From Ginzburg-Landau to Hilbert-Einstein via Yamabe

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Abstract

In this paper, based on some mathematical results obtained by Yamabe, Osgood, Phillips and Sarnak, we demonstrate that in dimensions three and higher the famous Ginzburg-Landau equations used in theory of phase transitions can be obtained (without any approximations) by minimization of the Riemannian-type Hilbert-Einstein action functional for pure gravity in the presence of cosmological term. We use this observation in order to bring to completion the work by Lifshitz (done in 1941) on group-theoretical refinements of the Landau theory of phase transitions. In addition, this observation allows us to develop a systematic extension to higher dimensions of known string-theoretic path integral methods developed for calculation of observables in two dimensional conformal field theories.

1 Introduction

1.1 Landau theory versus other theoretical methods for predicting crystal structure

An article \cite{1} in Nature written in 1988 referred to the inability, at that time, to predict the crystal structure of simple crystalline solids from their chemical composition as "a continuing scandal" in solid state physics. Recently, Oganov and Glass developed a method for prediction of the most stable structures along with some low energy metastable states for a given compound without hints supplied by experimental data for this compound \cite{2}. Their method combines \textit{ab initio} electronic structure calculations with an evolutionary algorithm. Only

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the chemical composition is needed as an input. The method allows prediction of crystal structures at any P-T conditions.

In view of these remarkable achievements, it is of interest to study to what extent much earlier phenomenological results by Landau [3] can help in solving the same problem of structure prediction. Landau’s results were subsequently improved by Lifshitz in 1941 [4] and used later by Ginzburg and Landau in 1950 [5] in connection with their study of superconductivity, as is well known. The Landau theory can be used only in a rather narrow domain of temperatures near criticality. Being thermodynamical in nature, it contains parameters whose actual numerical value is to a large degree arbitrary. In principle, they can be deduced from experimental data. The original motivation for such a theory came from experimental study of order-disorder phase transitions in alloys. The first paragraph of Chapter 14 of Vol. 5 of the famous Landau-Lifshitz course in theoretical physics [6] begins with description of the concept of order (to be defined below) in a typical CuZn alloy. For pure Cu, the lattice is face centered cubic (fcc), while for Zn, it is hexagonal closed packed (hcp) [7]. For an alloy composed of these two metals, the system must “decide” what kind of lattice to have. The decision is made based on thermodynamical considerations. Specifically, it is believed that if the system has reached an equilibrium at a given temperature and pressure, its free energy should be minimal. Since a system as simple as CuZn exhibits a very complicated phase diagram, depicted in Fig.1, such considerations are not too informative.

Empirically, it is known that about 3/4 of all elements in nature are metals. When mixed, about 3/4 of these crystallize into one of the three most frequently encountered lattices with almost equal probability [8]. These are: fcc, Fig.2a), bcc, Fig.3a), and hcp, Fig.2b). In addition, Fig.1 exhibits more complex lattices, e.g. \( \gamma \) and \( \delta \), whose group-theoretic description is given in Table 1.

| Phase | Composition(at % Zn) | Symbol and # | Prototype |
|-------|----------------------|--------------|-----------|
| \( \alpha \) | 0 – 38.27 | \( Fm\bar{3}m \) | 225 | fcc |
| \( \beta \) | 36.1 – 55.8 | \( Im\bar{3}m \) | 229 | bcc |
| \( \beta' \) | 44.8 – 50 | \( Pm\bar{3}m \) | 221 | \( Z^3 \) |
| \( \gamma \) | 57.0 – 70.0 | \( I4\bar{3}m \) | 217 | bcc |
| \( \delta \) | 72.45 – 76.0 | \( P6 \) | 174 | hcp |
| \( \varepsilon \) | 78.0 – 88.0 | \( P6_3/mmc \) | 194 | hcp |
| \( \eta \) | 97.17 – 100 | \( P6_3/mmc \) | 194 | hcp |

A brief summary of crystallographic terminology is provided in Appendix.

\(^2\)A large number of such binary alloys, their phase diagrams and their symmetry descriptions are listed in Ref.[8]. As compared to the textbook by Landau and Lifshitz [6], where actually only a small portion of CuZn phase diagram is discussed (e.g. \( \beta \) and \( \beta' \) phases in Fig.1), Ref.[8] indicates that most binary alloys, including CuZn, exhibit unexpectedly complex phase diagrams similar to that given in Fig.1. Subsection 6.2 contains additional information helpful for its understanding.
Figure 1: Phase diagram for CuZn alloy
Figure 2: a) Basic fundamental domain for the fcc lattice along with its primitive cell; b) the same for the hcp lattice and its primitive cell

A. The CuZn system was used in Ref. [6] as a good example of the second order phase transition. A phase transition for which the order parameter changes continuously (with concentration) till it becomes zero at the transition point is of second order (or continuous). In reality, however, such a transition takes place in a rather narrow concentration range (roughly, between 30 and 60% of Zn in Cu), as can be seen in Fig. 1. Nevertheless, this example was used by Landau to introduce the concept of an order parameter. To this purpose, using Fig.1, we fix the temperature so that the horizontal line will cross the phase boundary within the concentration range just mentioned. Then, on the l.h.s. with respect to this crossing we obtain the $\beta$-phase depicted in Fig. 3a) where both Cu and Zn can occupy each lattice site with equal probability (disordered state). To the r.h.s. of this crossing, the occupation probabilities for Cu and Zn become different (ordered state). Following Landau [3], we introduce the nonnegative order parameter $\varphi$ measuring the degree of such ordering. Clearly, it should be proportional to the difference between the occupation probability 1/2 in the disordered state (either for Cu or Zn) and that for the ordered state which should be less than 1/2. As Fig. 1 and Table 1 indicate, the symmetry of the low temperature $\beta'$-phase is that of two interpenetrating cubic lattices (as depicted in Fig. 3b)), while the symmetry of the high temperature $\beta$-phase is that of the bcc lattice and is higher. This fact is in accord with the general observation [6] that the higher symmetry phase usually occurs at higher temperatures. Having said this, one has to take into account that the order parameter $\varphi$ was defined without reference to temperature so that the order-disorder transition
Figure 3: The simplest example of superlattice formation: a bcc $\beta$–type lattice a) is converted into $\beta'$–type lattice made of two interpenetrating $\mathbb{Z}^3$–type lattices. To facilitate understanding, a two dimensional square lattice $\mathbb{Z}^2$ depicted in a') is splitting into two square sublattices in b')

thus described is only concentration-dependent. This means that infinitesimal changes in concentration can cause changes in symmetry.

To include both the temperature and concentration dependence, the notion of an order parameter should be generalized. This can be accomplished if, instead of fixing the temperature, we fix the concentration in the concentration range specified above. Then, a vertical line in Fig.1 also will cross the phase boundary so that the higher symmetry phase $\beta$ indeed occurs at higher temperatures. In view of this, to describe a phase diagram locally in the sense just described, Landau [3] proposed the following phenomenological expansion for the free energy functional $F\{\varphi\}$ valid in the vicinity of the transition temperature $T_c$:

$$F\{\varphi\} = F_0 + a\varphi + A\varphi^2 + C\varphi^3 + B\varphi^4 + \ldots . \quad (1.1)$$

It is expected, that for $T > T_c$ we are left only with $F\{\varphi\} = F_0$, while for $T < T_c$ we have to assume that coefficients $a$, $A$, etc. depend upon $T$, $P$ and concentration $c$. Such an expansion is non analytic, however, since the derivatives of the free energy with respect to $P$ and $T$ are discontinuous at $T = T_c$.

This fact allows us to define the order of transition using standard rules of thermodynamics. The system is undergoing a first order transition if the first order derivatives of $F\{\varphi\}$ with respect to $T$ and/or $P$ are discontinuous at $T_c$, while it undergoes a second order transition if the second derivatives of $F\{\varphi\}$ with respect to $P$ and/or $T$ are discontinuous at $T_c$. 

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To actually use the Landau theory under such circumstances, $F\{\varphi\}$ is minimized with respect to $\varphi$. Next, the first derivatives of $F\{\varphi\}$ are calculated with respect to $P$ and/or $T$. This minimum value of the order parameter $\varphi$ is substituted back into the derivatives in order to check their continuity at $T = T_c$. This requires making some additional assumptions on coefficients in the Landau expansion. For instance, for the second order transition, one should require $a = 0$ in Eq.(1.1) while $A = A(P,T)$ is expected to change sign at $T = T_c$ so that, by symmetry, it should become exactly zero at $T_c$. This implies that for temperatures $T$ close to $T_c$ the coefficient $A$ is expected to behave as $A(P,T) = \alpha(P)(T - T_c)/T_c \equiv \alpha \tau$. As for the coefficient $C$, it is also expected that it can be a function of $P$ and $T$. Its presence is not mandatory, however. It depends upon the symmetry of the system. The details were worked out by Lifshitz in 1941 [4].

\subsection*{1.2 Refinements by E.M. Lifshitz}

Although the textbook by Landau and Lifshitz [6] contains only one paragraph describing Lifshitz refinements, there are monographs, e.g. Refs. [9-11] and the references therein, elaborating on works by Lifshitz. Such elaborations are quite sophisticated, so we refer our readers to these monographs for details. Here we would like only to emphasize the key points essential for our work. Lifshitz improvements of Landau's theory were designed to explain phase transitions in superlattices. The $\beta'$ phase of CuZn mixture is an example of a superlattice. By definition, the superlattice, (or superstructure), is a lattice made of atoms of different kinds occupying existing lattice sites in an orderly fashion. When this happens, the lattice is subdivided into different sublattices, as depicted in Fig 2, so that different sublattices are occupied by different atoms in the alloy. To date, an enormous number of superlattices is known empirically [7,8]. In principle, Lifshitz theory allows these predictions provided that the symmetry of the high temperature phase is assigned. Then, the symmetry of the low temperature phase (superlattice) can be predicted. Many practical examples of such calculations can be found in Ref.[9-11]. It should be kept in mind, however, that such a theory can explain diagrams like that in Fig.1. only qualitatively. In its present form, it cannot make predictions about the exact location of the phase boundaries, which is also true of the method developed by Oganov. For this one needs a more detailed microscopic theory. Attempts to develop such theory were made (to our knowledge) only for specific systems, e.g. see Ref.[10,12]. It is hoped that the results of this paper and that by Oganov et al might stimulate further research in this area.

The probabilistic interpretation of the order parameter $\varphi$ suggests that it should be coordinate-independent. Yet, according to Lifshitz original work [4], it is allowed to be coordinate-dependent. Specifically, Lifshitz argues that the order parameter $\varphi$ is proportional to the crystalline density $\rho$ which can be presented as $\rho = \rho_0 + \delta \rho$, provided that $\rho_0$ serves as the basis of representation
of the prescribed symmetry group \( G_0 \) of the high temperature phase, and \( \delta \rho \) can be represented as

\[
\delta \rho = \sum_{n \neq 1} \sum_i \varphi_i^{(n)} \Psi_i^{(n)}.
\]

(1.2)

The first summation takes place over all irreducible representations (except trivial) while the second summation takes place over the bases of these irreducible representations. Clearly, \( \varphi_i^{(n)} \) is the analog of the earlier introduced \( \varphi \) while \( \rho_0 \) corresponds to the basis of unit representation for \( G_0 \). By design, \( \delta \rho \) is invariant under group \( G \) of lesser symmetry expected for the low temperature phase. For brevity, following Lifshitz, we shall suppress the superscript \( n \) in what follows. To make a connection with Eq.(1.1) Lifshitz suggests writing \( \varphi_i \) as \( \varphi_i = \varphi \gamma_i \) where the functions \( \gamma_i \) are chosen in such a way that

\[
\varphi^2 = \sum_i \varphi_i^2
\]

(1.3)

implying that \( \sum \gamma_i^2 = 1 \). Under such conditions, the expansion, Eq.(1.1), acquires the following form

\[
\mathcal{F}(\varphi) = \mathcal{F}_0 + A(P,T)\varphi^2 + \varphi^3 \sum_j C_j(P,T)f_j^{(3)}(\{\gamma_i\}) + \varphi^4 \sum_j B_j(P,T)f_j^{(4)}(\{\gamma_i\}) + ...
\]

(1.4)

where \( f_j^{(3)} \), \( f_j^{(4)} \) ... are the third, forth and higher order invariants of the group \( G \) made of \( \gamma_i \) s. The sums over \( j \) count all such respective invariants. This refinement by Lifshitz explains the group-theoretic nature of the coefficients in the original Landau expansion, Eq.(1.1). Thus, some of these coefficients are excluded from the expansion based on symmetry in addition to the thermodynamic stability requirements, discussed by Landau\(^3\). The results obtained thus far are still not too restrictive to determine the group \( G \) in the low temperature phase. Mathematically rigorous arguments leading to full determination of \( G \) can be found in the monograph by Lyubarsky \([9]\) and are too long to be used for these introductory remarks. To get a feeling for these arguments we provide some less rigorous (physical) arguments in spirit of the original paper by Lifshitz.

To this purpose, we assume that the order parameter is weakly coordinate-dependent in the following sense. The representation of any of 230 space groups (Appendix A) acts in the vector space whose basis is made of functions of the form

\[
\Psi_{k\alpha}(r) = u_{k\alpha} e^{i k \cdot r}.
\]

(1.5)

For a fixed \( k \), functions \( u_{k\alpha} \) are invariant under translations in the direct lattice, \( r \to r + a \), while the combination \( k \cdot r \) in the exponent changes to \( k \cdot r + k \cdot a \), so that if \( H \) is some vector of the reciprocal lattice, then the vectors \( k \) and

\(^{3}\)It should be noted that in Landau’s work these symmetry arguments are present already but without details.
\( \mathbf{k} + \mathbf{H} \) are equivalent. This equivalence leads to the exponent \( \exp(i \alpha \cdot \mathbf{H}) \) being equal to 1. The subscript \( \alpha \) in Eq.(1.5) numbers all functions with fixed \( \mathbf{k} \). Such a set of functions forms a basis for representation for the point group. The above expression for \( \Psi_{\mathbf{k} \alpha}(\mathbf{r}) \) can be simplified for superlattices according to the following arguments by Lifshitz. He noticed that lattices (expected to become superlattices) at higher temperature (in the disordered phase) should contain only one atom per unit cell \( \Lambda^4 \). At lower temperatures the points in such a lattice in different cells become non-equivalent thus signalling the formation of a superlattice. Because of this, the number of functions \( u_{\mathbf{k} \alpha} \) is reduced to one (i.e. \( \alpha = 1 \)). These arguments allow us to replace as well all \( u_{\mathbf{k} \alpha} \) s in Eq.(1.5) by unity. Next, applying all rotations related to the discrete subgroup (of \( \mathbf{G} \)) of point symmetries at fixed \( \mathbf{k} \) creates an orbit for such a subgroup, called a star. Since the expansion, Eq.(1.2), is made for a given star (the number of elements in a star thus forming a basis), it is only natural to require the coefficient \( A(P, T) \) to be \( \mathbf{k} \)-depenent. Suppose now that the low temperature phase corresponds to some \( \mathbf{k} = \mathbf{k}_0 \). Thermodynamically, for such a phase to be stable, one should look at \( A(P, T) \) as a function of \( \mathbf{k} \). When considered as a function of \( \mathbf{k} \), the coefficient \( A(P, T) \) should possess a minimum determining \( \mathbf{k}_0 \). Lifshitz recognized that such a condition is not constructive enough. In support of the necessity of such a condition the following chain of arguments can be used. If \( \mathbf{k}_0 \) would determine the structure, the density \( \delta \rho \) would be periodic with periodicity induced by \( \mathbf{k}_0 \). In view of Eq.s (1.2) and (1.5), such a requirement apparently looks completely satisfactory. Nevertheless, it is incomplete, since by itself, it is not sufficient for the lattice to be stable. For this to happen, one should take into account nearby structures with \( \mathbf{k} \)’s close to \( \mathbf{k}_0 \). Since the periodicity of \( \delta \rho \) is built into the expansion, Eq.(1.2), through its dependence on \( \Psi_{\mathbf{k} \alpha} \), the only option allowing structures with nearby \( \mathbf{k} \)’s to be considered lies in making \( \varphi_i \)s in Eq. (1.2) weakly coordinate-dependent. In this case the expression \( A(P, T)\varphi^2 \) should be replaced by a more general expression of the type

\[
\hat{A} = \int d\mathbf{r} \int d\mathbf{r}' \delta \rho(\mathbf{r})h(\mathbf{r}, \mathbf{r}')\delta \rho(\mathbf{r}')
\]

where the kernel is some function of \( P, T \) symmetric with respect to interchange of its spatial arguments. By construction, the \( \mathbf{k} \)-dependence of \( A(P, T) \) is built into the transformation properties of the kernel \( h(\mathbf{r}, \mathbf{r}') \). Specifically, for \( h(\mathbf{r}, \mathbf{r}') \) consider an eigenvalue problem of the type

\[
\int d\mathbf{r}' h(\mathbf{r}, \mathbf{r}')\phi(\mathbf{r}') = \lambda \phi(\mathbf{r}).
\]

The choice of the kernel \( h(\mathbf{r}, \mathbf{r}') \) is made in such a way that the function, Eq.(1.5), is identified with the eigenfunction \( \phi(\mathbf{r}) \) in Eq.(1.7). Keeping in mind that for superlattices, \( u_{\mathbf{k} \alpha} \) can be put equal to one and, taking into account the translational invariance, the above eigenvalue problem can be rewritten explicitly

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4It is known from solid state physics that the elementary cells displayed in Fig.s 2 and 3 should not be confused with the unit cells. The difference is well explained in the book by Ziman [13] for instance.
where summation over \( \mathbf{r}' \) is made over vectors of the direct lattice, while that over \( l \) is made over the \( \mathbf{k} \) vectors forming a star. From here we obtain,

\[
\delta_{mj} \lambda_j = \sum_{R} h_{jm}(R)e^{-i\mathbf{k}_m \cdot \mathbf{R}},
\]

(1.9)

where \( \mathbf{R} = \mathbf{r} - \mathbf{r}' \). For \( \mathbf{k} = \mathbf{k}_0 \), this lattice is expected to be stable. To check that this is the case, we use expansion, Eq.(1.2), for \( \delta \rho \) in Eq.(1.6). To actually do so, we need to be more specific about the expansion given by Eq.(1.2). To this purpose we write

\[
\delta \rho (\mathbf{r}) = \sum_i \phi_i (\mathbf{r}) e^{i\mathbf{k}_i \cdot \mathbf{r}} \tag{1.10}
\]

where \( \mathbf{k} = \mathbf{k}_0 + \kappa \) with \( \kappa \) being an infinitesimally small vector. Our order parameter function \( \phi_i (\mathbf{r}) \) can also be Fourier expanded in such a way that

\[
\phi_i (\mathbf{r}) = \sum_{\kappa} c_{k,\mathbf{0}} (\kappa) e^{i\kappa \cdot \mathbf{r}}. \tag{1.11}
\]

Using expansions Eq.s (1.10) and (1.11) in Eq.(1.6) produces

\[
\hat{A} = \sum_i \sum_{\kappa} \sum_j \sum_{\kappa'} c_{k,\mathbf{0}} (\kappa) c_{k',\mathbf{0}} (\kappa') \int d\mathbf{r} \int d\mathbf{r}' e^{i(\mathbf{k}_i + \kappa) \cdot \mathbf{r}} h(\mathbf{r} - \mathbf{r}') e^{i(\mathbf{k}_j + \kappa') \cdot \mathbf{r}'}.
\]

