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Statistical mechanics of ideal particles in null dimension and confinement

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(Received 1 June 1995)

The statistical mechanics of ideal particles in null dimension is obtained from a recently given polylogarithm formulation by analytic continuation. The chemical potential behaves anomalously as the dimensionality $d\rightarrow 0$, where $d=0$ appears to be an essential singularity of the reduced density. As a result, the temperature becomes irrelevant in null dimension. Also, the exclusion principle reappears in the coordinate space in the guise of an infinitely high energy barrier. Bose particles are not confinable. Standard thermodynamic quantities have been obtained. These results show some relevance to quantum dots in ultrasmall volumes. [S1063-651X(96)07707-0]

PACS number(s): 05.30.$-$d

There is considerable current interest in quasizero-dimension physics, which refers to the study of electrons and excitons in nanostructures [1(a)]. Known variously as quantum dots, Coulomb islands, etc., a finite number of these particles are confined in very small volumes quantized in all three directions. Efforts are being made to make the volumes of confinement ever smaller, possibly to the very limits of dimensions of these particles. As these volumes shrink, it has been found that (i) interacting particles increasingly behave like ideal particles, and (ii) the ground state energies are blueshifted. The emerging dominance of the ideal behavior recalls the underlying basis of the r_s expansion in the theory of the electron gas. To our knowledge the blueshift has not yet been satisfactorily explained [1(b)].

Physically it seems plausible to assume that shrinking the volume confining interacting particles is the same as lowering the dimensionality d of the system of ideal particles. A rigorous proof may be difficult to give. If assumed, the statistical mechanics of ideal particles in null-d could provide some useful insight and limits into the behavior of quantum dots. It may, of course, have some intrinsic interests of its own, such as, e.g., the classical spins in zero spin dimension [2].

In recent years some new methods [3–6] have been developed which have finally led to the theory of polylogarithms, and to a unification of the statistical mechanics of ideal Bose, Fermi, and classical particles [7]. The statistical, thermal, and dimensional properties of ideal particles can at once be related to the structural properties of the polylogarithms. Since this mathematics is seldom applied in physics [8], we shall first briefly introduce it.

The mth order polylogarithm in ζ, denoted $\mathrm{Li}_m(\zeta)$, where ζ may be a complex number, is a generalization of the dilogarithm $\mathrm{Li}_2(\zeta)$ due to Euler, itself a transcendental function [9]. It is real if ζ real and $\zeta\leqslant 1$, and complex if ζ real and $\zeta>1$. It is an analytic function of ζ, regular everywhere except on the branch cut from $\zeta=1$ to ∞. Classical polylogarithms are defined for integral orders only, $m=2,3,\ldots$. The dilogarithm is the seminal one, from which the trilogarithm is obtained, from which the quadrilogarithm, etc. There is a recurrence relation $\zeta\partial/\partial\zeta \mathrm{Li}_{m+1}(\zeta)=\mathrm{Li}_m(\zeta)$.

A very useful integral representation for the polylogarithm of order $m+1$ is as follows [7]:

$$\mathrm{Li}_{m+1}(\zeta)=\frac{1}{\Gamma(m+1)}\int_0^{\zeta}(a-\ln t)^m\,\frac{dt}{1-t},\quad a=\ln\zeta. \quad (1)$$

Using (1) we can deduce functional relations like the duplication formula $\mathrm{Li}_m(\zeta)+\mathrm{Li}_m(-\zeta)=2^{1-m}\mathrm{Li}_m(\zeta^2)$, asymptotic properties, bounds, etc. [9] Also, by (1) we can introduce polylogarithms of lower order [7], e.g., $\mathrm{Li}_1(\zeta)=-\ln(1-\zeta)$ and $\mathrm{Li}_0(\zeta)=\zeta/(1-\zeta)$, the monologarithm and nil-logarithm, respectively, which are the only polylogarithms of non-negative order expressible in closed form. We can define the polylogarithms of half-integral order by analytic continuation. Although not recognized in the classical theory, these specially defined polylogarithms are useful in physics.

