Riemannian geometry of the Pauli paramagnetic gas

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Abstract

We investigate the thermodynamic curvature resulting from a Riemannian geometry approach to thermodynamics for the Pauli paramagnetic gas which is a system of identical fermions each with spin $\frac{1}{2}$. We observe that the absolute value of thermodynamic curvature can be interpreted as a measure of the stability of the considered system only in the classical and semiclassical regime. But in quantum regime some exceptions are observed.

1 Introduction

Thermodynamic fluctuation theory whose basic goal is to express the time independent probability distribution for the state of a fluctuating system in terms of thermodynamic quantities, is usually attributed to Einstein who applied it to the problem of blackbody radiation \cite{1}. The full formalism for classical thermodynamic fluctuation theory was worked out by Green and Callen \cite{2} in 1951 and elaborated upon by Callen \cite{3}.

However, despite of a wide range of applicability, the classical fluctuation theory fails near critical points and at volumes of the order of the correlation volume and less.

In 1979 Ruppeiner \cite{4} introduced a Riemannian metric structure representing thermodynamic fluctuation theory, and related to the second derivatives of the entropy. His theory offered a good meaning for the distance between thermodynamic states. He showed that the breakdown of the classical theory occurs because it does not take into account local correlations\cite{5}. This deficiency of the classical theory is precluded in the covariant fluctuation theory of Ruppeiner by using a hierarchy of concentric subsystems, each of which samples only the thermodynamic state of the subsystem immediately larger than it\cite{6,7}. One of the most significant topics of this theory is the introduction of the Riemannian thermodynamic curvature as a qualitatively new tool for the study of fluctuation phenomena. It is this geometry which is the basis for this paper. Here we investigate the case of a Pauli paramagnetic gas that is a gas of identical spin $\frac{1}{2}$ fermions in the presence of an external magnetic field.
The outline of this paper is as follows. First the Riemannian geometry of thermodynamic fluctuation theory is summarized. Second, the Riemannian scalar curvature of the Pauli paramagnetic gas is evaluated. Finally the curvature of the classical ideal paramagnetic gas is calculated and is compared to the the curvature of Pauli paramagnetic gas in the classical limit.

2 Geometrical viewpoint of thermodynamics

In this section we review the Riemannian geometry of thermodynamics, discuss its connection to the covariant thermodynamic fluctuation theory, and summarize the resulting interpretation of thermodynamic curvature. Riemannian structure of the thermodynamic state space is defined by the second derivatives of a thermodynamic potential density as a metric tensor\[7\]. If we choose extensive densities as coordinates, we can use either energy or entropy density as the potential and these two descriptions are thermodynamically equivalent; but the metric tensor is different in these two representations. Here we work in entropy representation, because then the meaning of the distance, measured in units of average fluctuations, is very transparent. When some extensives are substituted by intensives, the potential is a Massieu function[3]. Now we consider an open subsystem \(\mathcal{A}_V\), with fixed volume \(V\), of a thermodynamic fluid system \(\mathcal{A}_{V_0}\) with a very large volume \(V_0\). The system \(\mathcal{A}_{V_0}\) consists of \(r\) fluid components and is in equilibrium. We denote by the \(n\)-tuple \(a_0 = (a^0_0, a^1_0, a^2_0, \ldots, a^r_0)\) the internal energy per volume and the number of particles per volume of the \(r\) components of \(\mathcal{A}_{V_0}\)[7]. These parameters are the standard densities in the entropy representation; they constitute the thermodynamic state of \(\mathcal{A}_{V_0}\).

The subsystem \(\mathcal{A}_V\) has the corresponding thermodynamic state \(a\). The Gaussian approximation of the classical thermodynamic fluctuation theory asserts that the probability of finding the thermodynamic state of \(\mathcal{A}_V\) between \(a\) and \(a + da\) is[7]:

\[
P_V(a|a_0)da^0da^1\cdots da^r = \left(\frac{V}{2\pi}\right)^{\frac{r+1}{2}} \exp\left[-\frac{V}{2}g_{\mu\nu}(a_0)\Delta a^\mu \Delta a^\nu\right] \times \sqrt{g(a_0)da^0da^1\cdots da^r},
\]

where

\[
\Delta a^\mu = a^\mu - a_0^\mu,
\]

\[
g_{\mu\nu} = -\frac{1}{K_B} \frac{\partial^2 s}{\partial a^\mu \partial a^\nu}\big|_{a=a_0},
\]

where \(s\) is the entropy per volume in the thermodynamic limit, \(K_B\) is Boltzmann’s constant, and \(g(a_0) = \det[g_{\mu\nu}(a_0)]\).

