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Bose–Einstein Condensation: A Mathematically Unsolved Problem[1]

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The interacting Bose gas with repulsive potential is considered in the polymer representation and some of the yet unsolved mathematical questions for establishing the existence of Bose condensation in this setting are discussed.

KEY WORDS: Bose gas; condensation; polymers; Brownian path.

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1. INTRODUCTION

In 1924, Einstein predicted that at low temperature massive bosons can macroscopically occupy a single microscopic quantum state (see Einstein (1925)). A direct observation of this wonderful consequence of Bose statistics was only obtained in 1995 in Boulder (Anderson *et al.* (1995)) in an ultracold gas of rubidium atoms confined in an harmonic trap. I strongly recommend a visit to the website "www.colorado.edu/physics/2000/bec/" where a pleasant presentation of the physics and experiments can be found. It may be of interest to look there at the picture of the condensate wave function (more precisely the modulus of its Fourier transform, the momentum distribution), showing that a quantum mechanical wave function can indeed be seen experimentally.

In the sequel I will discuss some aspects of the Bose–Einstein transition in three-dimensional infinitely extended space as originally considered by Einstein. Let me briefly recall the original argument for the existence of the transition in a noninteracting Bose gas. According to the principles of quantum statistical mechanics, the mean number of particles per unit volume having kinetic energy $p^2/2m = (\hbar k)^2/2m$ ($\mathbf{p} = \hbar\mathbf{k}$ is the momentum, $p = |\mathbf{p}|$, m is the mass of the

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particle, and $\hbar$ the Planck constant) is given by the Bose distribution

$$n(k,\mu)=\frac{1}{\exp[\beta((\hbar k)^2/2m-\mu)]-1}=\sum_{q=1}^{\infty}\exp[\beta(\hbar k)^2 q)/2m]\exp(\beta\mu q) \quad (1)$$

The series results of an expansion in the activity parameter $z=\exp(\beta\mu)$, which is convergent for $\mu<0$. The value of parameter μ (the chemical potential) fixes the particle density. The total number of particles per unit volume occupying excited states $\rho_{\mathrm{ex}}(\mu)$ is obtained from (1) by summing on all kinetic energies

$$\rho_{\mathrm{ex}}(\mu)=\frac{1}{(2\pi)^3}\int d\mathbf{k}n(k,\mu)=\frac{1}{(2\pi\lambda)^3}\sum_{q=1}^{\infty}\frac{e^{\beta\mu q}}{q^{3/2}},\quad \mu<0 \quad (2)$$

where $\lambda=\hbar\sqrt{\beta/m}$ is the de Broglie thermal length and $\beta=1/k_{\mathrm{B}}T$ the inverse temperature. The main observation is that starting from low density ($\mu\ll 0$) the density increases up to a finite value ρ_{c} (the critical density) as $\mu\to 0$

$$\lim_{\mu\to 0}\rho_{\mathrm{ex}}(\mu)=\frac{1}{(2\pi\lambda)^3}\sum_{q=1}^{\infty}\frac{1}{q^{3/2}}\equiv\rho_{\mathrm{c}}<\infty \quad (3)$$

This is the so called saturation mechanism. As a consequence, if the physical density ρ of the gas is larger than ρ_{c} then the exceeding particles, forming the condensate density $\rho-\rho_c$, must accumulate in the single zero kinetic quantum state $k=0$: this is the Bose condensation phenomenon. A more comprehensive rigorous treatment can be found in Van den Berg *et al.* (1986).

2. POLYMER REPRESENTATION OF THE INTERACTING GAS

It is not known if the saturation mechanism and the ensuing Bose–Einstein condensation survive the introduction of interactions between the particles. Suppose that the particles i an$j$ interact by means of a local positive and integrable pair potential $v(|\mathbf{x}_i-\mathbf{x}_j|),\ v(x)>0,\ a=\int d\mathbf{x}v(x)<\infty,\ x=|\mathbf{x}|$. The main quantity to be studied is the partition function

$$Z_{\Lambda,n}=\mathrm{Tr}_{\Lambda,\mathrm{sym}}\left[\exp\left(-\beta\left(\sum_{i=1}^{n}\frac{p_i^2}{2m}+\sum_{i<j}^{n}v(|\mathbf{x}_i-\mathbf{x}_j|)\right)\right)\right] \quad (4)$$

The trace is taken over the symmetrized tensor product $\mathcal{H}_{\mathrm{sym}}^{\bigotimes n}$ of the one-particle Hilbert space $\mathcal{H}$ and the particles are confined in the volume Λ by appropriate boundary conditions.