The statistical mechanics of ideal particles is unifiable in the following way: Let $\rho\equiv N/L^d$ be the number density and λ the thermal wavelength. Then the reduced density of a non-relativistic ideal gas in d dimensions may be given as [7]

$$\rho\lambda^d=\mathrm{sgn}(\zeta)\mathrm{Li}_{d/2}(\zeta),\quad \zeta=\begin{cases} z & \text{if Bose}\\ -z & \text{if Fermi,}\end{cases} \quad (2)$$

where the fugacity $z=\exp\beta\mu$, μ the chemical potential, $\beta=1/kT$, T temperature, and k the Boltzmann constant. The spin multiplicity $2s+1$ has been suppressed being inessential here. The grand partition function follows from (2): $Q=\exp\{\mathrm{sgn}(\zeta)(\lambda/L)^d\mathrm{Li}_{d/2+1}(\zeta)\}$.

The dimensionality d enters the polylogarithm through its order—an integral order if d is even, and a half-integral order if d is odd. The fugacity z alone determines the argument of the polylogarithm. The physically applicable domains for Fermi and Bose particles are, respectively, the intervals $\zeta=(-\infty,0)$ and $(0,1)$, whereupon the polylogarithm is real. (Any point in this interval represents an adiabatic line in thermodynamic planes.)

The thermodynamics of Fermi particles are regular since the polylogarithm is free of singularities on the negative real axis of ζ. The low-T properties of Fermi particles are simply the asymptotic properties of $\mathrm{Li}_{d/2}(\zeta)$, $\zeta\to-\infty$. The domain of Bose particles is also free of singularities except at the end point $\zeta=1$, which is a terminus of a branch cut if $d>0$. The branch point singularity at $\zeta=1$ is the mathematical source of the Bose-Einstein transition [3]. The branch cut running from $\zeta=1$ to ∞ corresponds to the Yang-Lee zeros in the thermodynamic limit [10]. The classical ideal gas is described by the condition $\zeta\to\pm0$, i.e., $\mathrm{Li}_{d/2}(\zeta)=\zeta$, where the polylogarithm is self-similar, hence generally d independent. The classical physics centers on the common point of the two domains $\zeta=0$, which partitions the interval of ζ according to statistics.

The thermodynamic functions can be expressed in polylogarithms through their relationship to the density. The pressure P, the energy U, the entropy S, and fluctuations in number of particles Y are, respectively, as follows [7]:

$$\beta\rho^{-1}P=\mathrm{Li}_{d/2+1}(\zeta)/\mathrm{Li}_{d/2}(\zeta), \tag{3}$$

$$\beta U/N=(d/2)\mathrm{Li}_{d/2+1}(\zeta)/\mathrm{Li}_{d/2}(\zeta), \tag{4}$$

$$S/Nk=(d/2+1)\mathrm{Li}_{d/2+1}(\zeta)/\mathrm{Li}_{d/2}(\zeta)-\ln|\zeta|, \tag{5}$$

$$Y=\mathrm{Li}_{d/2-1}(\zeta)/\mathrm{Li}_{d/2}(\zeta). \tag{6}$$

By the principle of analytic continuation, these results may be assumed valid for any d dimensions. In fact, by (3)–(6) all known results can be recovered. They denote a unification of the statistical thermodynamics of ideal particles.

If particles are extremely relativistic or if their dispersion relation is merely linear (i.e., $\epsilon_p=\nu p$, where ν is the velocity), the expression for the reduced density (2) changes as follows: λ is replaced by $\eta=\sqrt{\pi}\hbar\beta\nu[\Gamma(1/2)/\Gamma(d/2+1/2)]^{1/d}$ and the order of the polylogarithm $d/2$ by d. Now only the polylogarithms of integral order appear. There are no other changes. The thermodynamic relationships (3)–(6) remain the same, except for $d/2$ being replaced by d therein.

Although it would be difficult to construct the statistical mechanics of ideal particles in null-d in a conventional manner, our formalism allows us to obtain an equivalent one by the principle of analytic continuation. Also, if $d\to0$, it is immaterial whether the particles are nonrelativistic or extremely relativistic. Hence we shall consider only the nonrelativistic case.

The volume in null-d, a point or a dot, differs fundamentally from the volumes in $d>0$ which are hypercubical in length L. The density in null-d thus must refer to the number of particles per dot, i.e., an absolute fixed number, say n. It is not like the densities in $d>0$, which can be changed even if there are a fixed number of particles. This quantity n evidently is a measure of confinability. We shall assume it to be the same as the number of particles that remain within the enclosing volume when it shrinks to a point adiabatically.

