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ANOMALOUS BEHAVIOR OF IDEAL FERMI GAS BELOW 2D: THE "IDEAL QUANTUM DOT" AND THE PAUL EXCLUSION PRINCIPLE

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A physical interpretation is given to a curious "hump" that develops in the chemical potential as a function of absolute temperature in an ideal Fermi gas for any spatial dimensionality $d < 2$, integer or not, in contrast with the more familiar monotonic decrease for all $d \geq 2$. The hump height increases without limit as d decreases to zero. The divergence at $d = 0$ is shown to be a clear manifestation of the Pauli Exclusion Principle whereby two spinless fermions cannot sit on top of each other in configuration space. The hump itself is thus an obvious precursor of this manifestation, otherwise well understood in momentum space. It also constitutes an "ideal quantum dot" when $d = 0$.

Keywords: Ideal Fermi gas; arbitrary dimensions (integer or not); null dimension; ideal quantum dot; Pauli exclusion principle.

1. Introduction

The Pauli Exclusion Principle[1] plays a well-known role in constructing the Periodic Table of the Elements starting from hydrogen and then helium and etc. It is also crucial in explaining ionic and covalent bonding in molecules and solids, and in characterizing and distinguishing metals from insulators from semiconductors from superconductors. It accounts for nuclear shell structure and nuclear binding energies and even for a whole class of "compact astrophysics objects" such as white-dwarf stars, neutron stars, and black holes. It has been shown (see Refs. 2 and 3) to be

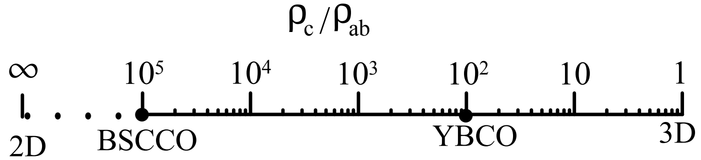

Fig. 1. Variation with the dimension d in high-temperature cuprate superconductors of the empirical ρ_c/ρ_{ab}, where ρ_{ab} is the resistivity parallel to the cooper-oxide planes and ρ_c that in the perpendicular direction, as d changes continuously from 2 to 3. Point marked $BSCCO$ corresponds to the experimental value found in the $Bi_{2+x}Sr_{2-y}CuO_{6+\delta}$ superconductor while point $YBCO$ stands for that commonly reported for the $YBa_2Cu_3O_{7-\delta}$ superconductor.

responsible for fact that ordinary bulk matter is stable and occupies volume. Here we present a novel proof of the Pauli Principle in ordinary space that starts from the d-dimensional ideal Fermi gas (IFG), for all $d \geqslant 0$, integer or not. As a by product, we propose a concrete example of what might be called an "ideal quantum dot."

It is well-known that the nonrelativistic ideal Bose gas (IBG) of quadratically-dispersive bosons undergoes a Bose-Einstein condensation (BEC) only for any dimensionality, integer or not, $d > 2$, with a cusp singularity in the temperature-dependent heat capacity for $2 < d \leqslant 4$ and a finite jump discontinuity for $d > 4$[4-6]. Since its theoretical prediction by Einstein in 1925 based on work in 1924 by Bose on photons, and after languishing many decades as a mere academic exercise in textbooks, BEC has been observed in the laboratory in laser- and evaporatively-cooled, magnetically-trapped ultra-cold bosonic atomic clouds of: $^{87}_{37}$Rb[7] and later of $^{7}_{3}$Li, $^{23}_{11}$Na, $^{1}_{1}$H, $^{85}_{37}$Rb, $^{4}_{2}$He , $^{41}_{19}$K , $^{174}_{70}$Yb, $^{133}_{55}$Cs, $^{52}_{24}$Cr and $^{50}_{24}$Cr. BEC has also been observed in lower d: Görlitz *et al.* [8] report BEC of $^{23}_{11}$Na atoms in 1D and 2D; Schreck *et al.* [9] observed it with $^{7}_{3}$Li atoms in 1D; Burger *et al.*[10] study the phase transition in cloud of $^{87}_{37}$Rb atoms in quasi-2D, to cite just a few instances.