The quadratic form in Eq.(2.1),

\[
(\Delta l)^2 = g_{\mu\nu}(a_0)\Delta a^\mu \Delta a^\nu
\]

constitutes a positive definite Riemannian metric on the thermodynamic state space. The positive definiteness results since the entropy is a maximum in equilibrium \(a =\)
Eqs. (2.1) and (2.3) denote the physical interpretation for the distance between two thermodynamic states. The less the probability of a fluctuation between the states, the further apart they are. The quantity 
\[ \sqrt{g(a_0)da^0da^1 \cdots da^r} \]
in Eq. (2.1), is the invariant Riemannian thermodynamic state space volume element. The form of Eq. (2.2) holds only in standard densities. To express the metric tensor in a general set of thermodynamic coordinates \( x = x(a) \), one can use the following transformation rule
\[ g'_{\alpha\beta}(x) = \frac{\partial a^\mu}{\partial x^\alpha} \frac{\partial a^\nu}{\partial x^\beta} g_{\mu\nu}(a). \] (2.4)

Having the metric we can calculate the Riemannian curvature tensor. For our metric, the scalar curvature \( R \), has units of real space volume, regardless of the dimension of the state space[11]. It is a measure of effective interaction between the components of the system, proportional to the correlation volume, and diverges near the critical point of the pure interacting fluid. Covariant thermodynamic fluctuation theory indicates that curvature is a measure of the smallest volume where classical thermodynamic fluctuation theory could work. This theory was proposed as the correct way to extend the classical thermodynamic fluctuation theory beyond the Gaussian approximation[7].

An alternative interpretation of the thermodynamic curvature was offered by Janyszek and Mrugala[8]. They suggested that the thermodynamic curvature is a measure of the stability of the considered system. The system is less stable if the curvature increases and vice versa. Also these authors calculated the curvature of ideal Fermi and Bose gases[9]. They show that these systems have the curvature with opposite signs.

In this paper we interpret the absolute value of the curvature as a measure of stability in order to come to an agreement with the curvature of the boson ideal gases that diverge to negative infinity (in the sign convention used here) where the Bose-Einstein condensation occurs[9].

3 Geometry of the Pauli paramagnetic gas

We now turn our attention to studying the equilibrium state of a gas of noninteracting fermions in the presence of an external magnetic field \( H \).

The extensive parameter which describes the magnetic properties of a system is \( M \), that is the component of the total magnetic moment parallel to the external field. The entropic intensive parameters are defined as[3],
\[ F^1 = \frac{\partial S}{\partial U} = \frac{1}{T}; \quad F^2 = \frac{\partial S}{\partial N} = -\frac{\mu}{T}; \quad F^3 = \frac{\partial S}{\partial M} = -\frac{H}{T}. \] (3.1)

We use the thermodynamic potential \( \phi \) which is defined as,
\[ \phi = s[\frac{1}{T}, -\frac{\mu}{T}, -\frac{H}{T}] = s - \frac{1}{T}u + \frac{\mu}{T}\rho + \frac{H}{T}m = \frac{P}{T}, \] (3.2)
where \( u, \rho, m \) and \( P \) are energy per volume, density, magnetization and pressure respectively. The energy of a particle, in presence of an external magnetic field \( H \), is given by
\[
E = \frac{p^2}{2m_0} - \vec{J}.\vec{H} \quad (3.3)
\]
where \( \vec{J} \) is the intrinsic magnetic moment of the particle and \( m_0 \) is its mass. For the case of the Pauli paramagnetic gas the spin of each particle is \( \frac{1}{2} \); the vector \( \vec{J} \) must then be either parallel to the vector \( \vec{H} \) or anti parallel. From the grand canonical distribution (using Fermi-Dirac statistics) one can obtain the following equations [13]:
\[
\ln Q = \frac{PV}{K_B T} = V \left( f^+_\frac{3}{2} + f^-_{-\frac{3}{2}} \right), \quad (3.4)
\]
\[
\rho = \frac{N}{V} = \frac{1}{\lambda^3}(f^+_\frac{3}{2} + f^-_{-\frac{3}{2}}) \quad (3.5)
\]
where
\[
f^\pm_n = f_n(\eta^\pm); \quad (3.6)
\]
\[
\eta^\pm = \eta \exp[\mp \frac{JH}{K_B T}] = \exp[\frac{\mu}{K_B T} \mp \frac{JH}{K_B T}] \quad (3.7)
\]
and \( \lambda = \frac{h}{(2\pi m_0 K_B T)^{\frac{3}{2}}} \) is the mean thermal wavelength of the particle, \( h \) is the Planck constant and
\[
f_n(\eta) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{X^{n-1}dX}{\eta + 1} \quad (3.8)
\]
we have used the standard symbol for the fugacity \( \eta = \exp(\frac{\mu}{K_B T}) \). From Eqs. (3.2) and (3.4) the thermodynamic potential is obtained
\[
\phi(x, y, z) = Ix^\frac{3}{2}[f^+_{\frac{3}{2}}(e^{y-Jz}) + f^-_{-\frac{3}{2}}(e^{-y+Jz})]. \quad (3.9)
\]
Where \( I = \frac{(2\pi m)^{\frac{3}{2}}}{h^3} \) and \( x = F^1, y = F^2, z = F^3 \). We have set \( K_B = 1 \).