The reduced density for spinless nonrelativistic Fermi particles in d dimensions follows from (2):

$$\rho\lambda^d=-\mathrm{Li}_{d/2}(-z), \quad 0<z<\infty. \tag{7}$$

Setting $d=0$, replacing ρ by n, we obtain

$$n=-\mathrm{Li}_0(-z)=\frac{z}{1+z}. \tag{8}$$

Now n must be T independent. The only way that this physical requirement can be met is if $z\to\infty$, resulting in $n=1$. In null-d evidently only one spinless Fermi particle (two if spin-1/2) can be accommodated, a restatement of the Pauli exclusion principle. It is equivalent to the coordinate space version of an electron in the $1S$ atomic orbital state.

The above result is obtained in effect by taking $d\to0$ first and $z\to\infty$ second, where the second limit is physically driven. That is, if $d\to0$, evidently z strongly depends on it such that $z\to\infty$ itself. Their relationship may be uncovered as follows: If $z\to\infty$, the polylogarithm in (7) may be replaced by its asymptotic form which can be obtained from (1) [7],

$$\rho\lambda^d=\frac{(\ln z)^{d/2}}{\Gamma(d/2+1)}+o((\ln z)^{d/2-1}). \tag{9}$$

We note that if $d\neq0$, $z\to\infty$ means $T\to0$, recalling that $\mu(T=0)=\epsilon_F$, $0<\epsilon_F<\infty$, and ϵ_F is the Fermi energy. In fact, through the above asymptotic form we recover the standard result

$$\rho=\frac{(k_F^2/4\pi)^{d/2}}{\Gamma(d/2+1)}, \tag{10}$$

where k_F is the Fermi wave vector. Now, if $d\to0$, we can recover the same previous result provided that $k_F^{-1}\to0$ not as fast. Thus from (9) we obtain the following two interesting conditions:

$$\lim_{z\to\infty,d\to0}(d/2)\ln\ln z=0, \tag{11a}$$

$$\lim_{z\to\infty,d\to0}(d/2)\ln z=\infty. \tag{11b}$$

Since the null-d volume is singular, it is not possible to give a Taylor expansion of (7) about $d=0$. The slope, which may be obtained from (9), behaves as $\frac{1}{2}\ln\ln z$ (the leading term only). The nth derivative with respect to d is in fact $(\frac{1}{2}\ln\ln z)^n$, so that all the derivatives are divergent as $z\to\infty$ and $d\to0$. This behavior suggests that $d=0$ is an essential singularity of the reduced density. One can construct the $d\to0$ form of the chemical potential which satisfies (11a) and (11b). Noting that $d\to0$ implies $z\to\infty$, let

$$\mu\sim d^{-x}, \quad x>1 \quad (d\to0). \tag{12}$$

Substituting (12) into (9), we obtain

$$\rho\lambda^d\sim e^{-(x/2)d\,\ln d} \quad (d\to0), \tag{13}$$

which has the requisite behavior of an essential singularity (e.g., the slope $\sim -\ln d$, $d \to 0$).

In null-d, thermodynamics in the ordinary sense would seem out of place. But if our formulation is analytically continued, what may be purely formal still seems to lend a consistent description. For example, $z \to \infty$ at any T means that $\mu \to \infty$ independently of T, i.e., T is not relevant in null-d. Since $\mu \to \infty$, it is energetically not possible to bring in another particle if one is already present. In null-d, the exclusion principle appears in the guise of an infinitely large chemical potential or, equivalently, an infinitely high potential barrier to particles in the reservoir. There is no classical analog.

The state of $z = \infty$, as noted, can also be realized in $d \neq 0$ if $T = 0$. Thus the ground state of Fermi particles in $d \neq 0$ should to some extent be mirrored in the thermodynamics in $d = 0$. For example, from (5), $S/k = \mathrm{Li}_1(-z)/\mathrm{Li}_0(-z) - \ln z \sim z^{-1} \ln z \to 0$ as $z \to \infty$. There is no entropy. From (6), $Y = \mathrm{Li}_{-1}(-z)/\mathrm{Li}_0(-z) \sim z^{-1} \to 0$ as $z \to \infty$. There are no fluctuations in number of particles. But from (4), $\beta U = (d/2)\mathrm{Li}_1(-z)/\mathrm{Li}_0(-z) \sim (d/2)\ln z \to \infty$ by (11b). Also from (3), $\beta P = \mathrm{Li}_1(-z)/\mathrm{Li}_0(-z) \sim \ln z \to \infty$ similarly or $P = \mu \to \infty$. An infinitely large energy or pressure implies an infinitely large momentum, necessary to preserve the uncertainty principle in null-d, where presumably there is no uncertainty in the position. Similarly a total uncertainty in the momentum of a particle in null-d implies that it is never in a stationary state, i.e., there always is a time evolution going from state to state. The energy and pressure increase very sharply with confinement as $U \sim d^{1-x}$ and $P \sim d^{-x}$, where $x > 1$ as $d \to 0$.

