate upper and lower bounds to energies, and thence to expectation values, is effective in a wide variety of problems [12], e.g., quantum spin systems in the large $S$ limit [5], the Dicke model [13], the strong coupling polaron [14], and the proof that Thomas-Fermi theory is exact in the large atom limit [15, 16]. For concreteness and relevance, we concentrate on the Bose gas problem here, and we discuss only the total, correct Hamiltonian. Nevertheless, the same conclusions hold also for variants, such as Bogoliubov’s truncated Hamiltonian (the “weakly imperfect Bose gas” [1, 3]) or other modifications, provided we are in the stability regime (i.e., the regime in which the models make sense). We are not claiming that any particular approximation is valid. That is a completely different story that has to be decided independently. The method can also be modified to incorporate inhomogeneous systems. The message is the same in all cases, namely that the $z$ substitution causes no errors (in the TL), even if there is no BEC, whenever it is applied to physically stable systems. Conversely, if the system is stable after the $z$ substitution then so is the original one.

We start with the well-known Hamiltonian for bosons in a large box of volume $V$, expressed in terms of the second-quantized creation and annihilation operators.
\begin{align}
H &= \sum_k k^2 a_k^\dagger a_k + \frac{1}{2V} \sum_{k,p,q} \nu(p) a_{k+p}^\dagger p a_{k-q} a_{p-q},
\end{align}

(with \( \hbar = 2m = 1 \)). Here, \( \nu \) is the Fourier transform of the two-body potential \( v(r) \). We assume that there is a bound on the Fourier coefficients \( |\nu(k)| \leq \varphi < \infty \).

The case of hard core potentials can be taken care of in the following way. First cut off the hard core potential \( v \) at a height \( 10^{12} \text{ eV} \). It is easy to prove, by standard methods, that this cutoff will have a negligible effect on the exact answer. After the cutoff \( \varphi \) will be about \( 10^{12} \text{ eV} \text{ A}^3 \), and according to what we prove below, this substitution will affect the chemical potential only by about \( \varphi / V \), which is truly negligible when \( V = 10^{23} \text{ A}^3 \).

If we replace the operator \( a_0 \) by a complex number \( z \) and \( a_0^* \) by \( z^* \) everywhere in \( H \) we obtain a Hamiltonian \( H'(z) \) that acts on the Fock-space of all the modes other than the \( a_0 \) mode. Unfortunately, \( H'(z) \) does not commute with the particle number \( \sum_{k \neq 0} a_k^\dagger a_k \). It is convenient, therefore, to work in the grand canonical ensemble and consider \( H_\mu = H - \mu N = H - \mu (a_0^\dagger a_0 + \sum_{k \neq 0} a_k^\dagger a_k) \) and, correspondingly, \( H'_\mu(z) = H'(z) - \mu (|z|^2 + \sum_{k \neq 0} |a_k|^2) \).

The partition functions are given by
\begin{align}
\Xi(\mu) &= \text{Tr}_\mathcal{H} \exp[-\beta H_\mu] \quad (2)
\Xi'(\mu) &= \int d^2z \text{Tr}_{\mathcal{H}'} \exp[-\beta H'_\mu(z)] 
\end{align}
where \( \mathcal{H} \) is the full Hilbert (Fock) space, \( \mathcal{H}' \) is the Fock space without the \( a_0 \) mode, and \( d^2z \equiv \pi^{-1} dx dy \) with \( z = x + iy \). The functions \( p(\mu) \) and \( p'(\mu) \) are the corresponding finite volume pressures.

The pressure \( p(\mu) \) has a finite TL for all \( \mu < \mu_{\text{critical}} \), and it is a convex function of \( \mu \). For the non-interacting gas, \( \mu_{\text{critical}} = 0 \), but for any realistic system \( \mu_{\text{critical}} = +\infty \). In any case, we assume \( \mu < \mu_{\text{critical}} \), in which case both the pressure and the density are finite.