The discovery of quasi-2D superconductors such as the cuprates[11,12], as well as quasi-1D superconductors like the organo-metallic (or Bechgaard) salts[13-16] and carbon nanotubes[17], has further motivated studying low-d quantum gases. For example, if the CuO_2 planes in cuprate superconductors are defined as the a, b plane while c is the perpendicular direction, anisotropies in the resistivities ratio $\rho_c/\rho_{a,b}$ as high as 10^5 have been reported[18] for $Bi_{2+x}Sr_{2-y}CuO_{6+\delta}$ ($BSCCO$) and are commonly quoted to be around 10^2 for $YBa_2Cu_3O_{7-\delta}$ ($YBCO$). According to the Drude model, Ref. 19 p. 7, of electric conductivity, the ratio $\rho_c/\rho_{a,b} = m_c/m_{a,b}$ where m_c and $m_{a,b}$ are the charge-carrier masses along the c and a, b-plane directions. Perfect isotropy then means $\rho_c/\rho_{a,b} = m_c/m_{a,b} = 1$, as characterizes an ideal 3D material. And if this ratio is infinite the charges "frozen" onto the a, b plane as in a perfectly 2D material. The *continuous* transition between 2D and 3D is illustrated in Fig. 1 where both $YBCO$ and $BSCCO$ lie in between. Indeed, two independent studies[20] [21] found $YBCO$ "living" in $d = 2.03$ dimensions.

2. Ideal Fermi Gases in Any $d \geqslant 0$

In contrast to the boson case, Fermi systems exhibit nontrivial anomalous behavior *below* 2D[22]. Low-d Fermi systems have found a host of practical applications in microelectronics[23]-[26] with quantum "wells" (2D), "wires" (1D) and "dots" (0D) [27].

The N-boson or N-fermion number equation for particles with energy $\varepsilon_{\mathbf{k}}$ is

$$N = \sum_{\mathbf{k}} n_{\mathbf{k}} = \sum_{\mathbf{k}} [\exp\{\varepsilon_{\mathbf{k}} - \mu(T)\}/k_B T \mp 1]^{-1} \tag{1}$$

with $\mu(T)$ the gas chemical potential. A peculiar rise in $1D$ of the fermion $\mu(T)$ as absolute temperature T increases from 0 was reported in a graph without further comment in Ref. 28. It was determined from the Sommerfeld low-T series expansion, Ref. 19 p. 45. For integer $d \neq 2$[29], and more generally for any $d \geqslant 0$[22] except $d = 2$, using the large-$z \equiv \exp \mu(T)/k_B T$ expansion[30] $f_\sigma(z) \simeq (\ln z)^\sigma/\Gamma(\sigma+1) + \left(\pi^2/6\right)(\sigma-1)(\ln z)^{\sigma-2}/\Gamma(\sigma) + \cdots$ (also known as Sommerfeld's lemma) for $\sigma = d/2$, the Sommerfeld expansion for $\mu(T)$ is found to become

$$\mu(T)/E_F \xrightarrow[T/T_F \to 0]{} 1 - (d-2)(\pi^2/12)\,(T/T_F)^2 + O(T^4) \tag{2}$$

where $T_F \equiv E_F/k_B$ is Fermi temperature and $E_F \propto \hbar^2 n^{2/3}/m$ (with n and m the fermion particle density and mass). Clearly, the first correction to unity on the rhs is negative (but *positive)* for all $d > 2$ ($d < 2$). For $d = 2$ one has the exact explicit expression (*not* expandable in powers of T/T_F by inspection)

$$\mu(T)/E_F = T/T_F \ln[\exp(T_F/T) - 1] \xrightarrow[T/T_F \to 0]{} 1. \tag{3}$$

Since for T large enough $\mu(T)$ must diverge negatively to approach the well-known classical ideal gas value

$$\mu(T)/E_F \xrightarrow[T/T_F \to \infty]{} -(d/2)(T/T_F)\ln(T/T_F) \tag{4}$$

a "hump" shape for $\mu(T)$ can be surmised in association with its initial rise at small T for all $d \leqslant 2$. Figure 2 illustrates this for several values of d, integer or not. This hump subsequently also appears[22] in the specific heat $C_V(T)$ curve.

In a volume L^d in any dimension d and in the continuum limit (1) becomes

$$N = (L/2\pi)^d [2\pi^{d/2}/\Gamma(d/2)] \int dk k^{d-1} [z^{-1}\exp(-\beta\varepsilon_{\mathbf{k}}) \mp 1]^{-1} \tag{5}$$

where $\beta \equiv 1/k_B T$, and the volume of a hypersphere of radius R in $d \geq 0$ dimensions

$$V_d(R) = \pi^{d/2} R^d/\Gamma(1 + d/2) \qquad \text{note: } V_0(R) \equiv 1 \tag{6}$$

was used. If the boson case holds for $a = -1$ and the fermion for $a = +1$, integrating over $x \equiv \beta\varepsilon_{\mathbf{k}}$ instead of over k in (5), via the density-of-states associated with $\varepsilon_{\mathbf{k}} = \hbar^2 k^2/2m$, one deals with the expression

$$\frac{1}{\Gamma(\sigma)} \int_0^\infty dx \frac{x^{\sigma-1}}{z^{-1}e^x + a} = -\frac{1}{a} \sum_{l=1}^{\infty} \frac{(-az)^l}{l^\sigma} \equiv -\,aLi_\sigma(-az) \qquad |z| < 1 \tag{7}$$