The reduced density for ideal nonrelativistic Bose particles in d follows from (2):

$$\rho \lambda^d = \mathrm{Li}_{d/2}(z), \quad 0 \leq z \leq 1. \tag{14}$$

By setting $d = 0$ and replacing ρ by n, we have

$$n = \mathrm{Li}_0(z) = \frac{z}{1-z}. \tag{15}$$

For the right-hand side of (15) to be T independent, as it must, it is necessary that $z = 0$, i.e., $\mu \to -\infty$ at any T. Hence T has no meaning here in null-d just as in the Fermi case. That $z = 0$ of course means that $n = 0$. We must conclude that ideal Bose particles cannot be confined in null-d because the chemical potential is negative infinite.

An infinitely large negative chemical potential places particles over edges of a potential precipice. They will fall out and escape from a confinement. In contrast, an infinitely large positive chemical potential acts as a potential barrier to the particles without and a confinement to the particles within. Also, $z = 0$ is the state of $T = \infty$, the ''ultimate'' classical limit. Recall that the classical chemical potential behaves as $\mu \sim T \ln T^{-1}$ as $T \to \infty$. Hence, equivalently, particles with so large a thermal energy cannot be confined to a point.

The other possibility $z = 1$ (i.e., $\mu = 0$) must be excluded since it would imply an existence of Bose-Einstein condensation at all T. Also recall that Bose-Einstein condensation exists if $d > 2$ only ($d > 1$ if extreme relativistic) [3]. If $z = 1$, $P = U = 0$ from (3) and (4). Hence there can be no particles out of the condensate. The existence of Bose-Einstein condensation in null-d then would imply a massive violation of the uncertainty principle.

As in the Fermi case, it is possible to shed some light on the behavior of the reduced density near $d = 0$. To obtain (15) we have taken $d \to 0$ first, then $z \to 0$ followed (physically required). Now reversing the order, let $z \to 0$ first. Then, using (1), one can prove that the polylog becomes self-similar, i.e.,

$$\rho \lambda^d = \mathrm{Li}_{d/2}(z) = z + o(z^2). \tag{16}$$

Now one can take $d \to 0$ recovering the same previous result. Being self-similar, the right-hand side of (16) is to order $o(z^2)$ d independent, and all derivatives vanish to this order. Since $\mu \to -\infty$ as $d \to 0$, let $\mu \sim -d^{-y}$, where $y > 0$ as $d \to 0$, structurally similar to the chemical potential for Fermi particles (12). Then

$$\rho \lambda^d \sim e^{-d^{-y}}, \quad y > 0 \quad (d \to 0), \tag{17}$$

also essentially singular at $d = 0$.

From (3) and (4), to order $o(z)$, $\beta U = N(d/2) \sim d$ and $\beta P = \rho \sim \exp - d^{-y}$, both vanishing as $d \to 0$. The strong vanishing of the slope of the reduced density as $d \to 0$ indicates that most particles will have escaped confinement with little energy well before $d \to 0$. This is in contrast to the behavior of Fermi particles, for which the null-d population is attained with a greatly rising energy only after $d \to 0$.

Are Bose particles really not confinable? Photons evidently are not because of the finite speed. Elementary excitations like phonons and plasmons—quasibosons—being extended over large regions of the physical space, are not confined. Excitons have a large Bohr radius [11]. They are, in fact, thought to be a realization of ideal Bose particles in $3d$ [12].

In conclusion, if the small volume limit of interacting particles and the low-dimensionality limit of ideal particles are equivalent, quantum dots in ultrasmall volumes [13] should be bounded by our null-d results. The blueshift in the ground state energy for the ''zero-dimension'' electrons may very well be foreshadowing the steep rise in the energy of ideal Fermi particles as $d \to 0$. The breakdown of excitons in the strong confinement regime [1(a)], however, does not necessarily indicate the nonconfinability of Bose particles, but more likely their shallow binding state. A more definitive test is needed.

The author thanks Dieter Hartmann and Robert L. Anderson for discussions. This work was supported in part by the NSF.

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