Let \( |z| = \exp(-|z|^2/2 + za_0^*|0\rangle \) be the coherent state vector in the \( a_0 \) Fock space and let \( \Pi(z) = |z\rangle \langle z| \) be the projector onto this vector. There are six relevant operators containing \( a_0 \) in \( H_\mu \), which have the following expectation values \[10\] (called lower symbols)
\begin{align}
|z\rangle a_0^\dagger a_0 |z\rangle &= |z|^2, \\
|z\rangle a_0^\dagger a_0^* a_0 |z\rangle &= |z|^2. \\
|z\rangle a_0 |z\rangle &= z^*, \\
|z\rangle a_0^* a_0^* a_0 |z\rangle &= z^{*2}, \\
|z\rangle a_0^* a_0 a_0 a_0 |z\rangle &= |z|^4.
\end{align}
Each also has an upper symbol, which is a function of \( z \) (call it \( u(z) \) generically) such that an operator \( F \) is represented as \( F = \int d^2z u(z) \Pi(z) \). These symbols are
\begin{align}
a_0 &\rightarrow z, \quad a_0 a_0^\dagger a_0^\dagger a_0 \rightarrow |z|^2 - 1 \\
a_0 &\rightarrow z^*, \quad a_0 a_0^* a_0 a_0 \rightarrow |z|^4 - 4|z|^2 + 2.
\end{align}

It will be noted that the operator \( H'_\mu(z) \), defined above, is obtained from \( H_\mu \) by substituting the lower symbols for the six operators. If we substitute the upper symbols instead into \( H_\mu \) we obtain a slightly different operator, which we write as \( H''_\mu(z) = H'_\mu(z) + \delta_\mu(z) \) with
\begin{align}
\delta_\mu(z) &= \mu + \frac{1}{2V} \left[ (-4|z|^2 + 2)\nu(0) - \sum_{k \neq 0} a_k^\dagger a_k (2\nu(0) + \nu(k) + \nu(\bar{0}) ) \right]. \quad (4)
\end{align}

The next step is to mention two inequalities, of which the first is
\begin{align}
\Xi(\mu) \geq \Xi'(\mu). \quad (5)
\end{align}
This is a consequence of the following two facts: The completeness property of coherent states, \( \int d^2z \Pi(z) = \text{Identity}, \) and
\begin{align}
\langle z | \phi e^{-\beta H_\mu} | z \rangle \geq e^{-\beta (z \phi | H_\mu | z \phi)} = e^{-\beta (\phi | H''_\mu(z) \phi)}, \quad (6)
\end{align}
where \( \phi \) is any normalized vector in \( \mathcal{H}' \). This is Jensen’s inequality for the expectation value of a convex function (like the exponential function) of an operator.

To prove (5) we take \( \phi = 1 \) (in (6)) to be one of the normalized eigenvectors of \( H''_\mu(z) \), in which case \( \text{exp} \{ (\phi - \beta H''_\mu(z) ) | \phi \} \). We then sum over all such eigenvectors (for a fixed \( z \)) and integrate over \( z \). The left side is then \( \Xi(\mu) \), while the right side is \( \Xi'(\mu) \).

The second inequality \[4-6\] is
\begin{align}
\Xi(\mu) \leq \Xi''(\mu) = e^{\beta p'(\mu)}, \quad (7)
\end{align}
where \( \Xi''(\mu) \) is similar to \( \Xi'(\mu) \) except that \( H''_\mu(z) \) is replaced by \( H'_\mu(z) \). Its proof is the following. Let \( |\Psi_j \rangle \in \mathcal{H} \) denote the complete set of normalized eigenfunctions of \( H_\mu \). The partial inner product \( \langle \Psi_j(z)| \rangle = \langle z| \Psi_j(z) \rangle \) is a vector in \( \mathcal{H}' \) whose square norm, \( c_j(z) = \langle \Psi_j(z)| \Psi_j(z) \rangle_{\mathcal{H}} \), satisfies \( \int d^2z c_j(z) = 1 \). By using the upper symbols, we can write \( \langle \Phi_j(z)|H''_\mu(z)| \Phi_j(z) \rangle = \int d^2z \langle \Psi_j(z)|H''_\mu(z)| \Psi_j(z) \rangle c_j(z), \) where \( |\Psi_j(z) \rangle \) is the normalized vector \( c_j(z)^{-1/2} | \Psi_j(z) \rangle \). To compute the trace, we can exponentiate this to write \( \Xi(\mu) \) as
\[ \sum_j \text{exp} \left\{ -\beta \int d^2z c_j(z) \langle \Psi_j(z)|H''_\mu(z)| \Psi_j(z) \rangle \right\}. \]
Using Jensen’s inequality twice, once for functions and once for expectations as in (6), \( \Xi(\mu) \) is less than
\[ \sum_j \int d^2z c_j(z) \text{exp} \left\{ -\beta H''_\mu(z) | \Psi_j(z) \rangle \text{exp} \left\{ -\beta H''_\mu(z) \right\} | \Psi_j(z) \rangle \right\}. \]
Since \( \text{Tr} \Pi(z) = 1 \), the last expression can be rewritten
\[ \int d^2z \sum_j |\Phi_j(z) \rangle \otimes \text{exp} \left\{ -\beta H''_\mu(z) \right\} | \Phi_j(z) \rangle = \Xi''(\mu). \]
Thus, we have that
\[ \Xi'(\mu) \leq \Xi(\mu) \leq \Xi''(\mu). \] (8)