Now it is straightforward to obtain the metric elements in \( F \) coordinates [7]:
\[
g_{\mu\nu} = \frac{\partial^2 \phi}{\partial F_{\mu} \partial F_{\nu}} \quad (3.10)
\]
According to Eqs. (3.9) and (3.10) and noting that, \( \frac{\partial f_n(\eta)}{\partial \eta} = \frac{1}{\eta}f_{n-1}(\eta) \), the components of the metric tensor are as follows
\[
g_{11} = \frac{15}{4}Ix^{-\frac{3}{2}}(a + b) \quad g_{12} = \frac{3}{2}Ix^{-\frac{3}{2}}(c + d) \quad g_{13} = -\frac{3}{2}IJx^{-\frac{3}{2}}(c - d) \quad g_{22} = Ix^{-\frac{3}{2}}(e + f) \quad g_{23} = -IJx^{-\frac{3}{2}}(e - f) \quad g_{33} = IJ^2x^{-\frac{3}{2}}(e + f) \quad (3.11)
\]
where \( a = f^+_\frac{3}{2}, b = f^-_{-\frac{3}{2}}, c = f^+_\frac{3}{2}, d = f^-_{-\frac{3}{2}}, e = f^+_\frac{3}{2}, f = f^-_{-\frac{3}{2}} \); they are functions of \( y \) and \( z \).
Their derivatives with respect to \( y \) and \( z \) are as follows:
\[
\frac{\partial a}{\partial y} = -c \quad \frac{\partial a}{\partial z} = Jc \quad \frac{\partial b}{\partial y} = -d \quad \frac{\partial b}{\partial z} = -Jd \quad \frac{\partial c}{\partial y} = -e \quad \frac{\partial c}{\partial z} = Je \quad \frac{\partial d}{\partial y} = -f \quad \frac{\partial d}{\partial z} = -Jf \quad \frac{\partial e}{\partial y} = -h \quad \frac{\partial e}{\partial z} = Jh \quad \frac{\partial f}{\partial y} = -k \quad \frac{\partial f}{\partial z} = -Jk \quad (3.12)
\]
where $h = f^+_n$, $k = f^-_n$, these quantities are used for obtaining the scalar curvature. The Riemann and the Ricci tensors and the scalar curvature are respectively

$$ R^\kappa{}_{\lambda\mu\nu} = \partial_\mu \Gamma^\kappa{}_{\nu\lambda} - \partial_\nu \Gamma^\kappa{}_{\mu\lambda} + \Gamma^\eta{}_{\nu\lambda} \Gamma^\kappa{}_{\mu\eta} - \Gamma^\eta{}_{\mu\lambda} \Gamma^\kappa{}_{\nu\eta} $$

$$ \text{Ric}_{\mu\nu} = R^\lambda{}_{\mu\lambda \nu} $$

$$ R = g^{\mu\nu} \text{Ric}_{\mu\nu} $$

(3.13)

where $\Gamma$s are the Christoffel symbols. The scalar curvature may be worked out with Eqs.(3.11),(3.12),(3.13):

$$ R = \frac{\lambda^3}{2(5e f + 5e f b - 3c f - 3d^2 e)^2} \left[ 55 f^2 e a^2 + 55 f^2 b e^2 ight. $$

$$ - 28 f^2 e c^2 - 25 f^2 a c h - 25 f^2 b c h - 28 f d^2 e^2 + 12 f d^2 e c $$

$$ - 25 e^2 d k e - 25 e^2 b d k + 12 c^2 d k e + 15 c d h k a + 15 c d b h k \right] $$

(3.14)

As it is seen from Eq.(3.14), $R$ is a symmetric function of $z$; this means that scalar curvature is independent of the orientation of external magnetic field, $R(-H) = R(H)$.