(1.12)

To simplify this expression we note that if \( \kappa' \)s in the double integral would be zero, the integral would reduce to the result given by Eq.(1.9). Since the free energy at equilibrium is minimal, by selecting the smallest eigenvalue \( \lambda(\mathbf{k}_0) \) from the set \( \{\lambda_j\} \) we obtain the following result for \( \hat{A} \),

\[
\hat{A} = \lambda(\mathbf{k}_0) \sum_i \sum_{\kappa} c_{k,\mathbf{0}} (\kappa) c_{k,\mathbf{0}}^* (\kappa), \tag{1.13}
\]

where \( c_{k,\mathbf{0}}^* = c_{-k,\mathbf{0}} \). In arriving at this result we kept only the diagonal (in \( \kappa \)) term and assumed (as Lifshitz did) that \( c_{k,\mathbf{0}} (\kappa) \)'s are very weakly dependent on \( \kappa \). Expanding the exponents in the double integral in Eq.(1.12) in powers of \( \kappa \), keeping only terms of the first order in \( \kappa \), and taking into account the perturbative nature of such a calculation leads to the following result:

\[
\int d\mathbf{r} \int d\mathbf{r}' e^{-i(\mathbf{k}_i + \kappa) \cdot \mathbf{r}} h(\mathbf{r} - \mathbf{r}') e^{i(\mathbf{k}_i + \kappa) \cdot \mathbf{r}'}
\]

\[
= \lambda_i + i\kappa \cdot \int d\mathbf{r} \int d\mathbf{r}' (\mathbf{r}' - \mathbf{r}) e^{-i\mathbf{k}_i \cdot \mathbf{r}'} h(\mathbf{r}' - \mathbf{r}) e^{i\mathbf{k}_i \cdot \mathbf{r}'} + O(\kappa^2)
\]

\[
= \lambda_i + i\kappa \cdot \int d\mathbf{r} \int d\mathbf{r}' h(\mathbf{r}' - \mathbf{r}) \{ e^{-i\mathbf{k}_i \cdot \mathbf{r}'} e^{i\mathbf{k}_i \cdot \mathbf{r}'} - e^{-i\mathbf{k}_i \cdot \mathbf{r}'} e^{i\mathbf{k}_i \cdot \mathbf{r}'} \}
\]

\[
+ O(\kappa^2). \tag{1.14}
\]
While the terms of order $O(\kappa^2)$ will be considered in the next subsection, here we would like to combine Eqs. (1.12), (1.14) in order to present our results in a physically suggestive form. Taking into account Eq.(1.9) we obtain:

\begin{equation}
\hat{A} = \sum_i \sum_\kappa \{ \lambda(k_0) + i(\kappa \cdot \partial_{\kappa} \lambda(k)) \big|_{k=k_0} + O(\kappa^2) \} c_{k_0\kappa}^* c_{k_0\kappa} \tag{1.15}
\end{equation}

where, clearly,

\begin{equation}
\frac{\partial}{\partial \kappa} \lambda(k) \big|_{k=k_0} = \sum_r \sum_{r'} r' h(r' - r) \{ e^{-i k_r^r} e^{i k_r^r} - e^{-i k_r^r} e^{i k_r^r} \} \tag{1.16}
\end{equation}

with integrals being replaced by lattice sums. Thus, in accord with Lifshitz [4,6], who only suggests (without derivation) that the requirement $\frac{\partial}{\partial \kappa} \lambda(k) \big|_{k=k_0} = 0$ is equivalent to the requirement of vanishing of invariants of the type $\{ e^{-i k_r^r} e^{i k_r^r} - e^{-i k_r^r} e^{i k_r^r} \}$, we have just demonstrated that this is indeed the case. This equivalence is absolutely essential for determination of the symmetry of the low temperature phase. Its existence also implies the vanishing of the coefficient $C$ in the Landau expansion, Eq.(1.1), [10]. These two conditions are the necessary and sufficient conditions for the second order (continuous) phase transition to take place. Violation of these conditions causes the order of phase transition change from second to first. The details can be found in previously cited literature. From the preceding discussion, it should be clear that both options depend crucially on the assigned symmetry of the disordered phase which should be artificially introduced into the theory.

1.3 Refinements by Ginzburg, Landau and Wilson. LGW free energy functional

Ginzburg and Landau [5] applied the Landau theory for study of superconductivity in restricted geometries. Subsequently (albeit in a different context) the Ginzburg-Landau (G-L) functional was reobtained by Kenneth Wilson, who not only recovered the G-L functional, but explained what approximations should be made in order to recover this functional from the microscopic (Ising) model. In view of his refinements, the G-L functional is frequently referred to as the Landau-Ginzburg-Wilson (LGW) functional [14]. It is written as

\begin{equation}
\mathcal{F} = \mathcal{F}_0 + \frac{1}{2} \int d\mathbf{x} \{ c(\nabla \varphi(\mathbf{x}))^2 + a \varphi^2(\mathbf{x}) + \frac{b}{2} \varphi^4(\mathbf{x}) - 2h(\mathbf{x})\varphi(\mathbf{x}) \}, \tag{1.17}
\end{equation}

where in the case of the Ising model the last term indirectly describes the coupling of the Ising spins to the external magnetic field. In the absence of such
a field the above functional describes the second order phase transition as discussed earlier. Usually, it is rather difficult to bring the coefficients of the Landau expansion in exact correspondence with parameters of respective lattice models [15,16]. This is especially true for the constant \( b \). It is expected, however, that under any circumstance, \( b \) is only very weakly temperature and pressure dependent, and normally it is greater than zero. The case when both \( a \) and \( b \) are zero is a special case. It determines the so called tricritical point in the \( P,T \) parameter space. Physically, there can be only one tricritical point \( (P_t, T_t) \) determined by the equations

\[
\begin{align*}
a(P_t, T_t) &= 0; \\
b(P_t, T_t) &= 0.
\end{align*}
\] (1.18)

Below the tricritical temperature \( T_t \) the parameter \( b \) becomes negative and the phase transition is of first order. In this case, it is necessary to introduce an extra term \( g\varphi \) into the LGW functional, Eq.(1.17), with \( g > 0 \). It is normally expected that the parameter \( g \) is practically constant below \( T_c \) [17].

Eq.(1.17) contains the magnetic field \( h \) whose role we would like to discuss now. To this purpose, let us consider the extremum of the LGW functional near \( T_c \). We obtain,

\[
\frac{\delta F}{\delta \varphi(x)} = -c \nabla^2 \varphi + a\varphi + b\varphi^3 - h = 0.
\] (1.19)

Consider a special case of a constant (coordinate-independent) field \( \varphi, \varphi(x) = \varphi_0 \). In this case, Eq.(1.19) is reduced to

\[
a\varphi_0 + b\varphi_0^3 = h.
\] (1.20)

For \( a > 0 \) and a weak magnetic field \( h \), we obtain \( \varphi_0 = h/a \). For \( a < 0 \) we obtain solutions even for \( h = 0 \). These are \( \varphi_0 = \pm\sqrt{|a|/b} \) and \( \varphi_0 = 0 \). The solution \( \varphi_0 = 0 \) is not a minimum of the free energy and, hence, should be discarded. Of the two other solutions, the system chooses one of them (which is interpreted in the literature as spontaneous symmetry breaking). They both have the same free energy. Let now \( \varphi(x) = \varphi_0 + \delta\varphi \equiv \varphi_0 + \eta(x) \), so that we can Taylor series expand \( F \{ \varphi \} \), thus obtaining

\[
F(\varphi) = F(\varphi_0) + \frac{1}{2} \int dV \int dV' \left[ \frac{\delta^2}{\delta \varphi(x) \delta \varphi(x')} F(\varphi) \bigg|_{\varphi=\varphi_0, h=0} \right] \eta(x)\eta(x') + ...,
\] (1.21)

where

\[
\frac{\delta^2}{\delta \varphi(x) \delta \varphi(x')} F(\varphi) \bigg|_{\varphi=\varphi_0, h=0} = (-c \nabla^2 + a + 3b\varphi_0^2) \delta(x - x').
\] (1.22)

\[5\] In this work we shall call the functional \( F \{ \varphi \} - F_0 \) (with \( h = 0 \)) as Ginzburg-Landau (or G-L) and we shall call it LGW if it is used in the exponent of the path integral, Eq.(1.27) below. Such distinction is needed for mathematical reasons: for the G-L functional the order parameter \( \varphi \) is strictly nonnegative as we had explained already in the main text. This allows us to relate the G-L and Yamabe functionals (Section 3) to each other.

\[6\] Once the choice is made, the order parameter can be considered in all subsequent calculations as positive.
Clearly, we are interested only in the phase with lowest free energy. In this case $a < 0$ and, therefore, we obtain, $-|a| + 3b\varphi_0^2 = 2|a|$. This result implies that, indeed, the selected minimum is stable since the spectrum of the operator given above contains only nonnegative eigenvalues. This fact was used by Levanyuk and then by Ginzburg in order to determine the limits of validity of the Landau theory. Details of their arguments can be found, for example, in Refs.[14,18]. Following these references, the Ginzburg number $G_i$ is defined in 3 dimensions as

$$G_i = b^2T_c^2/\alpha(P)c^3,$$

(1.23)

where $\alpha(P)$ was defined earlier, after Eq.(1.1). In order to explain its physical meaning, we need to introduce two characteristic lengths. This is accomplished by the use of Eqs.(1.21) and (1.22). Let $m^2 = a + 3b\varphi_0^2$, and consider the correlators defined by

$$\langle \eta(x)\eta(x') \rangle = \frac{\int D[\eta(x)]\eta(x)\eta(x') \exp(-\beta S[\eta(x)])}{\int D[\eta(x)] \exp(-\beta S[\eta(x)])},$$

(1.24)

where $S[\eta(x)] = \frac{1}{2} \int d^d r \left\{ c(\nabla \eta(x))^2 + m^2\eta^2(x) \right\}$ and $\beta = 1/T$, with $T$ being temperature (in the system of units in which Boltzmann’s constant $k_B = 1$). Calculation of such averages for temperatures $T$ close to $T_c$ is described in any textbook on path integrals [18,19] and is readily accomplished in any dimension $d$ due to the Gaussian nature of the respective path integrals in the numerator and denominator. In particular, for $d = 3$, the result is given by

$$\langle \eta(x)\eta(x') \rangle \simeq T_c e^{-r/\xi} \quad r = |x - x'|, \quad r/\xi \gg 1.$$

(1.25)

The above expression defines the correlation length $\xi$ via $\xi = (c/m^2)^{1/2}$. Consider the volume average of such a correlator

$$\frac{1}{V^2} \int d^3x \int d^3x' \langle \eta(x)\eta(x') \rangle > \sim \frac{\xi^2}{c^2 r_0^3} \quad (1.26)$$

where the characteristic length $r_0$ is given by $r_0^3 \sim V$ and can be estimated by equating this average with the previously obtained Landau result, $\varphi_0^2 = |a|/b \sim m^2/b$. This produces the following estimate for $r_0$: $r_0^3 \sim m^4/T_c b$. Consider now the ratio $(r_0/\xi)^6 \sim \tau^{-1}G_i$, with $\tau$ defined after Eq.(1.1). Clearly, the original Landau theory makes sense only if $m^2/b > \xi^2/c r_0^3$, that is, when fluctuations are negligible. This happens when $|\tau| >> G_i$, i.e. for the range of temperatures: $|T - T_c| >> T_c G_i$. When approaching $T_c$, this inequality is inevitably violated. In this case, fluctuation corrections should be taken into account as explained by Wilson, Fisher, Kadanoff and many others [14,18]. Theoretically, however, one can look at these results in different space dimensions. This allows one to introduce the upper $d_u$ and the lower $d_l$ critical dimensions. For $d > d_u$, the Landau-Lifshitz theory can be used with confidence since fluctuations become unimportant. For $d < d_l$ fluctuations are so significant at any nonzero temperatures that phase transitions do not occur. Exactly at $d_u$ fluctuations are
still important. Technically speaking, \( d_u \) is the dimensionality at which LGW model is renormalizable. This means that the functional integral of the type

\[
I = \int D[\varphi(x)] \exp\{-\beta \hat{S}[\varphi(x)]\}
\]

with \( \hat{S}[\varphi(x)] = \mathcal{F}\{\varphi\} - \mathcal{F}\{\varphi_0\} \) can be consistently calculated perturbatively by expanding the exponent in the above path integral in powers of the coupling constant \( b \), which is dimensionless exactly at \( d_u \)."Consistently" here means in such a way that the singularities occurring in perturbative calculations can be consistently removed, thus making the LGW model renormalizable. Details can be found in the literature \[15,19\]. The sophisticated machinery of the renormalization group method, a by-product of such a renormalization procedure, allows one to calculate the critical exponents associated with various thermodynamic observables.

1.4 Description of the problems to be solved and organization of the rest of the paper

The results just described allow us to formulate the following problems to be considered in the rest of our paper.

1. As the Fig. 1 and the Table 1 indicate, symmetry of the high temperature (disordered) phase for CuZn alloy is fcc as depicted in Fig.2a. The existing G-L theory needs this information to be supplied in advance as an input in order to determine the cascade of symmetry-breaking changes taking place either by lowering temperature at fixed concentration or by changing concentration at fixed temperature. Can such information be obtained by the proper re-interpretation of the G-L theory?

2. There is well a developed string-inspired formalism of conformal field theories in two dimensions. It takes into account full conformal invariance at criticality \[20\]. Can the G-L theory be modified in order to be in accord with the existing two dimensional formalism? That is to say, in higher dimensions the LGW functional is normally used in the exponent of the path integral, e.g. see Eq.(1.27). Can LGW theory be modified (to account for full conformal invariance) to be used in the exponent of such a string-inspired path integral? To what extent does such a modification allow us to develop the exact higher dimensional analogs of two dimensional manifestly full conformal invariant theories? By doing so, under what conditions can we recover known higher dimensional perturbative results for the LGW model?

In this work we provide affirmative answers to these problems. Based on this, we are able to consider the whole spectrum of physically interesting problems whose mathematical description is based entirely on solutions to problems just formulated. Specifically,

\[d_u = 4\] for the tricritical GLW functional, \( d_u = 3\] [17].

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a) In Section 2 we perform scaling analysis of the G-L model. We argue that in dimensions 3 and higher such scaling analysis is insufficient to insure the full conformal invariance of the G-L functional even at criticality (i.e. for $T = T_c$). Nevertheless, we argue that such analysis, when properly (re)interpreted, is helpful in finding the correct form of a conformally invariant G-L functional. It is found in Section 3, where it is shown to coincide with the Yamabe functional known in mathematics literature for some time\cite{21-25}.

b) In section 4 we argue that with respect to conformal variations, this functional is equivalent to the Hilbert-Einstein (H-E) functional for pure gravity in the presence of the cosmological term. The physical meaning of this cosmological term in the context of the G-L theory is explained in Sections 3 and 4. Its presence is of importance for both statistical and high energy physics.

c) To avoid confusion, only statistical physics applications are treated in this paper. In particular, to obtain better insight into the nature of the Yamabe functional (which can be used only in dimensions 3 and higher), in Section 5 we describe in some detail its two dimensional analog. This Yamabe-like functional was considered in detail in the work by Osgood, Phillips and Sarnak (OPS), Ref.[26]. Section 5 is not merely a review of the OPS work. In it, we accomplish several tasks. First, we connect the OPS results with those independently obtained in physics literature \cite{27,28}, where the OPS-type functional can be found in the exponents of string-theoretic path integrals. Such path integrals are used for calculation of observables (e.g. averages of the vertex operators) in CFT. They establish the most efficient direct link between the string and the CFT formalisms. Next, we argue that the OPS functional is the exact two dimensional analog of the Yamabe functional. The Yamabe should be used (instead of the OPS) in higher dimensions. This observation allows us to extend (later, in Section 6) the available two dimensional string-theoretic results to higher dimensions.

d) In particular, as a precursor to these 3 dimensional calculations, we reinterpret thermodynamically the inequalities obtained in OPS paper. Such a reinterpretation is essential in determining the symmetry of the high temperature phase thus allowing us to complete the work by Lifshitz. The results by Chowla and Selberg \cite{29} were used in order to recalculate exactly the values of functional determinants for 2 dimensional lattices of different symmetry. The logarithms of these determinants are associated with the respective free energies. The obtained exact spectrum of free energies in two dimensions provides us with useful reference for analogous 3 dimensional calculations done in the next section.

e) Even though the analytical expression for such a 3 dimensional spectrum can also be obtained formally in closed form, as we demonstrate, in practice, some numerical calculations were required in Section 6. The results of these calculations are in complete qualitative accord with the exact two dimensional results obtained earlier. Some details of our calculations are presented in appendices A through D.
2 Scaling analysis and conformal invariance of the Ginzburg-Landau functional

The conventional scaling analysis of the G-L functional routinely used in physics literature can be found, for example, in the book by Amit [15]. This analysis differs somewhat from that for the $\phi^4$ model as described in the monograph by Itzykson and Zuber [30]. For the sake of uninterrupted reading we would like to provide a sketch of arguments for both cases now.

We begin with the $\phi^4$ model. Let $L(x)$ be the Lagrangian of this scalar field model whose action functional in $d$ dimensions $S[\phi]$ is given by $S[\phi] = \int d^d x L(x)$. Let furthermore $\lambda$ be some nonnegative parameter. Then the requirement that $S[\phi]$ is independent of $\lambda$, i.e. $\int d^d x L(x) = \int d^d x \lambda^d L(\lambda x)$, leads to the constraint

$$\int d^d x (x \cdot \frac{\partial}{\partial x} + d) L(x) = 0 \quad (2.1)$$

obtained by differentiation of $S[\phi]$ with respect to $\lambda$ with $\lambda = 1$ at the end of calculation. For $L(x)$ given by

$$L(x) = \frac{1}{2} (\nabla \phi)^2 + \frac{m^2}{2} \phi^2 + \frac{\hat{G}}{4!} \phi^4 \quad (2.2)$$

the change of $L(x)$ under the infinitesimal scale transformation is given by

$$\frac{\delta L}{\delta \varepsilon} = (x \cdot \frac{\partial}{\partial x} + d) L(x) + (d-4) \frac{\hat{G}}{4!} \phi^4 - m^2 \phi^2. \quad (2.3)$$

Comparison between Eq.s (2.1) and (2.3) implies that the action $S[\phi]$ is scale invariant if $d = 4$ and $m^2 = 0$. The result just obtained raises the immediate question: given that the massless G-L action is scale invariant for $d = 4$, will it be also conformally invariant under the same conditions? We provide the answer to this question in several steps.