The next step is to try to relate \( \Xi''(\mu) \) to \( \Xi'(\mu) \). To this end, we have to bound \( \delta_{\mu}(z) \) in (4). This is easily done in terms of the total number operator whose lower symbol is \( N'(z) = |z|^2 + \sum_{k \neq 0} \xi_{z}^{k} \xi_{-z}^{k} \). In terms of the bound \( \varphi \) on \( \nu(p) \)
\[ |\delta_{\mu}(z)| \leq 2\varphi(N'(z) + \frac{1}{2})/V + |\mu|. \] (9)

Consequently, \( \Xi''(\mu) \) and \( \Xi'(\mu) \) are related by the inequality
\[ \Xi''(\mu) \leq \Xi'(\mu + 2\varphi/V)e^{\beta(|\mu| + \varphi/V)}. \] (10)

Equality of the pressures \( p(\mu), p'(\mu) \) and \( p''(\mu) \) in the TL follows from (8) and (10).

Closely related to this point is the question of relating \( \Xi(\mu) \) to the maximum value of the integrand in (3), which is \( \max_{\mu} \Tr_{\rho} \exp[-\beta H'_{\mu}(z)] \equiv e^{\beta V p^{\max}} \). This latter quantity is often used in discussions of the \( z \) substitution problem, e.g., in refs. [2, 3]. One direction is not hard. It is the inequality (used in ref. [2])
\[ \Xi(\mu) \geq \max_{z} \Tr_{\rho} \exp[-\beta H'_{\mu}(z)], \] (11)
and the proof is the same as the proof of (5), except that this time we replace the completeness relation for the coherent states by the simple inequality Identity \( \Xi(\mu) \geq \Pi(z) \) for any fixed number \( z \).

For the other direction, split the integral defining \( \Xi''(\mu) \) into a part where \( |z|^2 < \xi \) and \( |z|^2 \geq \xi \). Thus,
\[ \Xi''(\mu) \leq \frac{\xi}{|z|^2} \Tr_{\rho} \exp[-\beta H'_{\mu}(z)] \]
\[ + \frac{1}{\xi} \int_{|z|^2 \geq \xi} d^2z \frac{|z|^2}{2} \Tr_{\rho} \exp[-\beta H''_{\mu}(z)]. \] (12)

Dropping the condition \( |z|^2 \geq \xi \) in the last integral and using \( |z|^2 \leq N'(z) = N''(z) + 1 \), we see that the second line in (12) is bounded above by \( \xi^{-1} \Xi''(\mu) |\rho''(\mu)| + 1 \), where \( \rho''(\mu) \) denotes the density in the \( H''_{\mu} \) ensemble. Optimizing over \( \xi \) leads to
\[ \Xi''(\mu) \leq 2[V \rho''(\mu) + 1] \max_{z} \Tr_{\rho} \exp[-\beta H''_{\mu}(z)]. \] (13)

Note that \( \rho''(\mu) \) is order one, since \( p''(\mu) \) and \( p(\mu) \) agree in the TL (and are convex in \( \mu \)), and we assumed that the density in the original ensemble is finite. By (9), \( H_{\mu}' \geq H_{\mu}' + 2\varphi/V - |\mu| - \varphi/V \), and it follows from (7), (13) and (11) that \( p^{\max} \) agrees with the true pressure \( p \) in the TL. Their difference, is at most \( O(\ln V/V) \). This is the result obtained by Ginibre in [2] by more complicated arguments, under the assumption of superstability of the interaction, and without the explicit error estimates obtained here.

To summarize the situation so far, we have four expressions for the grand canonical pressure. They are all equal in the TL limit,
\[ p(\mu) = p'(\mu) = p''(\mu) = p^{\max}(\mu) \] (14)
when \( \mu \) is not a point at which the density can be infinite.

Our second main point is that not only is the \( z \) substitution valid for \( a_{\theta} \) but it can also be done for many modes simultaneously. As long as the number of modes treated in this way is much smaller than \( N \) the effect on the pressure will be negligible. Each such substitution will result in an error in the chemical potential that is order \( \varphi/V \). The proof of this fact just imitates what was done above for one mode. Translation invariance is not important here; one can replace any mode such as \( \sum_{k} g_{\theta} a_{k} \) by a \( c \)-number, which can be useful for inhomogeneous systems.