In the classical limit in the absence of the external magnetic field, we have $\eta^\pm \rightarrow \eta \rightarrow 0$ and $f^\pm_\eta(\eta) \rightarrow \eta$; so $R$ is obtained as follows:

$$ R = \frac{1}{2} \frac{\lambda^3}{\rho} $$

(3.15)

On the other hand in this limit, Eq.(3.5) results

$$ \rho = \frac{2 \lambda^3}{\eta^3} $$

(3.16)

From Eqs.(3.15) and (3.16) the classical limit of $R$ is given by

$$ R = \frac{1}{2\rho} $$

(3.17)

This surprising simple result, shows that in the classical limit the scalar curvature is in the order of the volume occupied by a single particle. It is in complete agreement with the scalar curvature obtained by Ruppeiner for multicomponent ideal gas[11]. It means that in the classical limit the scalar curvature of the Pauli paramagnetic gas behaves like that of a two-component ideal gas.

In Fig.1 we present the dependence of $R$ on $\eta$ for a fixed value of $H$, for an isotherm in units of $\lambda^3$. In the classical region where $\eta < 1$, $R$ diverges near $\eta = 0$. It relates to the fact that in this limit $\rho$ goes to zero (as Eq.(3.17) demonstrates), so there are not enough particles for a continuous thermodynamic description. In the quantum mechanical region, where $\eta \gg 1$, $R$ tends to a constant value.

Fig.2 shows the dependence of $R$ on $H$ for a fixed value of $\eta$, for an isotherm in units of $\lambda^3$. $R$ is a monotonically decreasing function of $H$. Physically, as the external magnetic field increases, the magnetization fluctuation decreases. So the system becomes more stable. Here we can interpret $R$ as a measure of the stability of the thermodynamic system. The less the magnitude of $R$, the more stable the system becomes.
In Fig. 3 there is something new that we can not explain it in terms of fluctuations. This figure shows the dependence of $R$ on $H$ for $\eta = 10$. As it is seen in this quantum regime, $R$ has maximum around $z = 2$. Fig. 4 shows that this maximum of $R$ occurs at higher values of $z$ as we increase the value of $\eta$. This behavior is in contrast with our intuition; because the magnetization fluctuation, $\langle (\Delta m)^2 \rangle / \langle m \rangle^2$ is a monotonically decreasing function of $H$ for all values of $\eta$. So it seems that the stability interpretation of thermodynamic curvature fails in strong quantum regime.

For the last point we allude to a relationship between $R$ and the correlation volume. We note that the correlation function of Fermi gas in classical regime ($\rho \lambda^3 \ll 1$ or $\eta \ll 1$) is given by the formula

$$\nu(r) = -\frac{1}{2} e^{-2\sigma^2 / \lambda^2}. \quad (3.18)$$

So one can see that the correlation volume in this regime is

$$V_{cor} = \frac{\lambda^3}{(2\pi)^{3/2}}. \quad (3.19)$$

It means that in the classical regime $R\eta$ is proportional to the correlation volume. The possible relationship between the curvature and the correlation volume in the quantum regime has not been explored.
4 Classical ideal paramagnetic gas

In this section we calculate the scalar curvature of a classical paramagnetic gas and compare it to the scalar curvature of the Pauli paramagnetic gas in the limit of low fugacity and low magnetic fields.

Consider a gas of identical, mutually noninteracting and freely orientable dipoles, each having a magnetic moment $J$. In the presence of an external magnetic field $H$, the dipoles experience a torque tending to align them in the direction of the field. The energy of a particle is given by

$$E = \frac{p^2}{2m_0} - JH \cos \theta \quad (4.1)$$

Here we have neglected the effect of the induced magnetic field. Mijatovic et al used the energy form of the metric to evaluate the geometry in the paramagnetic ideal gas[10]. They also used the particle number as the fixed scale. Here we use the energy form of the metric. we also use the volume as fixed scale. The logarithm of the grand canonical partition function (using Maxwell-Boltzman statistics) is obtained as follows:

$$\ln Q_c = \frac{PV}{K_B T} = 4\pi \eta \frac{V \sinh(Jz)}{Jz} \quad (4.2)$$

and the thermodynamic potential is again obtained from Eqs.(4.2) and (3.2)

$$\phi_c = 4\pi Ix^{-\frac{3}{2}}e^{-y} \frac{\sinh(Jz)}{Jz} \quad (4.3)$$

Where $x, y$ and $z$ are those that are defined in section 3 and $K_B = 1$. From Eq.(3.10) the metric elements are obtained