First, let $M$ be some Riemannian manifold whose metric is $g$. Then, any metric $\tilde{g}$ conformal to $g$ can be written as $\tilde{g} = e^{f} g$ with $f$ being a smooth real valued function on $M$ [23]. Let $\Delta_g$ be the Laplacian associated with metric $g$ and, accordingly, let $\Delta_{\tilde{g}}$ be the Laplacian associated with metric $\tilde{g}$. Richardson [31] demonstrated that

$$\Delta_{\tilde{g}} = e^{-f} \Delta_g - \frac{1}{2} \left( \frac{d}{2} - 1 \right) f e^{-f} \Delta_g - \frac{1}{2} \left( \frac{d}{2} - 1 \right) e^{-f} (\Delta_g f) + \frac{1}{2} \left( \frac{d}{2} - 1 \right) e^{-f} \Delta_g \circ f \quad (2.4)$$

8In arriving at this result we took into account Eq.(13-40) of Ref. [30] along with condition $D = \frac{d}{2} - 1$, with $D$ defined in Eq.(13-38) of the same reference. Also, we had changed signs (as compared to the original source) in $L(x)$ to be in accord with accepted conventions for the G-L functional.

9That is $\Delta_g \Psi = -(\det g)^\frac{1}{2} \partial_i (g^{ij} (\det g)^\frac{1}{2} \partial_j \Psi)$ for some scalar function $\Psi(x)$. 

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Using basic facts from bosonic string theory, we notice at once that only for \( d = 2 \) does one obtain the conformally invariant (string-type) functional \( S[X] = \int_M d^2 x \sqrt{g} (\nabla_g X) \cdot (\nabla_g X) \) (to be discussed later in Section 5). For \( d > 2 \), in view of Eq.(2.4), the conformal invariance of the \( \phi^4 \) model is destroyed. In particular, this means that Eq.(1.19) (for \( h = 0 \)) is not conformally invariant even at criticality (\( a = 0 \))! Thus, using conventional field-theoretic perturbational methods one encounters a problem already at the zeroth order (in the coupling constant \( \hat{G} \)) level, unless \( d = 2 \). This problem formally does not occur if one requires our physical model to be only scale invariant. This is undesirable however in view of the fact that in 2 dimensions an arbitrary conformal transformation of the metric tensor \( g \) of the underlying two dimensional manifold \( M \) is permissible at criticality [20]. Abandoning the requirement of general conformal invariance in 2 dimensions in favor of scale invariance in higher dimensions would destroy all known string-theoretic methods of obtaining exact results in two dimensions. Our general understanding of critical phenomena depends crucially on our ability to solve two dimensional models exactly. All critical properties for the same type of models in higher dimensions are expected to hold even in the absence of exact solvability. Fortunately, the situation can be considerably improved by reanalyzing and properly reinterpreting the scaling results for dimensions higher than 2.

This observation leads to the next step in our arguments. Using the book by Amit [15], we consider first scaling of the non interacting (free) G-L theory whose action functional is given by

\[
S[\phi] = \int d^d x \left( (\bigtriangledown \phi)^2 + m^2 \phi^2 \right). \tag{2.5}
\]

Suppose now that, upon rescaling, the field \( \phi \) transforms according to the rule [13]:

\[
\tilde{\phi}(Lx) = L^\omega \phi(x). \tag{2.6}
\]

If we require

\[
\int d^d x \left( (\bigtriangledown \phi)^2 + m^2 \phi^2 \right) = \int d^d x L^d \left( (\bigtriangledown \tilde{\phi})^2 + \tilde{m}^2 \tilde{\phi}^2 \right) \tag{2.7}
\]

and use Eq.(2.6) we obtain,

\[
S[\phi] = \int d^d x L^d \left( (\bigtriangledown \phi)^2 L^{2\omega - 2} + \tilde{m}^2 \phi^2 L^{2\omega} \right). \tag{2.8}
\]

In order for the functional \( S[\phi] \) to be scale invariant the mass \( m^2 \) should scale as: \( \tilde{m}^2 = m^2 L^{-2} \). With this requirement the exponent \( \omega \) is found to be \( \omega = 1 - \frac{d}{2} \).

This scaling of the mass is in accord with Amit [15], page 26, Eq.(2.72). It comes directly from the rescaling of the G-L functional, Eq.(1.17), causing the

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10 Notice that this is already a special kind of conformal transformation.
coefficient of the gradient term to become one. In the standard field-theoretic \( \phi^4 \)-type model, the coefficient of the gradient term is one already by the existing convention and, hence, the free field model \((\tilde{g} = 0)\) is scale-invariant only if the mass term is zero in accord with Eq.(2.3). Hence, although the field-theoretic methods are applicable to both \( S[\phi] \) and the G-L functionals, the G-L functional is not entirely equivalent to the standard \( \phi^4 \) model functional with respect to scaling properties.

The above scaling can be done a bit differently. This is also discussed in the book by Amit. We would like to use such different scaling to our advantage. Following Amit [15], we notice that although the action \( S[\phi] \) is scale invariant, there is some freedom of choice for the dimensionality of the field \( \phi \). For instance, instead of \( S[\phi] \) we consider

\[
S[\phi] = \frac{1}{a^d} \int d^d x \left\{ (\nabla \phi)^2 + m^2 \phi^2 \right\} \tag{2.9}
\]

with \( a^d \) being some volume, say, \( a^d = \int d^d x \). Then, by repeating arguments associated with Eq.(2.8) we obtain \( \omega = 1 \) (instead of previously obtained \( \omega = 1 - \frac{d}{2} \)), e.g. see Eq.(2-66) in the book by Amit [15]. Although, from the point of view of scaling analysis both results are actually equivalent, they become quite different if we want to extend such scaling analysis by considering general conformal transformations. Although, in view of Eq.(2.4), such a task seems impossible to accomplish, fortunately, this is not true, as we demonstrate below.

The next step can be made by noticing that the mass term scales as scalar curvature \( R \) for some Riemannian manifold \( M \), i.e. the scaling \( \tilde{m}^2 = m^2 L^{-2} \) is exactly the same as the scaling of \( R \) given by

\[
\tilde{R} = L^{-2} R. \tag{2.10}
\]

This result can be found, for example, in the book by Wald, Ref. [32], Eq.(D.9), page 446. In general, the scalar curvature \( R(g) \) changes under the conformal transformation \( \tilde{g} = e^{2f} g \) according to the rule [23]

\[
\tilde{R}(\tilde{g}) = e^{-2f} \{ R(g) - 2(d-1)\Delta_g f - (d-1)(d-2) |\nabla_g f|^2 \} \tag{2.11}
\]

where \( \Delta_g f \) is the Laplacian of \( f \) and \( \nabla_g f \) is the covariant derivative defined with respect to metric \( g \). From here we see that, indeed, for constant \( f \)'s the scaling takes place in accord with Eq.(2.10). Now, however, we can do more.

Following Lee and Parker [23], we would like to simplify the above expression for \( R \). To this purpose we introduce a substitution: \( e^{2f} = \varphi^{p-2} \), where \( p = \frac{2d}{d-2} \), so that \( \tilde{g} = \varphi^{p-2} g \). With such a substitution, Eq.(2.11) acquires the following form:

\[
\tilde{R}(\tilde{g}) = \varphi^{1-p} (\alpha \Delta_g \varphi + R(g)\varphi), \tag{2.12}
\]

with \( \alpha = 4d-4 \). Clearly, such an expression makes sense only for \( d \geq 3 \) and breaks down for \( d = 2 \). But we know already the action \( S[X] \) which is both scale and conformally invariant in \( d = 2 \). It is given after Eq.(2.4) and will be discussed further in Section 5. The results of this section will allow us to obtain
similar actions, which are both scale and conformally invariant in dimensions 3 and higher. This is described in the next section.

3 Ginzburg-Landau functional and the Yamabe problem

We begin with the following observation. Let $\tilde{R}(\tilde{g})$ in Eq.(2.11) be some constant (that this is indeed the case will be demonstrate shortly below). Then Eq.(2.12) acquires the following form

$$\alpha \Delta_g \varphi + R(g) \varphi = \tilde{R}(\tilde{g}) \varphi^{p-1}. \quad (3.1)$$

By noticing that $p-1 = \frac{d+2}{d-2}$ we obtain at once: $p-1 = 3$ (for $d = 4$) and $p-1 = 5$ (for $d = 3$). These are familiar Ginzburg-Landau values for the exponents of interaction terms for critical, Eq.(1.19), and tricritical G-L theories. Once we recognize these facts, the action functional producing the G-L-type Eq.(3.1) can be readily constructed. For this purpose it is sufficient to rewrite Eq.(2.9) in a manifestly covariant form. We obtain,

$$S[\varphi] = \frac{1}{\int M d^d x \sqrt{g} \varphi^p} \int M d^d x \sqrt{g} \{\alpha(\nabla_g \varphi)^2 + R(g) \varphi^2\} = \frac{E[\varphi]}{\|\varphi\|^2_p}. \quad (3.2)$$

Minimization of this functional produces the following Euler-Lagrange equation

$$\alpha \Delta_g \tilde{\varphi} + R(g) \tilde{\varphi} - \lambda \tilde{\varphi}^{p-1} = 0 \quad (3.3)$$

with constant $\lambda$ denoting the extremum value for the ratio:

$$\lambda = \frac{E[\varphi]}{\|\varphi\|^2_p} = \inf\{S[\varphi] : \tilde{g} \text{ conformal to } g\}. \quad (3.4)$$

In accord with Landau theory [3], it is expected that the conformal factor $\varphi$ is a smooth nonnegative function on $M$ achieving its extremum value $\tilde{\varphi}$. Comparison between Eq.s(3.1) and (3.3) implies that $\lambda = \tilde{R}(\tilde{g})$ as required. These results belong to Yamabe, who obtained the Euler-Lagrange G-L-type Eq.(3.3) upon minimization of the functional $S[\varphi]$ without knowledge of Landau theory. The constant $\lambda$ is known in literature as the Yamabe invariant [23,33]. Its value is an invariant of the conformal class $(M,g)$. The Yamabe problem lies in finding a compact Riemannian manifold $(M,g)$ of dimension $n \geq 3$ whose metric is conformal to metric $\tilde{g}$ producing constant scalar curvature.

Subsequent developments, e.g. that given in Ref.[34,35] extended this problem to manifolds with boundaries and to non compact manifolds. It is

\[\text{E.g. read the discussion after Eq.(1.18) and take into account that in the tricritical case } d_u = 3.\]
not too difficult to prove that the (Yamabe-Ginzburg-Landau-like) functional is manifestly conformally invariant. To this purpose, we need to rewrite Eq. (2.12) in the following equivalent form
\[ \phi^p \tilde{R} (\tilde{g}) = (\alpha \phi \Box g \phi + R(g) \phi^2). \] (3.5)

It can be used in order to rewrite \( E[\varphi] \) as follows:
\[ E[\varphi] = \int d^d x \sqrt{\tilde{g}} \tilde{R}(\tilde{g}). \]

Next, by noting that \( \int d^d x \sqrt{\tilde{g}} = \int d^d x \sqrt{g} \phi^p \), we can rewrite the Yamabe functional in the Hilbert-Einstein form
\[ S[\varphi] = \frac{\int d^d x \sqrt{\tilde{g}} \tilde{R}(\tilde{g})}{\left( \int d^d x \sqrt{\tilde{g}} \right)^{\frac{1}{p}}} \] (3.6)

where both the numerator and the denominator are invariant with respect to changes in the metric. This becomes especially clear if we recall that \( \tilde{R}(\tilde{g}) \) is a constant.

In order to use these results in statistical mechanics, we require that the extremum of the Yamabe functional \( S[\varphi] \) is realized for manifolds \( M \) whose scalar curvature \( R(g) \) in Eq. (3.3) is also constant. In view of the relation \( \int d^d x \sqrt{\tilde{g}} = \int d^d x \sqrt{g} \phi^p \), it is clear that for the fixed background metric \( g \) Eq. (3.3) can be obtained alternatively using the following variational functional
\[ \tilde{S}[\varphi] = \int d^d x \sqrt{g} \{ \alpha (\Box g \varphi)^2 + R(g) \varphi^2 \} - \tilde{\lambda} \int d^d x \sqrt{g} \phi^p \] (3.7)

where the Lagrange multiplier \( \tilde{\lambda} \) is responsible for the volume constraint. This form of the functional \( \tilde{S}[\varphi] \) brings this higher dimensional result in accord with that appropriate for two dimensions (e.g. see below Section 5, Eq. (5.24)).

Apart from the normalizing denominator, Eq. (3.6) represents the Hilbert-Einstein action for pure gravity in \( d \) dimensions. In the denominator, the volume \( V \) taken to power \( \frac{2}{p} \), serves to make \( S[\varphi] \) conformally invariant [22], page 150.

### 4 Ginzburg-Landau from Hilbert-Einstein

In this section we analyze significance of the cosmological constant in the Hilbert-Einstein action for gravity from the point of view of the G-L model. To this purpose, following Dirac [36], consider the extended Hilbert-Einstein action functional defined for some pseudo Riemannian manifold \( M \) of total space-time dimension \( d \), without boundary:
\[ S^c(g) = \int_M R \sqrt{g} d^d x + C \int_M d^d x \sqrt{g}. \] (4.1.)

\[ \text{Actually, } \tilde{\lambda} = \lambda \frac{2}{p} = \lambda \frac{d-2}{d}. \]
The (cosmological) constant $C$ is determined by the following arguments. Let $R_{ij}$ be the Ricci curvature tensor, so that the Einstein space is defined as a solution of the following vacuum Einstein equation

$$R_{ij} = \lambda g_{ij}$$

with $\lambda$ being constant. From this definition it follows that

$$R = d\lambda.$$ (4.3)

Following Dirac [36], variation of the action $S^c(g)$ produces

$$R_{ij} - \frac{1}{2}g_{ij}R + \frac{1}{2}Cg_{ij} = 0.$$ (4.4)

Combined use of Eq.s(4.3) and (4.4) produces as well,

$$C = \lambda(d - 2).$$ (4.5)

Again, using Eq.s(4.3) and (4.5) we can rewrite Eq.(4.4) as follows

$$R_{ij} - \frac{1}{2}g_{ij}R + \frac{1}{2}d(d - 2)Rg_{ij} = 0.$$ (4.6)

These results remain unchanged if we use the Riemannian manifold $M$ instead of pseudo Riemannian. This observation allows us to use many facts from the Yamabe theory [22-24], originally developed for Riemannian manifolds.

In view of this, we argue that Eq.(4.6) can be obtained as well by varying the Yamabe functional, Eq.(3.6). Indeed, following Aubin [22] and Schoen [24], let $t$ be some small parameter labeling the family of metrics $g_{ij}(t) = g_{ij} + th_{ij}$. Then, these authors demonstrate that

$$\left(\frac{dR_t}{dt}\right)_{t=0} = \nabla^i \nabla^j h_{ij} - \nabla^j \nabla_j h^i_t - R^{ij} h_{ij}$$ (4.7)

and

$$\left(\frac{d}{dt} \sqrt{|g|}\right)_{t=0} = \frac{1}{2} \sqrt{|g|} g^{ij} h_{ij}$$ (4.8)

where, as usual, $|g| = |\det g_{ij}|$.

Consider now the Yamabe functional, Eq.(3.6), but this time, written for the family of metrics. We have

$$\mathcal{R}(g(t)) = (V(t))^{-\frac{2}{d}} \int_M R(g(t))DV(t)$$ (4.9)

where the volume is given by $V(t) = \int_M d^dx \sqrt{g(t)}$ and, accordingly, $DV(t) = d^dx \sqrt{g(t)}$. Using Eq.s(4.7) and (4.8) in Eq.(4.9) and taking into account that the combination $\nabla^i \nabla^j h_{ij} - \nabla^j \nabla_j h^i_t$ is the total divergence, produces the following
result:

\[\left(\frac{d}{dt} \mathcal{R}(g(t))\right)_{t=0} = V(0)^{-2\frac{d-1}{d}} \left[ \int_M (Rg^{ij}/2 - R^{ij})h_{ij}DV(0) \int_M DV(0) \right. \]
\[\left. - \left(1 - \frac{1}{d}\right) \int_M DV(0) \int_M h_{ij}g^{ij}DV(0) \right]. \quad (4.10)\]

If the metric \(g\) is the critical point of \(\mathcal{R}(g(t))\), then

\[\left[R_{ij} - \frac{R}{2}g_{ij}\right] \int_M DV(0) + \left(\frac{1}{2} - \frac{1}{d}\right) \left(\int_M RDV(0)\right)g_{ij} = 0. \quad (4.11)\]

From here, multiplication of both sides by \(g^{ij}\) and subsequent summation produces at once

\[R - \frac{R}{2}d + \left(\frac{1}{2} - \frac{1}{d}\right) <R> = 0, \quad (4.12)\]

where \(<R> = \frac{1}{V(0)} \int RDV(0)\) is the average scalar curvature. Eq.(4.12) can be rewritten as \(R = <R>\). But this condition is exactly equivalent to the Einstein condition, Eq.(4.2), in view of Eq.(4.3)! Hence, under such circumstances, Eq.s (4.11) and (4.12) are equivalent. For the set of metrics of fixed conformal class (i.e. related to each other by \(\tilde{g} = e^{2f}g\)) the variational problem for the G-L functional, Eq.(3.7), is exactly equivalent to the variational problem for the Hilbert-Einstein functional, Eq.(4.1), for gravity field in the vacuum in the presence of the cosmological constant. Moreover, the result \(R = <R>\) just obtained coincides with the previously obtained Eq. 92.12) (in view of Eq. (3.4)). This equivalence is of major importance for application discussed in Sections 5 and 6.

The results displayed above become trivial for \(d = 2\). Physically, however, the case \(d = 2\) is important since it is relevant to all known statistical mechanics exactly solvable models treatable by methods of conformal field theories. Hence, we would like to discuss some modifications of the above results required for treatment of two dimensional analogs of the G-L theory.

5 Ginzburg-Landau-like theory in two dimensions

5.1 General remarks

From field-theoretic treatments of the G-L model [19] we know that straightforward analysis based on asymptotic \(\varepsilon\)-expansions from the critical dimension (4) to the target dimension (2) is impractical. At the same time, known results for CFT and exactly solvable models are useful thus far only in \(d = 2\). The question arises: is there an analog of the G-L Eq.(3.1) in two dimensions? And, if such an analog does exist, what use can be made of it? In the rest of
this section we provide affirmative answers to these questions. We demonstrate that: a) indeed, a two dimensional analog of the G-L equation does exist and is given by the Liouville Eq.(5.19) below, b) the functional, Eq.(5.14), whose minimization produces such an equation is the exact two dimensional analog of the G-L-Yamabe functional, Eq.(3.2), c) these results can be (re)obtained from the existing string-theoretic formulations of CFT developed entirely independently, d) in view of the noted correspondence, these string-theoretic CFT results can be extended to account for the Lifshitz-type problems discussed in the Introduction. This allows us to obtain a positive answer to the 1st Problem formulated in the Introduction.