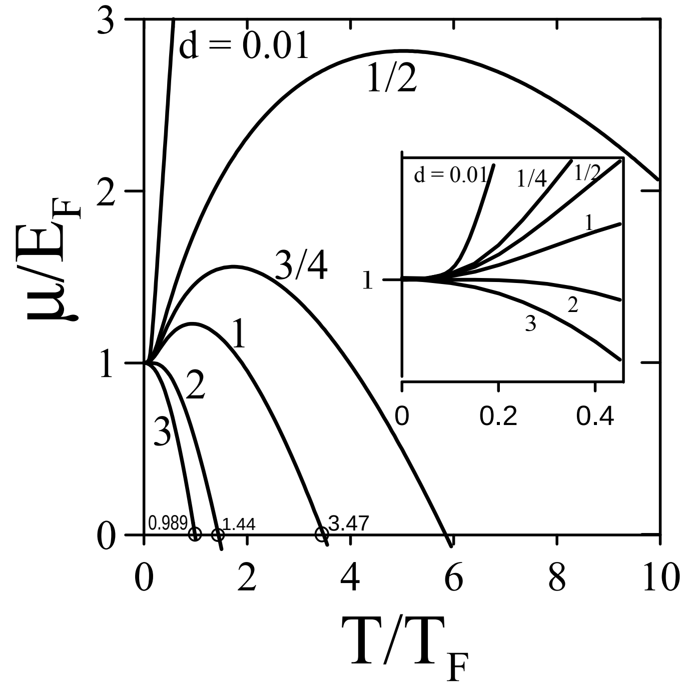

Fig. 2. Chemical potential $\mu(T)$ (in units of the Fermi energy E_F) of an IFG in $d = 3$, 2, 1, 3/4, 1/2 and 1/100 spatial dimensions as function of absolute temperature T (in units of Fermi temperature $T_F \equiv E_F/k_B$). The monotonically-decreasing curves for $d = 2$ and 3 are the familiar textbook curves which turn negative at $T/T_F \simeq 1.44$ and 0.989, respectively. Inset illustrates rise of $\mu(T)$ with T for $d < 2$, as opposed to its monotonic decrease for all $d \geq 2$.

where $z \equiv \exp[\mu(T)/k_BT] \equiv \exp \beta\mu(T)$ is the gas fugacity. The limitation $|z| < 1$ in convergence arises from the small-z binomial expansion of the integrand on the lhs of (7), which is then integrated term by term to get the summation term. Here we shall need to go beyond this unit circle of convergence in the z-plane, in fact the case $z \to \infty$ will be needed. For $a = -1$ (7) is the Bose integral $g_\sigma(z)$ which for $z = 1$ and $\sigma \geq 1$ becomes the Riemann Zeta function $\zeta(\sigma)$ of order σ. For $a = 1$ (7) is the Fermi integral $f_\sigma(z)$. Both Bose and Fermi integrals are extensively discussed in an Appendix of Ref. 30. In (7) $Li_\sigma(t) = \sum_{l=1}^{\infty} t^l/l^\sigma$ is the polylogarithm function designated as $PolyLog[\sigma, t]$ in Ref. 31.

Introducing the standard thermal wavelength

$$\lambda \equiv h/\sqrt{2\pi m k_B T} \tag{8}$$

one has for spinless fermions from (5) and (7) with $\sigma = d/2$ the reduced (i.e., dimensionless) number density

$$n\lambda^d = \frac{1}{\Gamma(d/2)} \int_0^\infty dx \frac{x^{d/2-1}}{\exp(x-\alpha)+1} \equiv I_{d/2}(\alpha) \tag{9}$$

where $n \equiv N/L^d$ and $\alpha(T) \equiv \beta\mu(T) \equiv \ln z$. Letting $\exp(\alpha - x) \equiv y$ in (9) and calling $d/2 - 1 \equiv m$ one gets the integral representation[32]

$$I_{m+1}(z) = \frac{1}{\Gamma(m+1)} \int_0^z \frac{dy}{y+1} (\alpha - \ln y)^m \qquad 0 < z < \infty \tag{10}$$

which is now valid for all nonnegative z. It can in fact be shown (Ref. 32, Eq. 10) that the integral defined in (9) is precisely