$$g_{11} = 15\pi Ix^{-\frac{3}{2}}e^{-y} \frac{\sinh(Jz)}{Jz}$$
$$g_{12} = 6\pi Ix^{-\frac{3}{2}}e^{-y} \frac{\sinh(Jz)}{Jz}$$
$$g_{13} = -6\pi Ix^{-\frac{3}{2}}e^{-y} \left( -\frac{\cosh(Jz)}{z} - \frac{\sinh(Jz)}{Jz^2} \right)$$
$$g_{22} = 4\pi Ix^{-\frac{3}{2}}e^{-y} \frac{\sinh(Jz)}{Jz}$$
$$g_{23} = -4\pi Ix^{-\frac{3}{2}}e^{-y} \left( -\frac{\cosh(Jz)}{z} - \frac{\sinh(Jz)}{Jz^2} \right)$$
$$g_{33} = 4\pi Ix^{-\frac{3}{2}}e^{-y} \left( \frac{J}{z^2} - 2\frac{\cosh(Jz)}{z^2} \right)$$

Using Eqs.(3.13) and (4.4), one can calculate the scalar curvature

$$R_c = \frac{1}{8\pi} \frac{\lambda^3}{\eta} \frac{Jz}{\sinh Jz} \quad (4.5)$$

Eqs. (4.3) and (4.5) show clearly that $R_c$ and $\phi_c$ satisfy the following equation.

$$R_c = \kappa \frac{K_B}{\phi_c} \quad (4.6)$$
where $\kappa = \frac{1}{2}$ and $K_B = 1$. This interesting result is nothing except the geometrical equation with $\kappa = \frac{1}{2}[7]$.

On the other hand, the equation of state of the classical ideal gas ($PV = NK_BT$) and Eqs.(4.6) and (3.2) results

$$R_c = \frac{1}{2\rho} \tag{4.7}$$

Eq.(4.7) shows that the curvature of the classical ideal paramagnetic gas is in order of the volume occupied by a single particle.

We can see the magnetic field dependence of $R_c$ through Eq.(4.5). It is a monotonically decreasing function of $z$ and has a maximum at $z = 0$. Here we can interpret the curvature as a measure of stability, since the magnetization fluctuation, $\frac{<(\Delta m)^2>}{<m^2>}$, is dominant near $z = 0$, and decreases monotonically as $z$ increases.

Now let us look at the Eq.(3.14) for the curvature of the Pauli gas in the limit of low fugacity and low magnetic field, where $f_n^\pm \to \eta^\pm$ then one can obtain

$$R_c = \frac{1}{4} \frac{\lambda^3}{\eta \cosh Jz}. \tag{4.8}$$

Eq.(4.8) is similar to Eq.(4.5), because the behavior of $\cosh z$ is similar to that of $\sinh z$; but they are somewhat different. The source of this difference is related to the fact that in the case of the classical ideal paramagnetic gas, each dipole is freely orientable whereas each particle in the Pauli paramagnetic gas can choose only two directions (even in the limit of low fugacity).

In fact, had we constrained the dipoles to choose only two directions (parallel or anti parallel to $H$) i.e. set $\cos \theta = \pm 1$ in Eq.(4.1) and used the classical grand partition function we would have obtained

$$\ln Q_c' = 2\eta \frac{V}{\lambda^3} \cosh Jz. \tag{4.9}$$

This is just Eq.(3.4) in the limit of low fugacity and low magnetic fields (where $f_n^\pm \to \eta^\pm = \eta e^{\pm Jz}$). The thermodynamic potential is

$$\phi'_c = 2Ix\frac{3}{2} e^{-y} \cosh Jz. \tag{4.10}$$

Again this is the classical limit of Eq.(3.9). Using Eqs.(3.10) and (3.13) one can obtain the scalar curvature which is just Eq.(4.8)

5 Conclusion

We have evaluated the thermodynamic curvature for the Pauli paramagnetic gas that is a system consisting of identical spin $\frac{1}{2}$ fermions.

In the classical limit (i.e. $\eta \ll 1$) in the absence of the external magnetic field this curvature reduces to that of a two-component ideal gas. In this regime we can find a simple relationship between the curvature and the correlation volume.
In the limit of low fugacity and for a finite value of external magnetic field the curvature of the Pauli gas coincides with that of the classical ideal paramagnetic gas which is a monotonically decreasing function of magnetic field; here we can interpret the curvature as a measure of stability. The system becomes more stable if the absolute value of the curvature decreases.

In the quantum mechanical regime (where $\eta \gg 1$) the curvature as a function of magnetic field has a maximum. This maximum occurs at stronger magnetic fields as the magnitude of fugacity is increased. Stability interpretation of curvature can not explain this maximum.

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