5.2 Designing the two dimensional G-L-Yamabe functional

To discuss topics related to items a) and b) just mentioned, we begin with the observation that in two dimensions, Eq.(2.4) acquires a very simple form

$$\Delta_{\tilde{g}} = e^{-2f} \Delta_g,$$  \hspace{1cm} (5.1)

where we use a factor of 2 to be in accord with Eq.(2.11) for scalar curvature. According to Eq.(2.11), the scalar curvature in two dimensions transforms like

$$\tilde{R}(\tilde{g}) = e^{-2f} \{ R(g) - \Delta g 2f \} \hspace{1cm} (5.2)$$

while the area $dA = d^2x\sqrt{g}$ transforms like

$$d\tilde{A} = e^{-2f}dA.$$  \hspace{1cm} (5.3)

These facts immediately suggest that the previously introduced action functional

$$S[X] = \int_M d^2x\sqrt{g} (\nabla g X) \cdot (\nabla g X)$$  \hspace{1cm} (5.4)

is conformally invariant. Using results by Polyakov [37] and noting that $(\nabla g X) \cdot (\nabla g X) = g^{\alpha\beta} \partial_{\alpha}X^{\mu} \partial_{\beta}X_{\mu}$, we need to consider the following path integral\footnote{Without loss of generality, we would like to consider the case of a one component field $\phi$ only.}

$$\exp(-\mathcal{F}(g)) = \int D[\phi] \exp(-\frac{1}{2} \int_M d^2x\sqrt{\tilde{g}} g^{\alpha\beta} \partial_{\alpha}\phi \partial_{\beta}\phi)$$  \hspace{1cm} (5.5)

where $\mathcal{F}(g)$ is the "free energy"\footnote{Usually, instead of $\mathcal{F}(g)$ one writes $\mathcal{F}(g)/k_BT$, where $T$ is the temperature and $k_B$ is the Boltzmann’s constant. In the present case, the problems we are studying do not require specific values for these constants. For this reason they will be suppressed. Also, one should keep in mind that the free energy is always defined with respect to some reference state. This will be the case in our calculations as well.}. Fortunately, this integral was calculated by Polyakov [37] for two dimensional manifolds $M$ without boundaries and by Alvarez [38] for manifolds with boundaries. In this work we shall be mainly concerned with manifolds without boundaries. Although in the original work by
Polyakov, one can find the final result of calculation of the above path integral, the details of this calculation can be found only elsewhere. In particular, we shall follow pedagogically written papers by Weisberger \[39,40\] and Osgood, Phillips and Sarnak \[26,41,42\] (OPS).

To begin, let $\tilde{g}_{\alpha\beta}$ be some reference metric, and let $g_{\alpha\beta}$ be a metric conformally related to it, i.e. $g_{\alpha\beta} = \exp(-2\varphi)\tilde{g}_{\alpha\beta}$. Should the above path integral be for the flat (i.e. $g_{\alpha\beta} = \delta_{\alpha\beta}$) two dimensional manifold, one would have at once the result:

$$F = \frac{1}{2} \ln \det \Delta_0,$$

where the prime indicates that the zero mode is omitted.

Because to assume such flatness in general is too restrictive, it is appropriate to pose a problem: how is the path integral for the metric $g$ related to that for the metric $\tilde{g}$? The paper \[26\] by OPS provides an answer, e.g. see Eq.(1.13) of this reference. To connect this equation with the free energy, we replace it by the equivalent expression

$$\ln \left( \frac{\det\Delta_{\tilde{g}}}{\det\Delta_g} \right) - \ln \left( \frac{\det\Delta_{\tilde{g}}}{\det\Delta_g} \right) = -\frac{1}{6\pi} \frac{1}{2} \int_M dA_g \left[ |\nabla g\varphi|^2 + R(g)\varphi \right]$$

(5.6)

useful in applications to strings and CFT, e.g see Ref.\[43\], page 637.

It is worthwhile to provide a few computational details leading to Eq.(5.6). Therefore, let $\hat{\psi}_i$ be eigenfunctions of the Laplacian $\Delta_g$ with eigenvalues $\lambda_i$ arranged in such a way that $0 = \hat{\lambda}_0 < \hat{\lambda}_1 \leq \hat{\lambda}_2 \leq \cdots$, i.e.

$$-\Delta_g \hat{\psi}_i + \hat{\lambda}_i \hat{\psi}_i = 0.$$  (5.7)

Then, we construct the zeta function

$$\zeta_g(s) = \sum_{i=1}^{\infty} \lambda_i^{-s}$$

(5.8)

in such a way that

$$\det \ '\Delta_g = \exp(-\zeta_g'(0))$$

(5.9)

with $\zeta_g'(0) = \left( \frac{d}{ds} \zeta_g(s) \right)_{s=0}$. Using Eq.(5.1), we obtain as well

$$- e^{-2\varphi}\Delta_g \psi_i + \lambda_i \psi_i = 0.$$  (5.10)

In particular, for a constant $\varphi = \bar{\varphi}$ we obtain

$$\zeta_{\bar{g}}(s) = \sum_{i=1}^{\infty} \left( e^{-2\varphi \hat{\lambda}_i} \right)^{-s} = e^{2s\bar{\varphi}} \zeta_g(s).$$

(5.11)

Use of Eq.(5.9) in Eq.(5.11) produces:

$$\zeta_{\bar{g}}'(0) = \zeta_g'(0) + 2\bar{\varphi} \left( \frac{\chi(M)}{6} - 1 \right).$$

(5.12)

This result was obtained with help of the known fact, Ref.\[26\], Eq.(1.9), that

$$\zeta_g(0) = \frac{\chi(M)}{6} - 1$$

(5.13)
with $\chi(M)$ being the Euler characteristic of two dimensional manifold $M$ without boundaries. In view of the definition, Eq.(5.9), and the Gauss-Bonnet theorem, we observe that Eq.(5.6) is reduced to Eq.(5.12) for the case of constant conformal factor $\varphi = \bar{\varphi}$, as required. It should be mentioned that Eq.(5.6) was used earlier in finite size scaling calculations [44-46]. Unfortunately, the authors of [45,46] did not take into account that the above formula is valid, strictly speaking, for manifolds $M$ without boundaries while the topology considered in these works was that for the punctured disc and/or annulus. Rigorous results for such topologies were obtained by Weisberger [40] and more general case of surfaces of higher genus with boundaries and/or punctures was discussed in detail by OPS [42]. To focus on the main goals of this paper, we shall not discuss the finite size scaling analysis further.

Using Eq.(5.6) and, following OPS [26], we would like consider the related functional $F(\varphi)$ defined by

$$F(\varphi) = \frac{1}{2} \int_M dA_g \left\{ |\nabla_g \varphi|^2 + R(g) \varphi \right\} - \pi \chi(M) \ln \int_M dA_g e^{2\varphi}.$$  \hfill (5.14)

This functional is the exact analog of the Yamabe functional, Eq.(3.2), in dimensions 3 and higher as we shall demonstrate shortly below. In the meantime, in view of Eq.(5.6), it can be rewritten in the following equivalent form

$$F(\varphi) = -6\pi \ln \det \ '\Delta_g + \pi (6 - \chi(M)) \ln A.$$  \hfill (5.15)

Let $a$ be some constant, then

$$F(\varphi + a) = F(\varphi).$$  \hfill (5.16)

This signifies that the above action is scale invariant. This property is in complete accord with Eq.s (2.7) and (2.8) discussed earlier. If we impose the constraint (fix the gauge): $A = 1$, then we end up with the Liouville-like action used in CFT. We would like to explain this in some detail now. Following OPS, it is convenient to replace the constraint $A = 1$ by the alternative constraint on the field $\varphi$:

$$\int_M \varphi dA_g = 0.$$  \hfill (5.17)

To demonstrate that such an imposed constraint is equivalent to the requirement $A = 1$, we note that, provided that the field $\psi$ minimizes $F(\psi)$ subject to the

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15 When comparing with the OPS paper, it should be noted that OPS use the Gaussian curvature $K$ while we use the scalar curvature $R = 2K$

16 Here one should understand the word “equivalence” in the sense that both functionals produce the same critical metrics upon minimization.
constraint Eq.(5.17), the field
\[ \varphi = \psi - \frac{1}{2} \ln \int_M \exp(2\psi) dA_g \] (5.18)
minimizes \( F(\varphi) \) subject to the constraint \( A = 1 \). Using these facts, minimization of \( F(\psi) \) produces the following Liouville equation
\[ -\Delta_g \psi + \frac{1}{2} R(g) - \frac{2\pi \chi(M) \exp(2\psi)}{\int_M \exp(2\psi) dA_g} = 0. \] (5.19)
Comparing this result with Eq.(5.2) and taking into account that
\[ 2\pi \chi(M) \int_M \exp(2\psi) dA_g = \tilde{R}(\tilde{g}) = \text{const}, \] (5.20)
we conclude that, provided that the background metric \( g \) is given so that the scalar curvature \( R(g) \) (not necessarily constant) can be calculated, the Liouville Eq.(5.19) is exactly analogous to the previously obtained Eq.(3.3), or equivalently, Eq.(2.12). In view of this analogy, use of Eqs (3.4) and (3.6) as well as Eqs(5.14),(5.15) causes the functional \( F(\varphi) \) to attain its extremum for metric \( \tilde{g} \) of constant scalar curvature \( \tilde{R}(\tilde{g}) \). To decide if the extremum is minimum or maximum, we have to consider separately cases \( \chi(M) > 0 \) and \( \chi(M) \leq 0 \).

In the case of \( \chi(M) > 0 \) we have only to consider manifolds homeomorphic to \( S^2 \) so that \( \chi(M) = 2 \). Fortunately, this case was considered in detail by Onofri \[47]\]. Using his work, the following inequality
\[ \ln \int_{S^2} dA_{\tilde{g}} \exp(\psi) \leq \int_{S^2} dA_{\tilde{g}} \psi + \frac{1}{4} \int_{S^2} dA_{\tilde{g}} |\nabla \tilde{\psi}|^2 \] (5.21)
attributed to Aubin \[22]\] and inspired by previous results by Trudinger and Moser \[48]\], is helpful for deciding whether the obtained extremum is minimum or maximum. Here \( \tilde{g} \) is the metric of the unit sphere \( S^2 \) with constant Gaussian curvature 1. The metric \( g \) conformal to \( \tilde{g} \) is given by \( g = \exp(2\psi) \tilde{g}, \) with \( \psi \) obeying the Liouville equation (just like Eq.(5.19)), where both \( R(g) \) and \( \tilde{R}(\tilde{g}) \) are constant by virtue of the initial choice of \( \tilde{g} \). By combining Eqs(5.6),(5.14) and (5.15) with the inequality (5.21) and taking into account that by design \( \ln A_{\tilde{g}} = 0 \) we obtain,
\[ -3\pi \ln \frac{\det' \Delta_g}{\det' \Delta_{\tilde{g}}} = \frac{1}{4} \int_{S^2} dA_{\tilde{g}} \{|\nabla \tilde{\psi}|^2 + 2\psi\} - \ln \int_{S^2} dA_{\tilde{g}} \exp(2\psi) \geq 0, \] (5.22)
with equality occurring only at the extremum \( \psi = \psi^* \), with the function \( \psi^* \) being a solution of the Liouville Eq.(5.19). It can be shown \[47]\] that: a) such a
solution involves only M"obius transformations of the sphere $S^2$ and that, b) the functional $F(\phi)$ is invariant with respect to such transformations. The case of $\chi(M) \leq 0$ is treated in Section 2.2 of the OPS paper, Ref.[26] and leads to the same conclusions about extremality of the functional $F(\phi)$.

The two dimensional results just obtained are in accord by design with results obtained in higher dimensions (discussed in Sections 3 and 6). In particular, the functional $F(\phi)$ is the exact analog of the Yamabe functional $S[\varphi]$, Eq.(3.2). Since in both cases the functionals are "translationally" (actually, scale) invariant, e.g. compare Eq.(3.6) with Eq.(5.16), in both cases, the extremum is realized for metric conformal to the metric of constant scalar curvature, e.g. compare Eq.(3.3) with the Liouville Eq.(5.19).

### 5.3 Connections with string and CFT

The results just obtained allow us now to discuss topic c) listed at the beginning of this section. Using known facts from string and conformal field theories, [27,28], it is of interest to consider averages of the vertex operators

$$\langle \prod_{i=1}^{n} \exp(\beta_i \phi(z_i)) \rangle \equiv \int D[\phi] \exp\{-S_L(\phi)\} \prod_{i=1}^{n} \exp(\beta_i \phi(z_i)),$$  \hspace{0.5cm} (5.23)

where the Liouville action $S_L(\phi)$ is given (in notation adopted from these references) by

$$S_L(\phi) = \frac{1}{8\pi} \int_M dA_\hat{\beta} [\nabla \phi]^2 - QR(\hat{\phi}) + 8\pi \hat{\mu} \exp(\alpha + \phi)].$$ \hspace{0.5cm} (5.24)

The actual values and the meaning of constants $Q$, $\hat{\mu}$ and $\alpha_+$ are explained in these references and are of no immediate use for us. Clearly, upon proper rescaling, we can bring $S_L(\phi)$ to the form which agrees with $F(\phi)$, defined by Eq.(5.14), especially in the trivial case when both $\chi(M)$ and $\hat{\mu}$ are zero. When they are not zero, the situation in the present case becomes totally analogous to that discussed earlier for the Yamabe functional. In particular, in Section 3 we noticed that the G-L Euler-Lagrange Eq.(3.3) can be obtained either by minimization of the Yamabe functional, Eq.(3.2) (or (4.9)), or by minimization of the G-L functional, Eq.(3.7), where the coupling constant $\lambda$ plays the role of the Lagrange multiplier enforcing the volume constraint. In the present case, variation of the Liouville action $S_L(\phi)$ will produce the Liouville equation, e.g. see Eqs. (5.19)-(5.20), which is the two dimensional analog of the G-L Eq.(3.3). This variation is premature, however, since we can reobtain $F(\phi)$ exactly using the path integral, Eq.(5.23). This procedure then will lead us directly to the Liouville Eq.(5.19).
To this purpose, we need to consider the path integral, Eq.(5.23), in the absence of sources, i.e. when all \( \beta_i = 0 \). Following ideas of Ref.s \([27,28]\), we take into account that: a) \[
\frac{1}{4\pi} \int_M dA_{\beta} R(\hat{g}) = \chi(M) = 2 - 2g
\]
with \( g \) being genus of \( M \) and, b) the field \( \phi \) can be decomposed into \( \phi = \phi_0 + \varphi \) in such a way that \( \phi_0 \) is coordinate-independent and \( \varphi \) is subject to the constraint given by Eq.(5.17). Then, use of the identity
\[
\int_{-\infty}^{\infty} dx \exp(ax) \exp(-b \exp(\gamma x)) = \frac{1}{\gamma} b^{-\frac{a}{\gamma}} \Gamma\left(\frac{a}{\gamma}\right) (5.27)
\]
(with \( \Gamma(x) \) being Euler's gamma function) in the path integral, Eq.(5.23), requires us to evaluate the following integral
\[
I = \int_{-\infty}^{\infty} d\phi_0 \exp(\phi_0 \frac{Q}{2} \chi(M)) \exp((\bar{\mu} \int_M dA_{\beta} \exp(\alpha + \varphi)) \exp(\alpha + \phi_0))
\]
\[
= \frac{\Gamma(-s)}{\alpha_+} (\bar{\mu} \int_M dA_{\beta} \exp(\alpha + \varphi))^s
\]
with \( s \) given by
\[
s = -\frac{Q}{2\alpha_+} \chi(M). (5.29)
\]
Using this result in Eq.(5.23), we obtain the following path integral (up to a constant)
\[
Z[\varphi] = \int D[\varphi] \exp(-\hat{F}(\varphi)) (5.30)
\]
with functional \( \hat{F}(\varphi) \) given by
\[
\hat{F}(\varphi) = S_L(\varphi; \bar{\mu} = 0) - \frac{Q}{2\alpha_+} \chi(M) \ln[\bar{\mu} \int_M dA_{\beta} \exp(\alpha + \varphi)]. (5.31)
\]
This functional (up to rescaling of the field \( \varphi \) is just the same as the Yamabe-like functional \( F(\varphi) \) given by Eq.(5.14).

Define now the free energy \( F \) in the usual way via \( F = -\ln Z[\varphi] \) (as was done after Eq.(5.5)) and consider the saddle point approximation to the functional integral \( Z[\varphi] \). Then, for a spherical topology, in view of Eq.(5.22), we (re)obtain \( F \geq 0 \) with equality obtained when \( \varphi = \psi^* \). Sources (or the vertex operators) can be taken into account also, especially in view of the results of \([42]\).\(^\text{18}\)

\(^{18}\)Since the results of this reference are useful as well as well for extension of the finite size scaling results given in works by Affleck \([46]\) and Blöte et al \([45]\), the detailed analysis of this case is left for further study.

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To better understand the physical significance of the obtained results, it is useful to reobtain them using a somewhat different method. The results obtained with this alternative method are also helpful when we shall discuss their higher dimensional analogs in the next section. To this purpose we write (up to a normalization constant)

\[
\int D[\phi] \exp\{-S_L(\phi)\} = \int_0^\infty dA e^{-\bar{\mu} A} Z_L(A) \tag{5.32}
\]

where

\[
Z_L(A) = \int D[\phi] \delta(\int_M dA_\hat{g} \exp(\alpha_+ \phi) - A) \exp(S_L(\phi; \bar{\mu} = 0)). \tag{5.33}
\]

If, as before, we assume that \(\phi = \phi_0 + \varphi\), then an elementary integration over \(\phi_0\) produces the following explicit result for \(Z_L(A)\):

\[
Z_L(A) = -\frac{1}{\alpha_+} A^\omega \int D[\varphi] \left[ \int_M dA_\tilde{g} \exp(\alpha_+ \varphi) \right]^{-(\omega+1)} \exp(-S_L(\varphi; \bar{\mu} = 0)), \tag{5.34}
\]

where the exponent \(\omega\) is given by

\[
\omega = \frac{\chi(M)Q}{2\alpha_+} - 1. \tag{5.35}
\]

Finally, using Eq.(5.34) in Eq.(5.32) produces back Eqs (5.30) and (5.31) (again, up to a constant factor). An overall "-" sign can be removed by proper normalization of the path integral. These results can be used for computation of the correlation functions of conformal field theories (CFT). Details can be found in [28].

### 5.4 Completion of the work by Lifshitz in 2 dimensions

Since in this work our main interest is investigation of higher dimensional analogs of the results just obtained, no further computational details related to two dimensional CFT will be presented in this work. Instead, we would like to complete our investigation related to item d) mentioned at the beginning of this section. It will enable us to develop similar treatments for higher dimensions to be considered in the next section.