A more delicate point is our third one, and it requires, first, a discussion of the meaning of ’condensate fraction’ that goes beyond what is usually mentioned in textbooks, but which was brought out in [1, 17, 19]. The ’natural’ idea would be to consider \( V^{-1} |\langle a_0 \rangle| \). This, however, need not be a reliable measure of the condensate fraction for the following reason. If we expand \( \exp\{-\beta H\} \) in eigenfunctions of the number operator \( n_{\theta} \) we would have \( \langle n_{\theta} \rangle = \sum_{\gamma} n_{\gamma}(n) \), where \( \gamma(n) \) is the probability that \( n_0 = n \). One would like to think that \( \gamma(n) \) is sharply peaked at some maximum \( n \) value, but we do not know if this is the case. \( \gamma(n) \) could be flat, up to the maximum value or, worse, it could have a maximum at \( n = 0 \). Recall that precisely this happens for the Heisenberg quantum ferromagnet [17]; by virtue of conservation of total spin angular momentum, the distribution of values of the \( z \)-component of the total spin, \( S_0^z \), is a strictly decreasing function of \( |S_0^z| \). Even if it were flat, the expected value of \( S_0^z \) would be half of the spontaneous magnetization that one gets by applying a weak magnetic field.

With this example in mind, we see that the only physically reliable quantity is \( \lim_{\lambda \to 0} \lim_{V \to \infty} V^{-1} |\langle a_0 \rangle|_{\mu,_{\lambda}} \), where the expectation is now with respect to a Hamiltonian \( H_{\mu,_{\lambda}} = H_{\mu} + \sqrt{V} (\lambda a_{0} + \lambda^* a_{0}^*) \) [1]. Without loss of generality, we assume \( \lambda \) to be real. We will show that for almost every \( \lambda \), the density \( \gamma(V_{0}) \) converges in the TL to a \( \delta \)-function at the point \( \rho_{0} : \lim_{V \to \infty} \lim_{\lambda \to 0} V^{-1}|\langle a_0 \rangle|_{\mu,_{\lambda}}^2 = V^{-1}|z_{{\max}}|^2 \) (15)
in the TL. This holds for those \( \lambda \) where the pressure in the TL is differentiable; since \( p(\mu,_{\lambda}) \) is convex (upwards) in \( \lambda \) this is true almost everywhere. The right and left derivatives exist for every \( \lambda \) and hence \( \lim_{\lambda \to 0} \lim_{V \to \infty} V^{-1}|\langle a_0 \rangle|_{\mu,_{\lambda}}^2 \) exists.

The expectation values \( \langle n_{0} \rangle_{\mu,_{\lambda}} \) and \( \langle a_0 \rangle_{\mu,_{\lambda}} \) are obtained by integrating (\(|z|^2 - 1\)) and \( z \), respectively, with
the weight $W_{\mu,\lambda}(z) \equiv \Xi(\mu, \lambda) \cdot \text{Tr}_{\mathcal{H}}(z| \exp[-\beta H_{\mu,\lambda}]|z)$.

We will show that this weight converges to a $\delta$-function at $z_{\text{max}}$ in the TL, implying (15). If we could replace $W_{\mu,\lambda}(z)$ by $W_{\mu,0}(z) e^{-\beta \sqrt{V}(z^2+z^2)}$, this would follow from Griffiths’ argument [17] (see also [18, Sect. 1]). Because $[H, a_0] \neq 0$, $W_{\mu,\lambda}$ is not of this product form. However, the weight for $\Xi''(\mu, \lambda)$, which is $W''_{\mu,\lambda}(z) = \Xi''(\mu, \lambda) \cdot \text{Tr}_{\mathcal{H}}(\exp[-\beta H''_{\mu,\lambda}(z)])$, does have the right form. In the following we shall show that the two weights are equal apart from negligible errors.