It is convenient to use an alternative mathematical representation of the partition function which has a classical like-form, the polymer representation, already initiated by Feynman. We only sketch a few steps, a detailed derivation can be found in Martin (2003), see also Brydges and Martin (1999) and references therein. The first step is to use the Feynman–Kac path integral representation of the kernel

$$\left\langle \mathbf{r}_1, \ldots, \mathbf{r}_n \right| \exp\left[-\beta\left(\sum_{i=1}^{n}\frac{p_i^2}{2m} + \sum_{i<j}^{n} v(|\mathbf{x}_i - \mathbf{x}_j|)\right)\right]\left|\mathbf{r}_{\pi(1)}, \ldots, \mathbf{r}_{\pi(n)}\right\rangle,$$

with π an element of the permutation group S_n. In the Feynman–Kac representation, the statistical weight of a quantum point particle at $\mathbf{r}$ in a potential $v(\mathbf{r})$ takes the classical-like form $\exp[-\beta\int_o^1 ds v(\mathbf{r}+\lambda\mathbf{x}(s))]$ with $\mathbf{x}(s)$ a closed Brownian path. Thus the particle can be viewed as a classical object at $\mathbf{r}$ equipped with an internal degree of freedom $\lambda\mathbf{x}(s)$), its quantum fluctuation whose size is controlled by the Broglie thermal lenth. To take Bose statistics into account, one decomposes each permutation π into cycles and groups together the particles belonging to the same cycle, so forming an extended Brownian path called a loop or a polymer. After some combinatorics the grand canonical sum

$$\sum_{n=0}^{\infty} e^{\beta\mu n} Z_{\Lambda,n} = \sum_{k=0}^{\infty}\frac{1}{k\,!}\int d\mathcal{L}_1 \cdots \int d\mathcal{L}_k z(\mathcal{L}_1)\cdots z(\mathcal{L}_k)$$

$$\exp\left[-\beta\sum_{i<j}^{k} v(\mathcal{L}_i, \mathcal{L}_j)\right] \tag{5}$$

can be rearranged into a sum on cycle numbers k. The basic objects entering in (5), the $q-$loops $\mathcal{L} = (\mathbf{R}, q, \mathbf{X}(\cdot))$ (or $q-$polymers), are specified by their locations in space $\mathbf{R}$, the number q of particles they contain, and their shapes $\mathbf{X}(s), 0 \le s \le q$. More precisely, $\mathbf{X}(\cdot)$ is a closed Brownian path (a Brownian bridge, $\mathbf{X}(0) = \mathbf{X}(q) = 0$) distributed according to the Gaussian measure with covariance

$$< X_\alpha(s) X_{\alpha'}(s') >= \delta_{\alpha,\alpha'} q\left(\inf\left(\frac{s}{q}, \frac{s'}{q}\right) - \frac{ss'}{q^2}\right), \quad \alpha, \alpha' = 1, 2, 3 \tag{6}$$

One can think of a loop as a classical object at $\mathbf{R}$, with internal degrees of freedom $q, \mathbf{X}(\cdot)$. The phase space integration on $\mathcal{L}$ is formally defined by

$$\int d\mathcal{L} \cdots = \sum_{q=1}^{\infty}\int_{\Lambda} d\mathbf{R} \int D_q(\mathbf{X}(\cdot)) \cdots \tag{7}$$

with $D_q(\mathbf{X}(\cdot))$ the Gaussian Brownian bridge measure. In this way the quantum grand canonical sum has been casted into a classical-like statistical sum with polymer activities $z(\mathcal{L}_i)$ and polymer pair-interactions $v(\mathcal{L}_i, \mathcal{L}_j)$, so that all powerful techniques of classical statistical mechanics are available. The polymer activity reads

$$z(\mathcal{L}) = \frac{e^{\beta\mu q}}{(2\pi q\lambda^2)^{3/2}} \exp(-\beta U(\mathcal{L})) \tag{8}$$

where

$$U(\mathcal{L}) = \frac{1}{2}\int_0^q ds_1 \int_0^q ds_2 \delta_p(s_1 - s_2) v(\lambda|\mathbf{X}(s_1) - \mathbf{X}(s_2)|) - \frac{q}{2} v(0) \tag{9}$$

is the self-energy of a polymer including all the pair-interactions of the q particles belonging to the same polymer. Here $\delta_p(s) = \sum_{n=-\infty}^{\infty} e^{2ins}$ is the periodic Dirac distribution arising from the "equal time" prescription in the Feynman–Kac formula. One has a similar formula for the potential $v(\mathcal{L}_i, \mathcal{L}_j)$ between two polymers including the pair-interactions of particles belonging to different polymers.