We begin with combining inequalities given by Eqs.(5.21) and (5.22). This produces,

\[-\ln \det '\Delta_g - (-\ln \det '\Delta_{\tilde{g}}) \geq 0, \tag{5.36}\]

with equality taking place only when the metric \(g\) is equal to that for the unit round sphere \(S^2\), i.e. to \(\tilde{g}\). This means that

\[\det '\Delta_g \leq \det '\Delta_{\tilde{g}} \tag{5.37}\]
implying that the determinant of the Laplacian for the round sphere provides the upper bound for determinants of Laplacians whose metric is conformally equivalent to that for the round sphere $S^2$. Calculation of the determinant of the Laplacian for the round sphere can be done with help of Eqs. (5.8) and (5.9). Specifically, for this case we need to calculate $Z'_\tilde{g}(0)$ where

$$Z_\tilde{g}(s) = \sum_{n=1}^{\infty} \frac{2n+1}{(n(n+1))^s}.$$  \hspace{1cm} (5.38)

This calculation is rather difficult and can be found, for example, in [49] along with its multidimensional generalization. For $S^2$ the final result is given by

$$Z'_\tilde{g}(0) = 4\zeta'(-1) - \frac{1}{2}. \hspace{1cm} (5.39)$$

From here we obtain, \[ \text{det}'\Delta_g \leq \exp\left\{ \frac{1}{2} - 4\zeta'(-1) \right\}. \] We deliberately avoid long discussion leading to this result since we are more interested in similar calculations for torus topology. In this last case the reference metric $\hat{g}$ is that for the flat torus $T^2 = \mathbb{C}/\Lambda$, where $\mathbb{C}$ is the complex plane and $\Lambda$ is some lattice. Evidently, $\chi(T^2) = 0$, so that $R(\hat{g}) = 0$. These facts produce at once

$$-\ln \text{det}'\Delta_g - (-\ln \text{det}'\Delta_{\tilde{g}}) = \frac{1}{12\pi} \int_M dA_{\tilde{g}} |\nabla_{\tilde{g}} \varphi|^2 \geq 0 \hspace{1cm} (5.40)$$

with equality when $\varphi = \text{const}$. From the point of view of applications to statistical mechanics (or better, to CFT), the above inequality is useful when calculating the path integral, Eq.(5.30), using the saddle point method. In this case, since $\hat{F}(\varphi)$ plays a role of the LGW free energy, in accord with general requirements of thermodynamics, the free energy attains its minimum at equilibrium, i.e., for $\varphi = \varphi^*$. Here $\varphi^*$ is a solution of the Liouville Eq.(5.19) in accord with previously obtained result, Eq.(5.22), for the sphere. In the present case of toral topology, it is known that $\chi(M) = 0$, so that $\varphi^* = \text{const}$ is an acceptable solution. Such a two dimensional result is formally in complete accord with the higher dimensional G-L result, Eq.(1.20), ($h = 0$) of Section 1. In the present case, the choice of the $\text{const}$ is dictated by Eq.(5.18). For such a choice, $\hat{F}(\varphi^*) = 0$. This is clearly the lowest possible value for the free energy, which in G-L theory corresponds to the free energy at criticality (i.e. at $T = T_c$). Expanding $\hat{F}(\varphi)$ around the equilibrium value of the field $\varphi$ in the path integral in Eq.(5.30) produces quadratic and higher order terms as usual [19]. If one ignores terms higher than quadratic, one obtains the standard Gaussian-type path integral discussed in the Introduction. It plays a major role in many two dimensional CFT models [20]. Justification of such a truncation is discussed in the next section. In the meantime, we would like to discuss calculation of this type of
path integral in some detail. Since the path integral is Gaussian, its calculation is essentially the same as calculation of \( \det \Delta \tilde{g} \). In view of Eq.(5.9), such a calculation involves use of the zeta function of the following type

\[
Z \tilde{g}(s) = \sum'_{\mathbf{l} \in \Lambda^*} \frac{1}{(4\pi^2 |\mathbf{l}|^2)^s}.
\]  

(5.41)

This result can be easily understood using some basic information from solid state physics [13]. Indeed, the eigenfunctions \( f(\mathbf{l}) \) of the Laplace operator for \( T^2 \) are given by \( f(\mathbf{l}) = \exp(i2\pi(l_1n_1 + l_2n_2)) \) with vector \( \mathbf{l} = \{l_1, l_2\} \in \Lambda^* \) being some vector of the dual (reciprocal) lattice \( \Lambda^* \), while the numbers \( \{n_1, n_2\} \) are related to some vector of the direct lattice \( \Lambda \). Accordingly, the corresponding eigenvalues are \( 4\pi^2 |\mathbf{l}|^2 \).

The method of calculation of \( Z \tilde{g}(s) \) presented in Ch 10 of Ref.[20] while being straightforward is not too illuminating, especially if one is contemplating its extension to dimensions higher than 2. We follow therefore the approach taken by OPS, Ref.[26], where the first Kronecker limit formula is used for evaluation of \( Z' \tilde{g}(0) \). To avoid duplications, our arguments (leading to the same results) are somewhat different than those used in the OPS paper. These arguments allow us to make additional useful connections with some facts from number theory.

It is well known [51] that for each torus \( T^2 \), the modular lattice \( \Lambda \) is given by

\[
\Lambda = \mathbf{Z}\omega_1 + \mathbf{Z}\omega_2 \text{ or, symbolically, } \Lambda = [\omega_1, \omega_2],
\]  

(5.42)

where the periods \( \omega_1 \) and \( \omega_2 \) are such that \( \tau = \frac{\omega_2}{\omega_1} > 0 \). That is, at least one of the periods should be complex. Different tori are related to each other by a modular transformation of the type

\[
\tau' = \frac{a\tau + b}{c\tau + d}
\]  

(5.43)

provided that \( ad - bc = 1 \) with \( a, b, c \) and \( d \) being some integers. The requirement \( ad - bc = 1 \) guarantees that the inverse transformation (i.e. \( \tau' \to \tau \)) also looks like Eq.(5.43), with respective constants being also integers. Invariance of the observables of CFT with respect to modular transformations is widely emphasized [20]. However, such invariance is too broad and leads to some inconsistencies in CFT and string theories discussed in Ref.[50]. These inconsistencies can be removed if we restrict values of the modular parameter \( \tau \) to those originating from complex multiplication (CM). The concept of CM can be easily understood based on the following example. Consider two lattices \( \Lambda \) and \( \Lambda' \) such that there is a matrix \( \mathbf{A} \)

\[
\mathbf{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}
\]  

(5.44)

Since this result can be extended immediately to 3 and higher dimensions it will be used in the next section as well.

Some of these facts have been presented already in our recent work, Ref.[50].
so that

\[
\begin{align*}
\omega'_2 &= a\omega_2 + b\omega_1, \\
\omega'_1 &= c\omega_2 + d\omega_1.
\end{align*}
\] (5.45)

Clearly, if we require \(ad - bc = 1\) and then form a ratio of the above two equations, we would obtain Eq.(5.43). This time, however, we would like to keep the requirement \(ad - bc = 1\) but avoid forming the ratio. This move is motivated by the fact that by making this ratio, we would lose the option: \(\omega'_2 = \alpha\omega'_2\) and \(\omega'_1 = \alpha\omega_1\) for some, yet unknown, \(\alpha\). Substitution of these relations into Eq.(5.45) leads to the following eigenvalue problem

\[
\alpha^2 - \alpha tr A - det A = 0.
\] (5.46)

But, we know already that \(det A = 1\). Hence, Eq.(5.46) can be rewritten as

\[
\alpha^2 - \alpha(a + d) + 1 = 0.
\] (5.47)

This is the equation for an integer in the quadratic number field. It is easy to demonstrate that such an integer must belong to the imaginary quadratic number field. To prove this fact, we write for the roots

\[
\alpha_{1,2} = \frac{a + d}{2} \pm \frac{1}{2} \sqrt{(a + d)^2 - 4}.
\] (5.48)

In order for \(\alpha\) to be an integer belonging to the imaginary quadratic field, the following set of options should be explored first. These are:

a) \(a = d = 0\), thus producing \(\alpha_{1,2} = \pm i\);

b) \(a = \pm 1, d = 0\) (or \(a = 0, d = \pm 1\)), thus producing \(\alpha_{1,2} = \frac{1}{2}(\pm 1 \pm \sqrt{-3})\);

c) \(a = d = \pm 1\), thus producing \(\alpha_{1,2} = \pm 1\).

Before analyzing these results it is helpful to recall the following definition from CM. A torus \(T^2\) admits CM if it admits an automorphism \(\Lambda \rightarrow c\Lambda\) so that \(c\Lambda \subseteq \Lambda\) for some \(c \neq Z\). The case when \(c\Lambda \subset \Lambda\) requires us to replace Eq.(5.48) by

\[
\alpha_{1,2} = \alpha\frac{a + d}{2} \pm \frac{1}{2} \sqrt{(a + d)^2 - 4n}
\] (5.49)

where the nonnegative integer \(n\) should be strictly greater than one.

To understand the physical implications of these results, recall that if \(a(\Lambda)\) denotes the area of the period parallelogram associated with \(\Lambda\), then it can be shown \([51]\) that

\[
a(\Lambda) = \frac{1}{2} |\omega_1\tilde{\omega}_2 - \omega_2\tilde{\omega}_1|.
\] (5.50)

If we now rescale \(\omega'\): \(\omega'_2 = \alpha\omega_2\), \(\omega'_1 = \alpha\omega_1\), this produces: \(a(\alpha\Lambda) = |\alpha|^2 a(\Lambda)\). If we require that the area upon rescaling remains unchanged, we are left with \(|\alpha|^2 = 1\). This is the only acceptable option in view of the constraint \(A = 1\) on
the area, which was imposed earlier. Above we obtained two types of integers (also units) of the imaginary quadratic field: a) the Gaussian units: \(\pm 1, \pm i\) of the Gaussian ring \(\mathbb{Z}[i]\) which are the 4-th roots of unity, i.e. \(1, i, i^2 = -1\) and \(i^3 = -i\), and, b) the units of the ring \(\mathbb{Z}[j]\) which are the 6-th roots of unity, i.e. \(1, -1, j, -j, j^2\) and \(-j^2\), where \(j = \frac{1}{2}(-1 + \sqrt{-3})\). Since these are units in the respective rings, automatically we get \(|\alpha|^2 = 1\). In view of the constraint \(ad - bc = 1\), no units from other imaginary quadratic fields can be used. Indeed, in the most general case of CM, we have to use Eq.(5.49) instead of Eq.(5.48). This is equivalent to replacing the constraint \(ad - bc = 1\) by \(ad - bc = n\) and leads to \(a(\alpha\Lambda) = na(\Lambda)\). Clearly, since by definition \(n \neq 1\), for physical reasons we are left only with the units of the two rings just discussed.

CM along with the area constraint is sufficient for determination of all regular lattices in two dimensions. These are: the square (associated with \(i\)), the hexagonal (associated with \(j\)) and the triangular (dual of the hexagonal). These are described in Refs[52, 53]. No other translationally invariant lattices exist in two dimensions [53].

Number-theoretically, these results can be reformulated as follows (e.g. see Appendix B). For the Gaussian lattice \(\Lambda_i\) we can take as basis \(\Lambda_i = [1, i]\) while for the cube root of unity (hexagonal) lattice \(\Lambda_j = [1, j]\). It should be clear that the usual complex numbers \(z = x + iy\) belong to \(\Lambda_i[53]\) so that the Gaussian integers are made of \(x\) and \(y\) being integral. Analogously, the "hexagonal" numbers are made of \(z = x + jy\) with "hexagonal integers" made accordingly from the integral \(x\)'s and \(y\)'s. The norm \(N(z)\) can be defined now as is done in complex analysis, i.e.

\[
N(z) = z\bar{z}.
\] (5.51)

The norm has a very useful property which can be formulated as follows. If \(z'' = z'z\), then \(N(z'') = N(z')N(z)\). In particular, if \(z\) is the unit of the complex imaginary quadratic field, then there is some \(z'\) in the same field such that \(zz' = 1\). This produces \(N(z')N(z) = 1\), so that \(N(z) = 1\). In the case of a Gaussian field this leads to the equation \(n^2 + m^2 = 1\), producing 4 Gaussian units: \(\pm 1, \pm i\). At this point it is useful to keep in mind that for the field of real numbers there are only 2 units: \(\pm 1\). In view of the results just presented we would like to rewrite the zeta function in Eq.(5.41) in the number-theoretic form. We obtain,

\[
Z_{\mathbb{R}}(s) = \frac{1}{(4\pi^2)^s} \sum_{z \in \mathbb{R}} \frac{1}{N(z)^s}
\] (5.52)

Apart from the factor \((4\pi^2)^{-s}\), the obtained result corresponds to the Dedekind zeta function. In the case of other (higher than quadratic order) number fields, the situation is more complicated as explained in the book by Terras [54], so that other methods should be used. These will be discussed in the next section. In the case of two dimensions, connections between the exactly solvable statistical
mechanical models and number theory have been known for some time. All these connections are based on the known fact that the Dedekind zeta function is related to the Dirichlet L-function via

$$\sum'_{z \in \Lambda^*} \frac{1}{N(z)^s} = \mu \zeta(s) \sum_{n=1}^{\infty} \frac{\chi(n)}{n^s}$$

(5.53)

where $\mu$ is the number of units in the number field and $\chi(n)$ is the Dirichlet character. In particular, for the Gaussian number field we obtain

$$\sum'_{z \in \Lambda^*} \frac{1}{N(z)^s} = 4 \zeta(s) \sum_{n=1}^{\infty} \frac{\chi_4(n)}{n^s}$$

(5.53)

with

$$\chi_4(n) = \begin{cases} 0 & \text{if } n \text{ is even} \\ (-1)^{(n-1)/2} & \text{if } n \text{ is odd} \end{cases}$$

(5.54)

while for the hexagonal number field we get

$$\sum'_{z \in \Lambda^*} \frac{1}{N(z)^s} = 6 \zeta(s) \sum_{n=1}^{\infty} \frac{\chi_3(n)}{n^s}$$

(5.55)

with

$$\chi_3(n) = \begin{cases} 0 & \text{if } n \equiv 0 \mod 3 \\ 1 & \text{if } n \equiv 1 \mod 3 \\ -1 & \text{if } n \equiv -1 \mod 3 \end{cases}.$$  

(5.56)

To obtain $\frac{d}{ds} Z_\theta(s)\big|_{s=0}$ using Eqs (5.53)-(5.55) is possible, but is not very illuminating. It is much better to use the 1st Kronecker limit formula valid for any quadratic number field [55]. In order to reveal the meaning of this formula and its relevance to our needs a few steps are required. First, we note that the area form given by Eq.(5.50) can be equivalently rewritten as

$$a(\Lambda) = \frac{1}{2} |\omega_1 \bar{\omega}_2 - \omega_2 \bar{\omega}_1| = |\omega_1|^2 \Im \tau$$

(5.57)

where $\tau = \frac{\omega_2}{\omega_1}$. Second, if $l$ is the vector of the reciprocal lattice $\Lambda^*$, then it can be decomposed as $l = l_1 \omega_1 + l_2 \omega_2$ with $l_1$ and $l_2$ being some integers. Accordingly,

$$|l|^2 = (l_1 \omega_1 + l_2 \omega_2)(l_1 \bar{\omega}_1 + l_2 \bar{\omega}_2)$$

$$= |\omega_1|^2 (l_1 + \tau l_2)(l_1 + \bar{\tau} l_2).$$

(5.58)

Next, since we have fixed the area $a(\Lambda)$ so that in our case, it is equal to one, we obtain

$$\Im \tau = \frac{1}{|\omega_1|^2}.$$  

(5.59)
By denoting $\text{Im} \, \tau = y$ we can rewrite Eq.(5.41) as follows

$$Z_{\tilde{g}}(s) = \sum_{l \in \Lambda^*} \frac{1}{(4\pi^2 |l|^2)^s} = \frac{1}{(2\pi)^{2s}} \sum_{l_1, l_2} y^s \frac{1}{|l_1 + \tau l_2|^{2s}}. \tag{5.60}$$

In mathematics literature [55] the derivation of the Kronecker 1st limit formula is given for the function

$$E(\tau, s) = \sum_{l_1, l_2} y^s \frac{1}{|l_1 + \tau l_2|^{2s}} \tag{5.61}$$

where the prime indicates that the summation takes place over all integers $(l_1, l_2) \neq (0, 0)$. For many applications, it is more convenient to consider the combination

$$E^*(\tau, s) = \pi^{-s} \Gamma(s) \frac{1}{2} E(\tau, s) \tag{5.62}$$

which possess the nice analytical property [56]

$$E^*(\tau, s) = E^*(\tau, 1 - s). \tag{5.63}$$

Kronecker found the Laurent expansion of $E^*(\tau, s)$ near $s = 0$. It is given by [57]

$$E^*(\tau, s) = -\frac{1}{2s} + \frac{\gamma}{2} - \ln 2\sqrt{\pi y} - \ln |\eta(\tau)|^2 + O(s) \tag{5.64}$$

where $\gamma$ is Euler’s constant and

$$\eta(\tau) = \exp(i\pi \tau / 12) \prod_{n=1}^{\infty} (1 - \exp\{i2\pi n\tau\}) \tag{5.65}$$

is the Dedekind eta function. By combining Eq.s (5.60)-(5.64) and taking into account that for $\varepsilon \to 0^+$

$$\Gamma(\varepsilon) = \frac{1}{\varepsilon}(1 - \gamma \varepsilon + O(\varepsilon^2))$$

and

$$\pi^\varepsilon = 1 + \varepsilon \ln \pi + O(\varepsilon^2)$$

after some straightforward algebra we obtain (for $s \to 0^+$),

$$Z_{\tilde{g}}(s) = -1 - s \ln y |\bar{\eta}(\tau)\eta(\tau)|^2, \tag{5.66}$$

in agreement with Weil [58], page 75. From here we get

$$\frac{d}{ds} Z_{\tilde{g}}(s) \big|_{s=0} = -\ln y |\bar{\eta}(\tau)\eta(\tau)|^2 \tag{5.67}$$

in agreement with OPS [26]. Eq.(5.9), when combined with Eq.(5.67), produces

$$\det \ '\Delta_{\tilde{g}} = y |\eta(\tau)|^4. \tag{5.68}$$
Comparison of this result with that given by Eqs (10.29), (10.30) of Ref.[20] indicates that the free energy $F$ for the Gaussian model on the torus is given by

$$F = \frac{1}{2} \ln y|\eta(\tau)|^2.$$  \hspace{1cm} (5.69)

For the hexagonal lattice A OSP found numerically that $\det \Delta_{\tilde{g}} = \sqrt{3} |\eta(j)|^4 = 0.35575$. In Appendix C it is shown that the hexagonal lattice provides the highest packing fraction: $q^2_{\Delta} = 0.9069$. We anticipate that there is a correlation between the packing fraction and the numerical value of the determinant (or, alternatively, the value of the free energy). For this to happen, according to Eq.(5.40) we must have

$$\det \Delta_g \leq \det \Delta_{\tilde{g}} = 0.35575 \hspace{1cm} (5.70)$$

for any lattice other than the hexagonal. In terms of the free energy defined by Eq.(5.69) this means that the free energy of the hexagonal lattice is the highest possible. This makes sense thermodynamically. Indeed, according to the G-L theory [6], at criticality, the symmetry of the system is higher than that in the low temperature phase. The free energy should be lower in the low temperature phase to make such a transition to lower symmetry thermodynamically favorable. In the next section we shall obtain analogous 3d results for the hexagonal close packed (hcp) and the face centered cubic lattices (fcc) whose symmetry is the highest. Such symmetry is typical for the high temperature phase (e.g. see Fig.1) and in accord with group-theoretic classification of successive second order phase transitions as predicted (in part) by Indenbom [59], e.g. see Fig.4 in his work. Further details are provided in Section 6 below.

The above inequality means that we have to prove that it holds for the square, hexagonal and triangular lattices. To accomplish this task, we follow the classical paper by Chowla and Selberg [29] (C-S) discussed also in our earlier work [50] in connection with the Veneziano amplitudes. To facilitate the reader’s understanding we note that from the point of view of algebraic geometry every torus $T^2$ can be associated with the projective version of the elliptic curve whose standard form is given by [51,55,60]

$$y^2 = 4(x - e_1)(x - e_2)(x - e_3). \hspace{1cm} (5.71)$$

Its periods $\omega_1$ and $\omega_2$ are given by

\textsuperscript{23}We shall recalculate this result below using different methods.