$$I_m(z) \equiv -Li_m(-z) \tag{11}$$

where the polylog function $Li_m(z)$ is defined by

$$Li_m(z) = \sum_{l=1}^{\infty} z^l / l^m \qquad |z| < 1 \tag{12}$$

and also by

$$= \int_0^z \frac{dt}{t} Li_{m-1}(t) \qquad 0 < z < \infty.$$

Or, alternately by

$$z \frac{\partial}{\partial z} Li_m(z) = Li_{m-1}(z). \tag{13}$$

This in turn immediately implies that

$$Li_1(z) = -\ln(1-z) \quad \text{and} \quad Li_0(z) = z/(1-z) \tag{14}$$

where the latter expression is to be used in the $d = 0$ IFG case to be discussed below. From (9) and (11) the number density n for N spinless fermions is thus given by

$$n\lambda^d = I_{d/2}(z) = -Li_{d/2}(-z). \tag{15}$$

For bosons, instead of (15) one has[33] $n\lambda^d = Li_{d/2}(z)$. For $z \equiv \exp \beta\mu = \exp \beta_c 0 = 1$ in $3D$ this implies $n\lambda_c^3 = Li_{3/2}(1) \equiv \zeta(3/2)$ which in turn immediately leads to

$$T_c = 2\pi\hbar^2 n^{2/3} / m\zeta(3/2)^{2/3} \tag{16}$$

or the familiar BEC critical temperature.

For fermions, if $T \to 0$ ($\beta \to \infty$) then $\alpha \equiv \beta\mu \equiv \ln z \to \infty$ and one can show (Ref. 32 Eq. 3) that

$$I_{m+1}(z_0) = (\alpha_0)^{m+1} / \Gamma(m+2) + O(\alpha_0) \tag{17}$$

where $\alpha_0 \equiv \beta\mu_0 \equiv \ln z_0$ with $\mu_0 \equiv E_F \equiv \hbar^2 k_F^2 / 2m$. For $m + 1 = d/2$ and since n is temperature-*independent* so that from (15) one may evaluate $I_{d/2}(z)/\lambda^d$ at $T = 0$ using (17). Since from (8) $\lambda \equiv h\sqrt{\beta/2\pi m}$, one can then write

$$n = \frac{1}{\lambda^d} I_{d/2}(\alpha_0) = \frac{1}{\lambda^d} \frac{(\alpha_0)^{d/2}}{\Gamma(d/2+1)}$$

$$= \frac{1}{(h\sqrt{\beta/2\pi m})^d} \frac{(\beta E_F)^{d/2}}{\Gamma(d/2+1)} = \frac{(k_F^2/4\pi)^{d/2}}{\Gamma(d/2+1)} \tag{18}$$

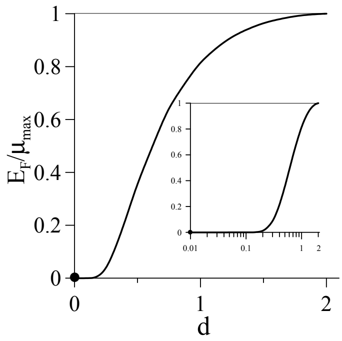

Fig. 3. Inverse of the maximum height of the $\mu(T)/E_F$ hump for an IFG for all $d < 2$. It exhibits how $\mu(T)/E_F$ must diverge when $d \to 0$, as follows from the analytical result (19) at precisely $d = 0$. Inset shows a semilog plot. Maximum value of $\mu(T)$ is just E_F (thin horizontal line at top) for all $d \geq 2$.

a known result. This reduces in $d = 3$ dimensions to the even more familiar expression $n = k_F^3/6\pi^2$ for spinless fermions.

3. Null-Dimensional (d = 0) IFG

At precisely $d = 0$ (15) and (18) imply that

$$n_{d\to 0} = \frac{(\alpha_0)^0}{\Gamma(1)} = 1 = -Li_0(-z) = \frac{z}{1+z} 0 < z < \infty \qquad (19)$$

where the last equality comes from the second relation in (14). At first sight, (19) implies that $1+z = z$ or that $1 = 0$—obviously impossible. One quickly realizes that infinite z is the *only* possible solution. And if $z \equiv \exp \mu(T)/k_B T = \infty$ this in turn implies that $\mu(T) = \infty$ for *all* T. Since the chemical potential μ is the energy that must be given the N-particle system to bring one particle to it, $\mu = \infty$ signifies an impossibly high energy barrier to add another fermion when one is already present, irrespective of T.

The analytical result (19)[33] for $d = 0$ is consistent with numerical results exhibited for all values of $d \geqslant 0$, integer or not, in Fig. 3.

4. Conclusion

The null-d ideal Fermi gas defines an "ideal quantum dot." Its infinite chemical potential is a statistical thermodynamic manifestation of the Pauli Exclusion Principle whereby two identical spinless fermions cannot be placed on top of each other in real space. The hump-shaped behavior in $\mu(T)$ for all $d < 2$ is evidently a precursor of this infinity. All of the above is reminiscent of the relevant and amusing quip: "Physics suggests that if the 2D realm is promising, then 1D or zero-D is even better[23]."

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