Equality (14) holds also for all distances $p(\mu, \lambda) = p''(\mu, \lambda) = p\max(\mu, \lambda)$ in the TL. In fact, since the upper and lower symbols agree for $a_0$ and $a_0^*$, the error estimates above remain unchanged. (Note that since $\sqrt{V}(a_0 + a_0^*) \leq \sqrt{\delta(N + \frac{1}{2})} + \sqrt{\delta}$ for any $\delta > 0$, $p(\mu, \lambda)$ is finite for all $\lambda$ if it is finite for $\lambda = 0$ in a small interval around $\mu$.) At any point of differentiability with respect to $\lambda$, Griffiths’ theorem [17] (see [18, Cor. 1.1]), applied to the partition function $\Xi''(\mu, \lambda)$, implies that $W''_{\mu,\lambda}(\zeta) \cdot \sqrt{V}$ converges to a $\delta$-function at some point $\zeta$ on the real axis as $V \to \infty$. (The original Griffiths argument can easily be extended to two variables, as we have here. Because of radial symmetry, the derivative of the pressure with respect to $\text{Im} \lambda$ is zero at any non-zero real $\lambda$.) Moreover, by comparing the derivatives of $p''$ and $p\max$ we see that $\zeta = \lim_{V \to \infty} z_{\text{max}}/\sqrt{V}$, since $z_{\text{max}}/\sqrt{V}$ is contained in the interval between the left and right derivatives of $p\max(\mu, \lambda)$ with respect to $\lambda$.

We shall now show that the same is true for $W_{\mu,\lambda}$. To this end, we add another term to the Hamiltonian, namely $\epsilon F \equiv \epsilon \mathcal{V} \int d^2z \Pi(z) f(z V^{-1/2})$, with $\epsilon$ and $f$ real if $f(\zeta)$ is a nice function of two real variables with bounded second derivatives, it is then easy to see that the upper and lower symbols of $F$ differ only by a term of order 1. Namely, for some $C > 0$ independent of $z_0$ and $V$,

$$V \int d^2z |(z|z_0\rangle|^2 \left[ f(z V^{-1/2}) - f(z_0 V^{-1/2}) \right] \right| \leq C.$$}

Hence, in particular, $p(\mu, \lambda, \epsilon) = p''(\mu, \lambda, \epsilon)$ in the TL. Moreover, if $f(\zeta) = 0$ for $|\zeta - \zeta| \leq \delta$, then the pressure is independent of $\epsilon$ for $|\epsilon|$ small enough (depending only on $\delta$). This can be seen as follows. We have

$$p''(\mu, \lambda, \epsilon) - p''(\mu, \lambda, 0) \equiv \frac{1}{\beta V} \ln \left\{ e^{-\beta \epsilon F(z V^{-1/2})} \right\},$$

where the last expectation is in the $\mathcal{H}''(\mu)$ ensemble at $\epsilon = 0$. The corresponding distribution is exponentially localized at $z/\sqrt{V} = \zeta$ [17, 18], and therefore the right side of (16) goes to zero in the TL for small enough $\epsilon$. In particular, the $\epsilon$-derivative of the TL pressure at $\epsilon = 0$ is zero. By convexity in $\epsilon$, this implies that the derivative of $p$ at finite volume, given by $V^{-1}\langle F \rangle_{\mu,\lambda} = \int d^2z f(z V^{-1/2}) W_{\mu,\lambda}(z)$, goes to zero in the TL. Since $f$ was arbitrary, $V \int_{|\zeta - \zeta| \geq \delta} d^2\xi W_{\mu,\lambda}(\zeta \sqrt{V}) \to 0$ as $V \to \infty$. This holds for all $\delta > 0$, and therefore proves the statement.

Our method also applies to the case when the pressure is not differentiable in $\lambda$ (which is the case at $\lambda = 0$ in the presence of BEC). In this case, the resulting weights $W_{\mu,\lambda}$ and $W''_{\mu,\lambda}$ need not be $\delta$-functions, but Griffiths’ method [17, 18] implies that they are, for $\lambda \neq 0$, supported on the real axis between the right and left derivative of $p$ and, for $\lambda = 0$, on a disc (due to the gauge symmetry) with radius determined by the right derivative of $p$ and, for $\lambda = 0$, on a disc (due to the gauge symmetry) with radius determined by the right derivative of $p$. This, together with convexity, implies that $(n_0)_{\mu,\lambda}$ is monotone increasing in $\lambda$ in the TL and, in particular, $\lim_{V \to \infty} V^{-1}(n_0)_{\mu,\lambda} = \lim_{V \to \infty} V^{-1} ||(a_0)_{\mu,\lambda}||^2$, a fact which is intuitively clear but has, to the best of our knowledge, not been proved so far [19] in this generality. In fact, the only hypothesis entering our analysis, apart from the bound $\varphi$ on the potential, is the existence of the TL of the pressure and the density.

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[20] *Note added in proof*: After we submitted this paper A. Sütő presented a different proof of item 3 (math-ph/0412056).