\textsuperscript{24}After Eq.(5.3) we have noticed that the free energy is defined with respect to some reference state. To be in accord with the G-L theory we can choose as the reference state the state at criticality. In this case the value of the free energy for the hexagonal lattice should be taken as zero so that the square lattice will have lower free energy typical for the lower temperature phase in accord with the G-L theory. Inequality (5.70) indicates that transformation from the higher symmetry hexagonal lattice to the lower symmetry square lattice is conformal in accord with OSP [26].

\textsuperscript{25}It is tempting to conjecture that the values of respective determinants are proportional to the packing fractions. Unfortunately, this is not the case as we shall demonstrate below.
\[ \omega_1 = \int_{e_1}^{\infty} dx \left[ (x - e_1)(x - e_2)(x + e_1 + e_2) \right]^{-\frac{1}{2}} = \frac{2K(k)}{\sqrt{e_1 - e_3}} \]  
(5.72a)

\[ \frac{\omega_2}{\sqrt{-1}} = \int_{e_2}^{e_3} dx \left[ (e_1 - x)(x - e_2)(x + e_1 + e_2) \right]^{-\frac{1}{2}} = \frac{2\sqrt{-1}K'(k)}{\sqrt{e_1 - e_3}} \]  
(5.72b)

where \( k^2 = \frac{e_2 - e_3}{e_1 - e_3} \). For the sake of comparison with the results of C-S it is useful to keep in mind that the values of integrals \( K(k) \) and \( K'(k) \) can be rewritten in the alternative (Legendre) form, e.g.

\[ K(k) = \frac{\pi}{2} \int_0^{\pi/2} \frac{d\varphi}{1 - k^2 \sin^2 \varphi} \]  
(5.73a)

and

\[ K'(k) = K(k') = \frac{\pi}{2} \int_0^{\pi/2} \frac{d\varphi}{1 - k'^2 \sin^2 \varphi} \]  
(5.73b)

where \( 0 < k < 1 \) and \( k^2 + k'^2 = 1 \). Nevertheless, in the actual calculations shown below it is sufficient to use Eqs. (5.72a), (5.72b) as defining equations for \( K(k) \) and \( K'(k) \). Using these definitions we obtain as well,

\[ \tau = \sqrt{-1} \frac{K'}{K} = \frac{\omega_2}{\omega_1} \]  
(5.74)

Naturally, we are interested only in \( \tau \) belonging to the imaginary quadratic field. In our case it is either \( i \) or \( j \). Hence, if \( \tau \) is assigned, it is sufficient to know only one period in order to determine another. By means of straightforward manipulations with elliptic functions C-S demonstrate that for \( \Delta(\tau) = |\eta(\tau)|^{24} \) the following equality holds

\[ \Delta(\tau) = \left( \frac{2K}{\pi} \right)^{12} 2^{-8} (kk')^4. \]  
(5.75a)

From here, in view of Eq. (5.70), we obtain

\[ (\Delta(\tau))^\frac{1}{8} = \left( \frac{2K}{\pi} \right)^2 2^{-\frac{8}{2}} (kk')^{\frac{2}{2}}. \]  
(5.75b)

In the case of the square lattice the associated elliptic curve is \( y^2 = x^3 - x \) [60]. This allows us to obtain the period \( \omega_1 = \int_{e_1}^{\infty} \frac{dx}{\sqrt{x^3 - x}} \). Use of substitutions
\[ x = 1/y \text{ and } 1 - y^2 = z, \text{ produces } \omega_1 = \frac{1}{\sqrt{2}} \int_0^1 dz z^{-\frac{1}{2}} \left( 1 - z \right)^{-\frac{1}{2}} = -\frac{1}{2} \frac{\Gamma(1/4)\Gamma(1/2)}{\Gamma(3/4)}. \]

The remaining calculations are straightforward and are based on definitions made in Eqs.(5.72) and next to it. This allows us to obtain \( k^2 = k'^2 = 1/2 \) and, accordingly, \( K(1/\sqrt{2}) = \frac{1}{2\sqrt{2}} \omega_1 = \frac{1}{4} \frac{1}{\sqrt{\pi}} [\Gamma(1/4)]^2 \). Collecting terms and using Eq.(5.75b) we obtain,

\[ (\Delta(\tau))^\frac{1}{2} = \frac{1}{16 \pi^4} [\Gamma(1/4)]^4 \]  

(5.76)

and, since for the square lattice \( y = 1 \), in view of Eqs.(5.70) and (5.75), we obtain, \( \text{det} \ '\Delta_g = 0.3464 \). Hence, for the square lattice, inequality Eq.(5.70) indeed holds. The OPS result, Eq.(5.70), is given for the hexagonal lattice whose dual lattice \( \Lambda^*_0 \) is triangular. Hence, the result, Eq.(5.70), represents the determinant for the hexagonal lattice, while the actual calculations were made using the reciprocal (dual) lattice, which is triangular. For the triangular lattice the associated elliptic curve is \( y^2 = x^3 - 1 \) [60]. Therefore, one finds \( k^2 = \frac{1}{2}(1 - \sqrt{-3}) \) and, because \( k'^2 = 1 - k^2 \), one finds \( kk' = 1 \), which is used in Eq.(5.75). Also, for the period \( \omega_1 \) one obtains \( \omega_1 = \int_{1}^{\infty} \frac{dx}{\sqrt{x^3 - 1}} \). Substitutions

\[ x = 1/y \text{ and } 1 - y^3 = z \text{ produce } \omega_1 = \frac{1}{3} \int_0^1 dz z^{-\frac{3}{2}} \left( 1 - z \right)^{\frac{1}{2}}. \]

Accordingly, \( K(k) = \frac{1}{6} \sqrt{\frac{3}{2}} \left( \sqrt{3} - \sqrt{-1} \right) \frac{\Gamma(1/6)\Gamma(1/2)}{\Gamma(2/3)}. \)  

(5.77)

Using Eq.(5.75b) and, taking into account that for the triangular lattice \( y = \sqrt{x^2} \), we obtain

\[ \text{det} \ '\Delta_g = \sqrt{\frac{3}{2}} \frac{1}{36 \pi^2} \frac{\sqrt{3}}{24/3} \left[ \frac{\Gamma(1/6)\Gamma(1/2)}{\Gamma(2/3)} \right]^2 = 0.357567, \]  

(5.78)

to be compared with Eq.(5.70)\(^{26}\).

The packing fraction \( q_2^\square \) for the square lattice (e.g., see Appendix c) can be obtained using simple arguments presented in Ref.[61] and is given by: \( q_2^\square = 0.7853 \). Accordingly, the ratio \( q_2^\triangle / q_2^\square = 1.154845 \) while the ratio of determinants is \( \text{det} \ '\Delta_g / \text{det} \ '\Delta_\triangle = 1.032237 \). From here we conclude that, although the inequalities between the packing fractions and the inequalities between the respective determinants are in accord with each other, one cannot claim that the values of determinants are proportional to their respective packing fractions. Also, there is no need to recalculate determinants for the hexagonal lattice because the \( \tau \) parameter is the same as for the triangular lattice [53] and so is

\(^{26}\)Apparently, there is a minor typographical error in the bound, Eq.(5.70), taken from the OPS paper [26].
its imaginary part. We can, loosely speaking, call such lattices self-dual. We shall encounter the same kind of self-duality in 3 dimensions as well. This will be discussed in the next section.

6 Ginzburg-Landau theories in dimensions 3 and higher

6.1 Designing higher dimensional CFT(s)

6.1.1 General Remarks

In the previous section we explained a delicate interrelationship between the path integrals Eq.(5.5) and (5.23). From the literature on CFT cited earlier it is known that, actually, both are used for designing of different CFT models in 2 dimensions. For instance, if one entirely ignores the effects of curvature in Eq.(5.5), then one ends up with the Gaussian-type path integral whose calculation for the flat torus is discussed in detail in Ref.[20], pages 340-343, and, by different methods, in our Section 5. By making appropriate changes to the boundary conditions (or, equivalently, by considering appropriately chosen linear combinations of modular invariants) it is possible to build partition functions for all existing CFT models. For the same purpose one can use the path integral given by Eq.(5.23), but the calculation proceeds differently as we explained in Section 5. Since in 2 dimensions conformal invariance is crucial in obtaining exact results, use of the Gaussian-type path integrals is, strictly speaking, not permissible. Fortunately, saddle point-type calculations made for the path integral, Eq.(5.23), produce the same results since the extremal metrics happens to be flat. If one does not neglect curvature effects in Eq.(5.5), one ends up with the integrand of the path integral, Eq.(5.23). This result is a consequence of Eq.(5.6) known as a conformal anomaly. If one would like to proceed in analogous fashion in dimensions higher than two one finds that there is a profound difference between calculations done in odd and even dimensions. We would like to explain this circumstance in some detail now. By doing so we shall provide a positive solution to the 2nd Problem formulated in the Introduction.

In 2 dimensions the conformal invariance of the action, Eq.(5.4), has been assured by the transformational properties of the 2 dimensional Laplacian given by Eq.(5.1). In higher dimensions, the Laplacian is transformed according to Eq.(2.4), so that even the simplest Gaussian model is not conformally invariant! This observation makes use of traditional string-theoretic methods in higher dimensions problematic. In two dimensions these are based on a two stage process. First one calculates the path integral, Eq.(5.5), exactly and, second,
one uses the result of that calculation (the conformal anomaly) as an input in another path integral, e.g. Eq.(5.23), which is obtained by integrating this input over all members of the conformal class. Since in odd dimensions there is no conformal anomaly as we shall demonstrate momentarily, such a two stage process cannot be used. Moreover, absence of a conformal anomaly in odd dimensions also affects the results of finite scaling analysis\textsuperscript{28}. The situation can be improved considerably if we do not rely on the two stage process just described. We would like to explain this fact in some detail now.

Even though the transformational properties (with respect to conformal transformations) of the Laplacian, Eq.(2.4), in dimensions higher than 2 are rather unpleasant, they can be considerably improved if, instead of the usual Laplacian, one uses the conformal (Yamabe) Laplacian $\Box_g$ defined by

$$\Box_g = \Delta_g + \hat{\alpha} R(g)$$

where $\hat{\alpha} = \alpha^{-1} - \frac{d-2}{2(d-1)}$. By construction, in 2 dimensions it becomes the usual Laplacian. In higher dimensions its transformational properties are much simpler than those for the usual Laplacian (e.g see Eq.(2.4)). Indeed, it can be shown\textsuperscript{62} that

$$\Box_{e^{2f}g} e^{-\left(\frac{d}{2}+1\right)f} \Box_g \left( e^{\left(\frac{d}{2}-1\right)f} \right).$$

(6.2a)

This result can be easily understood if we use results of Section 2. Indeed, since $e^{2f} = \varphi^{p-2}$ and $p = \frac{2d}{d-2}$, we obtain at once $e^{\left(\frac{d}{2}-1\right)f} = \varphi$, while the factor $e^{-\left(\frac{d}{2}+1\right)}$ is transformed into $\varphi^{1-p}$. From here, it is clear that Eq.(2.12) for scalar curvature can be equivalently rewritten as

$$\tilde{R}(\tilde{g}) = \alpha \varphi^{1-p}(\Delta_g \varphi + \alpha^{-1} R(g) \varphi),$$

(6.3)

where $\tilde{g} = e^{2f}g$, so that

$$\tilde{R}(\tilde{g}) = \alpha \Box_{e^{2f}g}.$$

(6.4)

In practical applications it could be more useful to consider two successive conformal transformations made with conformal factors $e^{2f}$ and $e^{2h}$. If $e^{2f} = \varphi^{p-2}$ and $e^{2h} = \psi^{p-2}$ then, we obtain,

$$\Delta_\tilde{g} \psi + \alpha^{-1} R(\tilde{g}) \psi = \varphi^{1-p}[\Delta_g (\varphi \psi) + \alpha^{-1} R(g) (\varphi \psi)].$$

(6.2b)

This result is, of course, equivalent to Eq.(6.2a).

Consider now the following path integral

$$\exp (-\mathcal{F}(g)) = \int D[\varphi] \exp \{-S_{\Box_g}(\varphi)\}$$

(6.5)

where

$$S_{\Box_g}(\varphi) = \int_M d^d x \sqrt{g} \{(\nabla_g \varphi)^2 + \alpha^{-1} R(g) \varphi^2\}$$

$$= \int_M d^d x \sqrt{g} \varphi \Box_g \varphi = \int_M d^d x \sqrt{g} \tilde{R}(\tilde{g}).$$

\textsuperscript{28}As mentioned in Section 5.2, even in 2 dimensions the results of calculations of conformal anomalies were used incorrectly in the finite size scaling analysis.
The conformal factor $\varphi^{-p}$ in Eq. (6.3) is eliminated by the corresponding factor coming from the volume factor of $\sqrt{g} = \sqrt{\exp(2f)g} = \varphi^p \sqrt{g}$, as explained after Eq. (3.5). Thus, Eq. (6.5) is the exact higher dimensional analog of the two dimensional path integral, Eq. (5.5). Thus, problems related to higher dimensional CFT are those of Riemannian (quantum) gravity [25]. In this paper we are not considering the pseudo Riemannian case associated with Einsteinian gravity.

The question arises: If the path integral, Eq. (6.5), is such an analog, is there a higher dimensional analog of Eq. (5.6)? The answer is “yes”, if the dimension of space is even and ”no” if the dimension of space is odd [62].

Because Eq. (5.6) is used heavily in finite size calculations [44], the absence of similar results in 3 dimensions should be taken into account. Earlier attempts to generalize these two dimensional results to higher dimensions [44] were made without such consideration.

### 6.1.2 Lack of conformal anomaly in odd dimensions

In view of its importance, we would like to provide a sketch of the arguments leading to the answer ”no” in dimension 3, important for developments in this paper. Clearly, the same kind of arguments will be of use in other odd dimensions. In doing so, although we follow arguments of Refs. [62,63], some of our derivations are original. We begin by assuming that there is a one parameter family of metrics: $\tilde{g}(x) = \exp(2xf)g$. Next, we define the operator $\delta_f$ via

$$\delta_f \Box_g = \frac{d}{dx} \big|_{x=0} \Box_{\exp(2xf)g}. \tag{6.7}$$

Taking into account Eq. (6.2) we obtain explicitly

$$\delta_f \Box_g = -2f \Box_g \tag{6.8}$$

and, accordingly,

$$\delta_f e^{-t\Box_g} = -t(\delta_f \Box_g)e^{-t\Box_g}. \tag{6.9}$$

These results allow us to write for the zeta function (Appendix B)

$$\delta_f \zeta_{\Box_g}(s) = \frac{1}{\Gamma(s)} \int_0^\infty dt t^{s-1} \delta_f Tr(e^{-t\Box_g})$$

$$= \frac{1}{\Gamma(s)} \int_0^\infty dt t^{s} Tr(-2f \Box_g e^{-t\Box_g})$$

$$= \frac{-2s}{\Gamma(s)} \int_0^\infty dt t^{s-1} Tr(f e^{-t\Box_g}). \tag{6.10}$$
The last line was obtained by performing integration by parts. Since for small $t$’s it is known that, provided that $\dim \ker □_g = 0$,

$$\text{Tr}(fe^{-t□_g}) \simeq \sum_{k=0}^{\infty} \left( \int_M f(x)u_k(x) dvol \right) t^{k-d/2}. \quad (6.11)$$

Using this result in Eq.(6.10) produces

$$δ_fζ □_g(0) = -\frac{2s}{Γ(s)} \left( \int_0^1 dt t^{s-1} \text{Tr}(fe^{-t□_g}) \right) + \int_1^{∞} dt t^{s-1} \text{Tr}(fe^{-t□_g}) ) \right) \] (6.12)

Since for $s \to 0^+$ we have $(1/Γ(s)) \sim s$, the second (regular) term in brackets will become zero when multiplied by the combination $\frac{2s}{Γ(s)}$, while the first term will become zero even if it might acquire a pole (when $d = 2k$). Hence, for all dimensions $d \geq 3$ we obtain $δ_fζ □_g(0) = 0$ or

$$ζ □_g(0) = ζ □_\tilde{g}(0). \quad (6.13)$$

This result can be used further now. Indeed, if we write

$$δ_f \left[ Γ(s)ζ □_g(s) \right] = Γ(s)[δ_fζ □_g(0) + sδ_fζ □_g(0) + O(s^2)] \quad (6.14)$$

and take into account Eq.(6.13) and the fact that $sΓ(s) = 1$ we obtain,

$$δ_fζ □_g(0) = δ_f \int_0^{∞} dt t^{s-1} \text{Tr}(e^{-t□_g}) \big|_{s=0} = -2s \sum_{k=0}^{∞} \frac{∫_M f u_k dvol}{s + k - d/2} + \int_1^{∞} dt t^{s-1} \text{Tr}(fe^{-t□_g}) \big|_{s=0}. \quad (6.15)$$

Applying the same arguments to Eq.(6.15) as those which were used for Eq.(6.12) we conclude that, provided that $\dim \ker □_g = 0$, in odd dimensions, $δ_fζ □_g(0) = 0$. That is

$$ζ □_g(0) = ζ □_\tilde{g}(0). \quad (6.16)$$

In view of Eq.(5.9) this leads also to

$$\det □_g = \det □_{\tilde{g}}, \quad (6.17)$$

QED.

$^{29}$For path integrals this is always assumed since zero modes of the corresponding operators are associated with some kind of translational, rotational, etc. symmetry. To eliminate the undesirable dilatational symmetry, one actually should use the Yamabe functional, Eq.(3.6), as explained in Section 3. Although this is silently assumed thus far, arguments additional to those in Section 3 will be introduced further below.
6.1.3 3d CFT path integrals

The previously obtained results can be refined further if we recall Eqs. (5.9)-(5.11). In particular, let $e^{2\phi}$ in Eq. (5.11) be rewritten as some nonnegative constant $l$. Then we obtain

$$\tilde{\zeta}_g(s) = l^s \zeta_g(s). \quad (6.18)$$

This result is consistent with Eq. (6.13) for $s = 0$. Differentiation with respect to $s$ produces

$$\zeta'_g(0) = \zeta_g(0) \ln l + \zeta'_g(0). \quad (6.19)$$

In view of Eq. (5.9), this result is equivalent to $\ln \det \Box_{\tilde{g}} = \ln \det \Box_g - \zeta_g(0) \ln l$. This result apparently contradicts Eq. (6.17), but the contradiction is only apparent in view of the earlier footnote. The situation is easily correctable if in the path integral, Eq. (6.5), we replace the action functional $S_{\Box}(\phi)$ by that of Yamabe given by Eqs. (3.2) (or (3.6)). This, by the way, allows us to fix the value of $\zeta_g(0)$ in Eq. (6.19): provided that we identify the constant $l$ with the volume $V$, the value of $\zeta_g(0) = \frac{2}{p}$. After this, the situation in the present case becomes similar to that encountered in the previous section, e.g. see Eqs. (5.12 and (5.13). Now, instead of the functional $F(\phi)$ given by Eq. (5.15), we consider the related functional given by

$$F(\phi) = \ln \det \Box_g - \zeta_g(0) \ln V = \ln \det \Box_g - \frac{2}{p} \ln V. \quad (6.20)$$

For the path integral calculations, a functional defined in such a way is not yet sufficient. To repair this deficiency we have to impose a volume constraint. That is we need to consider the path integral of the type

$$Z_Y(V) = \int D[\phi] \delta(\int_M d^4x \sqrt{g} \phi^4 - V) \exp(-S[\phi]) \quad (6.21)$$

with $S[\phi]$ given by Eq. (3.2) (or (3.6)).