3. THE SELF-CONSISTENT EQUATION FOR THE DENSITY

Our goal is to investigate the possible saturation mechanism in the interacting gas. For this we need first to recall the notion of Mayer graph in classical statistical mechanics (see, e.g., Ford and Uhlenbeck (1962)). The partition function as well as the density can be expanded in series of Mayer graphs. To a vertex (i) of the graph is associated the weight $z(\mathcal{L}_i)$ and to a bond (i, j) the weight $f(i, j) = \exp[-\beta v(\mathcal{L}_i, \mathcal{L}_j)] - 1$. The value of the graph is obtained by integrating on loops at internal vertices according to the rule (7); nonintegrated vertices are the root points of the graph. It is useful to split $f(i, j) = f_\ell(i, j) + f_{n\ell}(i, j)$ with $f_\ell(i, j) = -\beta v(\mathcal{L}_i, \mathcal{L}_j)$ the part linear in the interaction. Then a Mayer graph is said to be irreducible (or multiply connected) if it cannot be disconnected by cutting a $f_\ell(i, j)$-bond. Define $\mathcal{I}(\mathcal{L})$ to be the value of sum of all irreducible graphs with one root point and

$$F(\mu) = \sum_{q=1}^{\infty} q \int D_q(\mathbf{X}) \mathcal{I}(\mathcal{L}) \tag{10}$$

Note that because of translation invariance $\mathcal{I}(\mathcal{L})$ does not depend on the location $\mathbf{R}$ of the polymer. The following propositions are proved in Martin and Piasecki (2003, 2005)

Proposition 1. *The Mayer series converge absolutely for $\mu < -a\rho_c$ with ρ_c the critical density of the free gas (3).*

Proposition 2. *The density $\rho(\mu)$ as function of the chemical potential μ is determined as the solution of the implicit equation*

$$\rho(\mu) = F(\mu - a\rho(\mu)) \tag{11}$$

in the range of convergence of the Mayer series, with $F(\mu)$ defined in (10) .

Equation (11) can now be used to compute the density $\rho(\mu)$ as a function of the chemical potential in the interacting gas.

4. THE SINGLE POLYMER PROBLEM

An exact determination of the function $F(\mu)$ necessitates the resummation of all irreducible Mayer graphs, a formidable task. The simplest graph consists of a single root point, with attached activity $z(\mathcal{L})$ (8) depending on the self-energy of a polymer. All the other irreducible graphs involve the polymer pair interaction $v(\mathcal{L}_i, \mathcal{L}_j)$. A simple approximation $F^{(0)}$ to F is to disregard the pair interactions and to only retain the effect of the polymer self-energy, i.e., to neglect all graphs except the single root point. According to the definitions (7), (8), one has

$$F^{(0)}(\mu) = \sum_{q=1}^{\infty} q \int D_q(\mathbf{X}) z(\mathcal{L}) = \frac{1}{(2\pi\lambda)^3} \sum_{q=1}^{\infty} \frac{e^{\beta\mu q}}{q^{3/2}} \kappa(q) \tag{12}$$

where

$$\kappa(q) = \int D_q(\mathbf{X}) \exp[-\beta U(q, \mathbf{X})] \tag{13}$$

is the Brownian bridge expectation of the statistical weight of a polymer of size q self-interacting with the repulsive interaction (9). Comparing with the free gas density (2) one sees that the only difference in (12) is the occurence of the new factor $\kappa(q)$. The saturation mechanism for $F^{(0)}(\mu)$ requires to know the range of convergence of the series (12), say $\mu \in (-\infty, \mu_c)$ for some μ_c, and to have $\lim_{\mu\to\mu_c} F^{(0)}(\mu) = F^{(0)}(\mu_c)$ finite. By solving the self-consistent Eq. (11) with $F^{(0)}(\mu)$ in place of $F(\mu)$ one then will find that, within the single polymer approximation, the density will saturate at $\mu = \mu_c + aF^{(0)}(\mu_c)$ thus providing a strong indication for Bose condensation in the presence of interactions.[3]