Clearly, the path integral $Z_Y(V)$ (Y in honor of Yamabe) is the exact higher dimensional analog of the "stringy" path integral $S_L(A)$ given by Eq. (5.33). In view of Eq. (3.7), it also can be viewed as the path integral for pure gravity in the presence of the cosmological constant. Because of this, the standard path integral for the self interacting scalar $\phi^4$ (or LGW) field theory is obtainable now in complete analogy with Eq. (5.32), i.e.:

$$\int D[\phi] \exp\{-S_{\text{LGW}}(\phi)\} = \int_0^\infty dV e^{-bV} Z_Y(V) \quad (6.22)$$

But, since the variation of the Yamabe functional produces the same Eq. (3.3) as can be obtained with LGW functional, $S_{\text{LGW}}(\phi)$, one can develop things
differently, but surely equivalently. To this purpose, instead of the functional $S[\varphi]$ given in Eq.(3.2) we use

$$S_V[\varphi] = \frac{1}{V^2} \int_M d^d x \sqrt{g} \left\{ (\nabla_g \varphi)^2 + R(g) \varphi^2 \right\}$$

(6.23)

and replace $S[\varphi]$ in the exponent of the path integral in Eq.(6.21) by $S_V[\varphi]$ from Eq.(6.23). Then, instead of Eq.(6.22), we obtain,

$$\int D[\varphi] \exp\left\{ -S_{LGW}(\varphi) \right\} \doteq \int_0^\infty dVZ_Y(V),$$

(6.24)

where the sign $\doteq$ means "supposedly". This is so, because, at the level of saddle point calculations the left hand side and the right hand side produce the same G-L equation. Beyond the saddle point, calculations are not necessarily the same. Although we plan to discuss this issue in detail in subsequent publications, some special cases are further discussed below in this section.

It should be clear, that at the level of saddle point calculations, replacement of the functional $S[\varphi]$ in Eq.(6.21) by $F(\varphi)$ from Eq.(6.20) is completely adequate, so that the sequence of steps in analysis performed for the two dimensional case in Section 5 are transferable to higher dimensions without change. This can be summarized as follows.

Although in 3 dimensions we have the result given by Eq.(6.17), which forbids use of identities like that in Eq.(5.6), still, based on arguments just presented, the functional $F(\varphi)$ defined by Eq.(6.20) should be used in the exponent of the corresponding path integral replacing that given in Eq.(5.15) in 2 dimensions. Since by doing so one will be confronted with the same type of minimization problems as discussed earlier in Section 5, this defined functional integral is an exact 3 dimensional analog of the path integral, Eq.(5.30).

### 6.2 Completion of the work by Lifshitz in 3 dimensions

#### 6.2.1 General remarks

The results just obtained allow us to proceed with the rest of our developments in complete accord with results of Section 5. This means that our task from now on will be to provide an affirmative answer to the 1st Problem formulated in Section 1.4 following logical steps developed previously. To this purpose, it is helpful to use some results from the classical paper by Hawking on zeta function regularization of path integrals in curved spacetime [65] in view of the fact that, typically, the calculation of path integrals is done by the saddle point...
method. In the present case, the saddle point level of approximation for the path integral, Eq.(6.21), is equivalent to minimization of the functional $F(\phi)$ given by Eq.(6.20). In turn, this is equivalent to minimization of the Yamabe functional, Eq.(3.2). The following theorem (attributed to Aubin, Trudinger and Yamabe) is very helpful for this task.

For any $d$-dimensional compact manifold $M$

$$\lambda(M) \leq \lambda(S^d)$$

(6.25)

where $\lambda(S^d)$ is the Yamabe invariant for $d$-dimensional sphere.

The proof of this result can be found in Refs.[22,23].

The previously obtained inequality, Eq.(5.37), indicates that, at least in two dimensions, the same type of inequality exists for determinants. These two dimensional results for determinants cannot be readily extended to higher dimensions however since, in view of Eq.(6.17), there is no conformal anomaly in 3 dimensions (but there is in dimension 4 [66,67]). Therefore, in Refs. [66,67] extremal properties of these determinants with respect to changes in the background metric have been studied. These studies produced inequalities analogous to that given in Eq.(6.25), which take place only locally, i.e. in the vicinity of some point on $p \in M$.

The Yamabe constant $\lambda(S^d)$ has been calculated. In particular, for $S^3$ it is found to be $\lambda(S^3) = 6(2\pi^2)^{\frac{2}{d}}$, Ref.[33]. Calculation of $\lambda(M)$ for manifolds other than those diffeomorphic to $S^3$ has been found to be surprisingly difficult. Only few explicit examples are known to date [33]. Fortunately for us, they are just sufficient for our current purposes. In particular, Gromov and Lawson [68] have demonstrated that $\lambda(T^d) = 0$ for $d \geq 3$ and, moreover, the same result holds for the connected sum ($T^d \# T^d$, etc.) of $d$–dimensional tori. Aubin Ref.[22], pages 150-152, proved the following theorem

Let $M$ be $d$-dimensional $C^\infty$ compact Riemannian manifold, then there is a conformal metric whose scalar curvature is either a nonpositive constant or is everywhere positive.

From the results of Section 1 and 2 it should be clear that in the case of the G-L functional, based on physical arguments (e.g. read the discussion related to Eq.(1.20)), one should look at cases of nonpositive constant scalar curvatures. That is, one should look at the mass term $m^2$ representing constant negative scalar curvature for temperatures below criticality (and zero scalar curvature at criticality) in accord with Eq.(2.10)\[32\].

Using the above Theorem by Aubin and taking into account details of its proof we conclude that for manifolds admitting constant curvature (spherical(s), hyperbolic(h) or flat (0)) one should expect

\[31\] In $d$-dimensions this result is replaced by $\lambda(M) \leq d(d-1)\left[Vol(S^d)\right]^\frac{2}{d}$.

\[32\] In our recent work, Ref.[69], we have studied the connections between the hyperbolicity and conformal invariance. Development of such connections is linked with the study of properties of hyperbolic 3-manifolds and orbifolds. Examples of such connections can be found in the same reference in the context of AdS-CFT correspondence.
\[ \lambda_h \leq \lambda_0 \leq \lambda_s. \] (6.26)

This result is consistent with that known in two dimensions. Indeed, formally using Eq. (3.6) in two dimensions and employing the Gauss-Bonnet theorem we obtain

\[ \lambda(M) = 4\pi \chi(M). \] (6.27)

As discussed in Section 1 in this work, we are interested mainly in determining symmetries of the high temperature phase. In this phase the G-L order parameter is zero and so is the free energy at the saddle point level of approximation (e.g. read the comments after Eq. (5.31)). This implies that the Yamabe constant is zero, i.e. that \( \lambda(T_d) = 0 \). Next, using Eq. (6.16), valid only if the volume constraint is imposed as we explained above, for a given background metric \( g \) we can choose the metric \( \tilde{g} \) as flat. With such a choice of metric we can use the results of Richardson, Ref. [31], which we would like to summarize briefly now.

Let \( \tilde{g}(u) = e^{\phi(u)} g \) be 1-parameter family of metrics of fixed volume and such that \( \tilde{g}(0) = g \). This implies that \( \phi(0) = 0 \) and \( \int_M e^{\phi(u)} dV_0 = V \). In two dimensions, using results of OPS [26], especially their Eq. (1.12), it is straightforward to obtain the following result

\[ \frac{d}{du} \left( -\ln \det \left( \Delta_{\tilde{g}(u)} \right) \right) \bigg|_{u=0} = \hat{\zeta}'_g(0) = \frac{1}{12\pi} \int_M \hat{\phi} K(g) dV_g, \] (6.28)

where \( K(g) \) is the Gaussian curvature for the metric \( g \). \( \hat{\zeta}_g(0) \) and \( \hat{\phi} \) represent \( \frac{d}{du} \zeta_{g(u)}(0) \bigg|_{u=0} \) and \( \frac{d}{du} \phi(u) \bigg|_{u=0} \) respectively. Volume conservation implies

\[ \frac{d}{du} \int_M e^{\phi(u)} dV_g \bigg|_{u=0} = \int_M \hat{\phi} dV_g = 0 \] (6.29)

in accord with the earlier result, Eq. (5.17). If the Gaussian curvature \( K(g) \) is constant, then Eq. (6.28) and Eq. (6.29) produce the same result. This implies that \( \frac{d}{du} \zeta_{g(u)}(0) \bigg|_{u=0} = 0 \). That is \( g \), is the "critical" (extremal) metric. In view of Eq. (6.28), this also means that for such a metric the free energy attains its extremum. We encountered such extremal situations in the previous section when we demonstrated that the triangular and hexagonal lattices have the highest possible free energies as compared to other lattices. We shall demonstrate below that the same holds in 3 dimensions where the hcp and fcc lattices possess the highest possible free energies as compared to other lattices. To this purpose, we need to generalize the above two dimensional results to higher dimensions. Formally, this is not an easy task mainly because of the differences in properties of the Laplacian under conformal transformations in two and higher dimensions, e.g. see Eq. (2.4), causing absence of the Moser-Trudinger type of inequalities in dimensions higher than two. Nevertheless, some of the difficulties can be easily
overcome with help of the results we have already. For instance, by combining Eq.s (6.10), (6.14) and (6.15) we obtain at once

\[ \delta_f \zeta'(g)(0) = \delta_f \int_0^\infty dt t^{n-1} Tr(e^{-t\Box_g}) \bigg|_{s=0} \]

\[ = \int_0^\infty dt t^s Tr(-2f\Box_g e^{-t\Box_g}) \bigg|_{s=0} \]  

(6.30)

From here we obtain essentially the same result as the main theorem by Richardson \[31\], i.e.

\[ \zeta'(g)(0) \big|_{u=0} = 0 = \int_M dV \hat{\phi}(x) \Box_g \zeta(1, x, x). \]  

(6.31)

That is, provided that we replace \(\Box_g\) by \(\Delta_g\) and require that \(\text{locally } \zeta(1, x, x) = \text{const}\), with the heat kernel \(\zeta(s, x, x)\) given (as usual) by

\[ \zeta(s, x, x) = \sum_{k=1}^{\infty} \frac{\psi_k^2(x)}{\lambda_k^s}, \]  

(6.32)

we obtain the main result by Richardson, Ref.\[31\], e.g. see his Theorem 1 and Corollary 1.1. Here \(\psi_k(x)\) are eigenfunctions of the Laplacian (or Yamabe Laplacian respectively) corresponding to eigenvalues \(\lambda_k\) with \(0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k \leq \cdots\). In two dimensional case the condition for criticality is given by \(\hat{\zeta}'(0) = 0\) is local meaning that, provided the the volume is constrained, the constancy of the Gaussian curvature \(K(g)\) at given point of \(M\) is caused by the metric \(g\) for which \(\hat{\zeta}'(0)\) is extremal. In 3 and higher dimensions, the constancy of curvature at the point of \(M\) is replaced by constancy of \(\zeta(1, x, x)\) under the same conditions of volume conservation. This condition is necessary but is not sufficient now, since the analog of the Moser-Trudinger inequality (used to prove sufficiency in 2 dimensions) does not exists. Instead, one should study locally the second variation of \(\zeta'(g)(0)\) with respect to the underlying background metric in order to decide if such (local) extremum is maximum or minimum. Fortunately, this task was accomplished in Ref.s \[31, 64\]. In particular, Richardson \[31\] obtained the following theorem of major importance for our work:

The Euclidean metric on a cubic 3-torus is a local maximum of determinant of the Laplacian with respect to fixed-volume conformal variations of the metric.

This Theorem is proven only for the cubic 3-torus. The word ”local” means that there could be (or, there are, as we shall demonstrate) other 3-tori also providing local maxima for determinants. In fact, according to the result by Chiu \[70\], all determinants of flat 3-tori possess local maxima so that the determinant for the face centered cubic (fcc) lattice has the largest determinant. Unfortunately, his results are nonconstructive and hence, cannot be used in
physical applications. Therefore, below we provide an entirely different way to reach the same conclusions.

The second variation of the Yamabe functional was calculated by Muto \cite{71} (see also Ref.\cite{25}) with the result:

\[
\left( \frac{d^2}{dt^2} \mathcal{R}(g(t)) \right)_{t=0} = \frac{d - 2}{2} \left[ \int_M dV_g (\sigma (\nabla g \varphi)^2 - R(g) \varphi^2) \right], \tag{6.33}
\]

where the constant $\sigma = d - 1$. As in the case of quadratic actions in the flat space \cite{15,19} the second variation (with volume constrained to be equal to one) looks very much the same as the original quadratic Yamabe functional, except for the "wrong" sign in front of scalar curvature. Following Muto \cite{71} we conclude that: a) if $R(g)$ is positive, the second variation can be made positive for appropriately chosen $\varphi$; b) if $R(g)$ is negative, it is positive for the same reasons.

The positivity of second variation implies that the extremal constant curvature metric $g$ provides a locally stable minimum for $\mathcal{R}(g(t))$ (that is, using results of Section 4, the Einstein metric obtained as solution to Eq.(4.2) is stable among nearby metrics).

It is interesting to notice that calculation of higher order fluctuation corrections to the Yamabe path integral, Eq.(6.21), involves calculations on the moduli space of Einsteinian metrics, Ref.\cite{72}. This observation provides a strong link between higher dimensional LGW theory and two dimensional string inspired CFT discussed in the previous section. Naturally, Eq.(6.24) can be used to investigate to what extent the final results of conventional field-theoretic calculations, Ref.\cite{19}, may differ from more sophisticated string-theoretic calculations in the style of Ref.s \cite{27,28,72}. This task is left for further study.

For the same reasons as in the two dimensional case considered in the previous section, we are not interested in a positive constant curvature metric typical for $S^n$ even though such metric do provide a local maximum for determinants of both Laplace and Yamabe operators \cite{64}. Thus, we are left only with zero and negative curvature metrics characteristic for physical systems at and below criticality (i.e. below $T_c$). Thermodynamically, the system at criticality should possess higher free energy than the system below criticality. In our case, at criticality the free energy $F = \frac{1}{4} \ln \det \Delta_3$ (e.g. see Appendix D). Hence, the above cited theorem by Richardson guarantees that for cubic 3-tori the free energy is larger as compared to that below criticality (which corresponds to negative

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33 This "wrong" sign has significance, however. It is in accord with existing calculations of the fluctuation corrections to G-L theory in the low temperature phase, e.g. see Eqs.(1.20), (1.22). Moreover, given that the low temperature "mass" term in Eq.(1.22) is $2|a|$ and comparing the expansion, Eq.(1.21), with Eq.(6.33) we obtain (for $d = 4$) exactly the same fluctuation kernel using Eq.(6.33). This is so since in $d = 4$ the combination $\frac{d - 2}{2} R(g) = 2R(g)$ and $R(g)$ is negative in the low temperature phase. The constant $c$ in front of Laplacian is 6 in the present case while it was left unspecified in Eq.(1.22).

34 This can be easily understood if we expand $\varphi$ into Fourier series made of eigenfunctions of the Laplacian and take into account that for any closed Riemannian manifold the spectrum of the Laplacian is nonnegative and nondecreasing \cite{22}.

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curvatures) and Chiu's results [70] imply (by analogy with two dimensions) that among 3-torus lattices the fcc lattice possess the highest free energy. Below we shall provide more direct demonstration of this fact and, in addition, we shall demonstrate that the spectra of both fcc and hcp lattices possess the same value for determinants, thus implying the possibility of phase transitions between these lattices. Such transitions have been indeed observed in nature [73], but their description falls outside of the scope of this paper.

Thus, in the rest of this section we shall concentrate on explicit calculations of the toral determinants for different 3-dimensional lattices. Such calculations involve the use of the 3-dimensional version of the zeta function, Eq.(5.41). Unlike the two dimensional case considered earlier, we cannot apply directly the 1st Kronecker limit formula in order to obtain the corresponding values for determinants. We are also unable to extend the ideas of complex multiplication in order to determine the types of allowable lattices. For even dimensional spaces, where one can use the concept of the Abelian variety such a task can be accomplished. Some of these varieties possess complex multiplication and can be mapped into even dimensional tori [74]. We are not aware of similar results for odd dimensional spaces. Thus, we have calculated determinants numerically using a procedure to be discussed below. The results obtained are in complete qualitative agreement with those obtained in two dimensions.

In order to introduce our readers to issues involved in such calculation, we would like to discuss the 3 dimensional analog of the 1st Kronecker limit formula now. It was considered by Bump and Goldfield [57] and later summarized in the paper by Efrat [75].

We begin with the following observation. As it is shown by Sarnak [76], the function $E(\tau, s)$ in Eq.(5.61) is an eigenfunction of the hyperbolic two dimensional Laplacian $\Delta = -y^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right)$, i.e.

$$\Delta E(\tau, s) = s(1-s)E(\tau, s).$$

We discussed this type of eigenvalue equation extensively in our earlier work, Ref.[69]. In the same work we discussed the $d-$dimensional extension of such an eigenvalue problem. Unfortunately, these results cannot be used in the present case. As it is demonstrated by Bump [77], instead of looking for eigenfunctions of the 3 dimensional hyperbolic Laplacian, one should consider a more complicated eigenvalue problem. It is important to realize at this point that this eigenvalue problem should be of the same relevance to all exactly solvable 3 dimensional statistical mechanics models as two dimensional eigenvalue problem, Eq.(6.34), to two dimensional exactly solvable models discussed in Ref.[20]. Since we are not aware of exact solutions of non trivial 3 dimensional models, we believe that discussing the issues involved in such calculations might shed some new light on the whole problem of exact solvability in dimension 3. In addition, we would like to present these results in order to compare them against our calculations of determinants presented below.