The answer to these questions clearly depends on the knowledge of the asymptotic behavior of $\kappa(q)$ as $q \to \infty$. The determination of this asymptotic behavior is a nontrivial problem in Brownian motion theory, which has received much attention in the context of classical polymers. Classical polymers are modeled as Brownian paths interacting by means of the repulsive interaction

$$U_{\text{clas}}(\mathcal{L}) = \frac{1}{2} \int_0^q ds_1 \int_0^q ds_2 v(\lambda|\mathbf{X}(s_1) - \mathbf{X}(s_2)|) \tag{14}$$

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[3] It can be seen that solving (11) in this approximation is equivalent to approximate the density by the sum of tree graphs with linearized bonds $f_\ell(i, j)$.

For such polymers, it is established on firm grounds that the corresponding Brownian expectation behaves as (Duplantier (1994) and references therein)

$$\kappa_{\mathrm{clas}}(q) = \int D_q(\mathbf{X}) \exp(-\beta U_{\mathrm{clas}}(q, \mathbf{X})) \sim C \frac{e^{-\beta A}}{q^{\eta}}, \quad \eta > 0 \tag{15}$$

as $q \to \infty$ where A and C are constants depending on the form of the potential v. The quantum self-energy (9) differs from $U_{\mathrm{clas}}(\mathcal{L})$ (a part from a constant) by the presence by the $\delta-$distribution $\delta_p(s_1 - s_2)$ that limits the interaction at "equal time" segments of the polymer. This limitation, which does not occur classically (all segments interact pair-wise), originates in the Feynman–Kac formula and is the signature of the quantum mechanical nature of the system. If one could prove that $\kappa(q)$ has the same asymptotic behavior as its classical counterpart (15) one could conclude that the saturation mechanism discussed above holds with $\mu_{\mathrm{c}} = A$. At the moment we can only prove the existence of exponential lower and upper bounds (Martin and Piasecki (2003, 2005))

$$C_1 e^{-\beta A_1 q} \leq \kappa(q) \leq C_2 e^{-\beta A_2 q} \tag{16}$$

which are not precise enough to settle the question. In addition to the saturation problem in the framework of the single polymer model, one would also have to treat the effects of mutual interaction between different polymers. Contrary to other types of phase transitions, the Bose–Einstein condensation is already present in a gas of free quantum particles as the sole result of Bose statistics. It is still an open challenge to show that it is not destroyed when interactions are present.

5. OUTLOOK

Rigorous proofs of Bose–Einstein condensation have been provided in the following cases:

- for the inhomogeneous gas in a trap (i.e., in a confining potential) at zero temperature and in a low density scaling limit (Lieb and Seiringer (2002)); this correponds to the experimental situation described in the Introduction,
- for the homogeneous gas when there is a gap in the one-particle energy spectrum (Lauwers *et al.* (2003)),
- for the homogeneous gas (without spectral gap) with interaction of the mean field type (de Smedt and Zagrebnov (1987); Lewis (1986)).

The case considered in this paper (the original Einstein prediction, namely the homogeneous gas without energy gap and with genuine short-range interactions) is not yet under control. The related literature is immense and discusses a variety of approximate treatments. Our approach relies on a classical-like representation of the system by means of path integral formalism. The representation maps the Bose gas onto a system of self and mutually repulsive polymers. To identify the onset of the saturation mechanism needed for Bose condensation requires in this language the knowledge of the asymptotic behavior of the partition function of a long self-repelling polymer, a difficult problem not yet fully solved even in the classical polymer theory.

The polymer representation is particularly well suited to the investigation of the immediate vicinity of the mean field limit characterized by a scaled potential (Kac potential) $v_\gamma(\mathbf{x}) = \gamma^3 v(\gamma\mathbf{x})$, γ small (γ^{-1} is a measure of the potential range of $v_\gamma(\mathbf{x})$), see Martin and Piasecki (2003). Some exact results on the small γ asymptotics in the noncondensed region can be found in Martin and Piasecki (2005). Although not conclusive about the existence of Bose–Einstein condensation, our study offers at least a new viewpoint on this old problem.

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