To begin, we need to write the 3 dimensional analog of $E(\tau, s)$ (e.g. compare
with Eq.(5.61)). It is given by
\[
E(\tau, s) = \sum_{(m,n,k)=1}^{(y_1^2 y_2)^s \prod_{m,n \neq 0} \left| 1 - \exp(-y_2^2 y_2 |mz_1 - m| + 2\pi i (mz_1 + nz_4)) \right|}.
\]

(6.35)

In Appendix B we introduce the Epstein zeta function, Eq.(B.5). It can be demonstrated [57,75] that
\[
E(\tau, s) = \sum_{(m,n,k)=1}^{(y_1^2 y_2)^s \prod_{m,n \neq 0} \left| 1 - \exp(-y_2^2 y_2 |mz_1 - m| + 2\pi i (mz_1 + nz_4)) \right|}.
\]

(6.36)

where \( |A| = \det A \) and \( z_2 = x_2 + iy_2, y_1, y_2 \in \mathbb{R}_{>0}, x_1, x_2, x_3 \in \mathbb{R} \). By analogy with the two dimensional case, one can establish a very important functional equation for the combination \( E^*(\tau, s) = \pi^{\frac{3}{2}} \Gamma(\frac{3}{2}) \zeta(3s)E(\tau, s) \). Namely, \( E^*(\tau, s) = E^*(\tau, 1 - s) \) [57]. This equation allows us to extract the \( s \to 0^+ \) limit for \( E(\tau, s) \) using the associated result for \( s \to 1^+ \) obtained in Efrat’s paper [75]. For the combination \( \zeta(3s)E(\tau, s) \), which he also denotes as \( E^*(\tau, s) \), he obtains
\[
E^*(\tau, s) = \frac{2/3}{s-1} + (C - 2/3 \ln (y_1 y_2^2) - 4 \ln g(\tau)) + O(s-1),
\]

(6.37)

where
\[
g(\tau) = \exp(-\frac{y_1^{1/2} y_2^2 E^*(z_1, s)}{8\pi}) \prod_{(m,n)\neq 0} \left| 1 - \exp(-2\pi i (mz_1 + nz_4)) \right|
\]

(6.38)

with \( z_1 = x_1 + iy_1 \) and \( z_4 = x_3 - x_1 x_2 \) and \( C \) being a known constant. The limiting expression \( (s \to 0^+) \) can be found in the work by Chiu [70]. Since neither Chiu nor Efrat have provided any explicit examples of actual calculations involving formulas just presented, we have chosen another approach to the whole calculation of these limits. Before discussing our calculations we would like to mention that Bump [77] and, following him, Efrat [75] have demonstrated that \( E(\tau, s) \) defined in Eq.(6.35) is an eigenfunction of two operators \( \Delta_1 \) and \( \Delta_2 \) (whose explicit form is rather complicated [77]) so that
\[
\Delta_1 E(\tau, s) = 3s(s-1)E(\tau, s)
\]

(6.39a)

\[
\Delta_2 E(\tau, s) = -(s-1)(2s-1)E(\tau, s)
\]

(6.39b)

to be compared with Eq.(6.34).

6.2.2 Calculation of determinants: general discussion of the numerical algorithm

So far in this paper calculation of determinants has been done with the help of zeta functions, e.g. see Eq.(5.9). This method required use of the first
Kronecker limit formula in two dimensional calculations. Generalization of this result to higher dimensions was formally accomplished by Epstein at the turn of 20th century [79]. However, his results were too general to allow any practical calculations. This fact caused many attempts to improve/simplify his calculations. The result, Eq.(6.37), is one of many [70,80], etc. It can be derived directly from the 3 dimensional Epstein zeta function [75,77]. However, subsequent results by Chiu [70] stop short of actual use of Eq.(6.37) in order to produce numerical values for lattice determinants, as it is done in two dimensions. In view of this, we are going to develop another method of calculation of lattice determinants, which does not involve the use of zeta function. The reliability of this alternative method is tested against exactly known results obtained, again, with the help of some ideas from physics. In Appendix D we provide the simplest example of this type of calculation, so that readers are encouraged to read this appendix before proceeding with the rest of this subsection.

Assuming this, we need to calculate the 3 dimensional version of Eq.(5.41), i.e.

\[ Z_\tilde{g}(s) = \sum_{\lambda \in \Lambda^*} \frac{1}{4\pi^2 |l|^2} |l|^2 s. \]  

(6.40)

As in Appendix D, we disregard the constant $4\pi^2$ in the denominator and consider the following regularized sum instead

\[ S = \sum_{l^*} \frac{1}{|l^*|^2 + \kappa^2}, \]  

(6.41)

where now the summation takes place over all lattice cites of the reciprocal lattice $\Lambda^*$ due to the presence of the small parameter $\kappa^2$, which will be put to zero at the end of calculations. Evidently, as in Appendix D, we have

\[ \beta \mathcal{F} = \lim_{\kappa^2 \to 0} \frac{1}{2} \ln \frac{\det \Delta_\tilde{g}(\kappa^2)}{\det \Delta_\tilde{g}(0)} = \int_{\mathbb{R}^3} \kappa^2 \sum l^* \frac{1}{|l^*|^2 + \kappa^2}. \]  

(6.42)

Again, as in the Appendix D, to proceed, we need to evaluate somehow the sum at the r.h.s. of Eq.(6.42). To this purpose we would like to take advantage of the Poisson summation formula [81]. In the present case we obtain,

\[ \sum_{l^*} \frac{1}{|l^*|^2 + \kappa^2} = \sqrt{\frac{vol(\Lambda)}{vol(\Lambda^*)}} \sum_{l} e^{-\kappa |l|}, \]  

(6.43)

where we take into account that in 3 dimensions the summand on the l.h.s. represents the Fourier transform of the screened Coulomb (also known as the Debye-Hückel (D-H)) potential displayed as the summand on the r.h.s. The parameter $\kappa$ is known in the literature on electrolyte solutions [6,82] as the D-H inverse screening length. Treated from such perspective, our calculations are reminiscent of those for the Madelung constant in solid state physics [13,83]. Using
Eq. (6.43) in Eq. (6.42) and taking into account results of the Appendix A we obtain upon integration over $\kappa$ the following result:

$$\beta F = \lim_{\kappa \to 0} (-1)\kappa \sqrt{\text{disc}(\Lambda)} \sum_{l} \frac{\exp(-\kappa |l|)}{|l|^2}. \quad (6.44)$$

This result is still very inconvenient to use. To simplify matters further we make use of the expansion Eq. (B.9) for the theta function and take also into account Eq.s (B.5)-(B.8). This produces the following result to be used in numerical calculations:

$$\beta F = \lim_{\kappa \to 0} (-1)\kappa \sqrt{\text{disc}(\Lambda)} \sum_{n=1}^{\infty} a(n) \frac{n}{n} \exp(-\kappa \sqrt{n}). \quad (6.45)$$

As in Eq. (B.7), we have subtracted one so that the series starts with $n = 1$. The coefficients $a(n)$ have been tabulated for various lattices [52, 84]. The difficulty in evaluating such sums lies in the fact that there is only a finite number of $a(n)$’s which are available in literature. The difficulty with calculations containing finite number of terms can be seen already in evaluation of much simpler sums such as, for example,

$$S(\kappa) = \kappa \sum_{n=0}^{\infty} \exp(-\kappa n). \quad (6.46)$$

Clearly, evaluating the geometric progression and taking the limit: $\kappa \to 0^+$ produces 1 as expected but, should we keep a finite number of terms and take the same limit, we would obtain an entirely wrong result. The results can be considerably improved if we correlate the number of terms in the sum $N$ with the optimal value of $\kappa$ for such $N$. This can be achieved by minimizing the above sum with respect to $\kappa$. This leads to the following minimization equation:

$$\sum_{n=0}^{N} \exp(-\kappa^* n) = \kappa^* \sum_{n=0}^{N} n \exp(-\kappa^* n) \quad (6.47a)$$

or, equivalently,

$$\frac{1}{\kappa^*} = \langle n \rangle. \quad (6.47b)$$

The best results are obtained with still additional refinement. Since we are interested in the limit $\kappa \to 0^+$, it is convenient to look at the obtained values of $\kappa^*$ as function of $N$, i.e. we look for $\kappa^*(N)$. We expect that for $N_2 > N_1$ the optimal $\kappa^*$’s should behave as $\kappa^*(N_2) < \kappa^*(N_1)$, etc. This indeed happens. Moreover, we expect that $S(\kappa^*(N))$ behaves in a similar way, i.e. if we have successive sums including $N_1 < N_2 < N_3 < \cdots$, we expect that $|S(\kappa^*(N_1)) - S(\kappa^*(N_2))| > |S(\kappa^*(N_2)) - S(\kappa^*(N_3))| > \cdots$ so that the series is converging in the desired direction. For the sum like that given in Eq. (6.46) this is easy to check, but for the sum, Eq. (6.45), this is less obvious (although numerically we obtained exactly the same type of convergence). So, additional
arguments need to be invoked. For instance, the sum in Eq.(6.44) can be analyzed as is typically done in solid state physics. Here, one routinely replaces such sums by integrals \[13,83\]. In our case we obtain,

\[
\kappa \sum_1 \frac{\exp(-\kappa |l|)}{|l|^2} \sim \kappa \int_0^\infty dx \frac{x^2}{x^2} \exp(-\kappa x) \sim 1.
\] (6.48)

As plausible as it is, one can obtain a much better estimate based on the work by Jones and Ingham \[85\]. It is more accurate when used for the sum, Eq.(6.45). According to these authors, if one thinks about a selected atom at the lattice site chosen as the origin, then at large distances \(R\) from the origin, it is permissible to assume that the atoms are more or less homogeneously distributed on the sphere of radius \(R\). In view of this, the factor \(a(n)\) is proportional to the area of a sphere of radius \(R\) while the factor of \(n \sim R^2\). Hence, in our case the sum

\[
\tilde{S}(\kappa) = \kappa \sum_{n=1}^\infty \exp(-\kappa \sqrt{n})
\] (6.49)

provides an upper bound for the sum in Eq.(6.45). The lower bound can be estimated if we replace all \(a(n)'s\) in Eq.(6.45) by 1 thus obtaining the sum

\[
\hat{S}(\kappa) = \kappa \sum_{n=1}^\infty \frac{1}{n} \exp(-\kappa \sqrt{n}).
\] (6.50)

6.2.3 Use of designed algorithm for calculation of various lattice determinants

The convergence procedure for the sums defined above can be easily tested for any \(N\) and, indeed, it satisfies the convergence criteria just described. A numerical check provided assurance that the sum, Eq.(6.45), is indeed bounded by the above two sums for lattices we are interested in. The numerical values for coefficients \(a(n)'s\) are taken from Ref.\[84\]. Specifically, Table 7 of this reference provides 80 entries for the cubic lattice, Table 11 provides 80 entries for the fcc lattice, Table 16 provides 80 entries for the hcp lattice and Table 24 provides 80 entries for the bcc lattice. The book by Conway and Sloane (C-S), Ref. \[52\], provides the values of discriminants for lattices of unit edge length. In particular, for the bcc lattice we find: \(\sqrt{\text{disc}(\Lambda)} = 4\), and accordingly 1 for the cubic, 2 for the fcc and \(\sqrt{2}\) for the hcp lattices. In actual computations the following information was taken into account. First, both the cubic and hcp lattices are self-dual \[52\]. Second, the bcc lattice is dual to fcc \[13,52\]. This means, for instance, that one should be careful when using the relation \(\text{vol}(\Lambda)\text{vol}(\Lambda^*) = 1\) (or, as in solid state physics, Ref.\[13\], \(\text{vol}(\Lambda)\text{vol}(\Lambda^*) = (2\pi)^3\)) since, if one chooses \(\text{vol}\Lambda_{\text{bcc}} = 4\) then, one formally gets \(\text{vol}\Lambda_{\text{fcc}}^* = 1/4\) (or \((2\pi)^3/4\) as compared with 2 for fcc just presented. To resolve this "paradox" we use results from the solid state physics \[13\]. For instance, the basis vectors of the fcc lattice
are known to be: \(a_1 = \frac{a}{2}(-a_x + a_z), a_2 = \frac{a}{2}(a_y + a_z), a_3 = \frac{a}{2}(-a_x + a_y)\). From here the volume is obtained as \(V_{fcc} = a_1 \cdot (a_2 \times a_3) = \frac{a^3}{2}\). Using this result for \(a = 1\), we obtain: \(V_{fcc} = \frac{1}{V_{bcc}}\) where \(V_{bcc} = 4\) in accord with C-S. At the same time, C-S provide the value 2 for \(V_{fcc}\). As a final example, let us consider the bcc lattice. In this case we have the basis vectors \(a_1 = \frac{a}{2}(-a_x - a_y + a_z), a_2 = \frac{a}{2}(a_y + a_y + a_z), a_3 = \frac{a}{2}(-a_x - a_y - a_z)\) so that the volume is obtained as \(V_{bcc} = \frac{a^3}{2}\). From here, we obtain \(V_{bcc} = \frac{1}{V_{fcc}}\) where \(V_{fcc} = 2\) in accord with C-S. Since the hcp lattice is selfdual \([52]\), we obtain \(V_{hcp} = 1/V_{hcp} = 1/\sqrt{2}\). These examples illustrate the relationships between the (C-S) and the accepted solid state (SS) conventions. They are summarized in the Table 2 below.

Table 2

| Lattice      | Vol | Lattice      | Vol |
|--------------|-----|--------------|-----|
| bcc (C-S)    | 4   | fcc* (SS)    | 1/4 |
| fcc (C-S)    | 2   | bcc* (SS)    | 1/2 |
| Z^3 (C-S)    | 1   | Z^* (SS)     | 1   |
| hcp (C-S)    | \sqrt{2} | hcp* (SS)   | 1/\sqrt{2} |

It should be clear from this table and the examples just presented that the conventional solid state direct lattice results are dual to that given in C-S monograph \([52]\). To make sense out of our numerical results, we use the C-S results in our calculations compatible with C-S data for \(a(n)'s\). Using the numerical procedure outlined above the following results for the free energies are summarized in Table 3 below.

Table 3

| Lattice \(\Lambda^*\) | Free energy | Packing fraction |
|-----------------------|-------------|-----------------|
| hcp                   | -6.669431   | 0.74            |
| fcc                   | -6.65616    | 0.74            |
| bcc                   | -8.68137    | 0.68            |
| Z^3                   | -9.27008    | 0.52            |

These results are in qualitative agreement with those obtained earlier in two dimensions where we observed that the respective free energies are arranged in accordance with their respective packing fractions. The accuracy of our calculations is supported by the fact that we have obtained numerically practically the same free energies for the hcp and fcc lattices whose packing fractions are the same (e.g. see Appendix C). As in two dimensions, the earlier made assumption that the free energies are proportional to their respective packing fractions happens to be wrong. The obtained results provide an affirmative answer to the 1st Problem formulated in Section 1.4.

The equality of free energies between the hcp and fcc lattices has been established in recent computer simulation methods \([86]\) and apparently is of
great practical interest. Such an equality between the free energies might lead to the phase transition between these lattices and, indeed, they were observed and theoretically discussed [73].

The equality between the hcp and fcc free energies has been achieved with account of the following observation. On page 114 of C-S book, Ref.[52] it is said that: "The hcp is not itself a lattice, but may be defined as a union of a lattice L.....and the translate...". Such an opinion is not shared by solid state physicists for whom hcp is a legitimate lattice [8,13,83]. If one compares between C-S and SS definitions, then one should multiply $\sqrt{2}$ in Table 2 by a factor of 2. After such multiplication the free energies of both hcp and fcc lattices become the same. The data of Table 3 reflect this observation and are in accord with experimental results depicted in Fig.1, which we would like to discuss now.

6.2.4 6.3. A brief walk across the CuZn phase diagram.

As is mentioned in the Introduction, the CuZn phase diagram is a typical equilibrium phase diagram for a binary alloy. Many such alloys make superlattices under appropriate concentration/temperature conditions[8,87]. Apparently, this fact was a motivation for Lifshitz original work, Ref.[4]. Taking this into account, we would like to complete this section by connecting the phase diagram depicted in Fig.1 with the results summarized in Table 3.

To do so, we would like to remind our readers about how such phase diagrams are obtained in real life and what they are actually supposed to convey. Initially, a typical phase diagram, like that depicted in Fig.1, is determined experimentally by preparing an array of samples of varying composition at room temperature and then heating each to temperatures above that required for complete homogeneous melting. Upon cooling, detection of a first order transition is possible by simple calorimetric methods. Much more sophisticated methods (including calorimetric, X-ray diffraction, etc.) must be used for detection of the second order transitions. Once the phase diagram is complete, the fraction of each component in a given phase can be extracted directly from the diagram at a specified temperature $T$ and composition $C_0$.

For the sake of illustration, we begin with the simplest typical case of a two component (A and B) system existing in two phases, say $\alpha$ and $\beta$, as depicted in Fig.4. If such a system is kept under constant pressure, depending on temperature, we expect it to be either in the $\alpha$ or the $\beta$ phases or in both. It is of interest to know the fraction of a given phase in the overall system, but it is not always possible to measure this directly. Normally, only the overall composition $C_0$ is known. Although for a single-phase region on the phase diagram the composition is $C_0$, for a two-phase region, the composition of each phase is obtained by first placing a horizontal line $l$ through the point $(C_0,T)$ on the diagram. At each end, this horizontal line intersects the boundary separating the two phase region from a single phase region. The two-phase region is always bounded by two single-phase regions. Any larger diagram, like that depicted in Fig.1, is assembled of alternating fragments of this kind. The composition of a given phase is then obtained as an abscissa of the above mentioned intersection.
point. Thus, the compositions of the \( \alpha \) and \( \beta \) phases are \( C_\alpha \) and \( C_\beta \), respectively as depicted in Fig.4.

We would like to connect this information with the Landau order parameter \( \phi \). To this purpose, we introduce the following notation. Let \( l_\beta = |C_\beta - C_0| \) and \( l_\alpha = |C_0 - C_\alpha| \) so that \( l_\beta + l_\alpha = |C_\beta - C_\alpha| \equiv l \). With this notation, we let the total fraction \( w_\alpha \) of the \( \alpha \) phase be \( w_\alpha = \frac{l_\beta}{l} \) and accordingly, \( w_\beta = \frac{l_\alpha}{l} \).

By construction, \( w_\alpha + w_\beta = 1 \) so that the Landau order parameter \( \phi \) can now be defined as \( \phi = |w_\alpha - w_\beta| \). To check that such a definition makes sense, it is sufficient to notice that since at criticality \( C_\beta = C_\alpha = C_0 \), we obtain \( w_\alpha = w_\beta = 1/2 \) in accord with Section 1. Such a picture assumes existence of a well defined single critical point as discussed in Ref.[6], page 257. On the next page of this reference one finds the following statement: "Strictly speaking, there can be said to be two phases only when they exist simultaneously and in contact, that is at points lying on the equilibrium curve. It is clear that the critical point can exist only for phases such that the difference between them is purely quantitative, for example a liquid and a gas ..." Applying this statement to Fig.4, one can say that two phases (co)exist as long as \( l \neq 0 \) and the critical point corresponds exactly to the case when \( l = 0 \). Next, on the same page we read "...such phases as liquid and solid (crystal), or different crystal modifications of substance, are qualitatively different, since they have
different internal symmetry. It is clear that we can say only that a particular symmetry...element exists or does not exist; it can appear or disappear only as a whole, not gradually. In each state the body will have one symmetry or the other, and so we can always say to which of the two phases it belongs. Therefore the critical point cannot exist for such phases, and the equilibrium curve must either go to infinity or terminate by intersecting the equilibrium curves of other phases.”

The background information we have just supplied is sufficient for understanding of the CuZn phase diagram depicted in Fig. 1. We begin with the region where Zn concentrations are less than 31.9% and temperatures $T > 900^\circ C$. In this domain the horizontal (temperature) line intersects two coexistence curves so that locally the picture looks exactly the same as in Fig. 4. Under such conditions we have a phase coexistence between the CuZn liquid and the Cu Zn solid alloy, whose crystal structure $\alpha$ is that for Cu, i.e. fcc, Fig. 2a). By lowering the temperature below $900^\circ C$ and increasing the concentration of Zn we observe the phase coexistence between two solid phases $\alpha$ and $\beta$ where, according to the Table 1, the $\beta$ phase is bcc, Fig. 3a). This fact is in accord with results of Table 3 indicating that the free energy of the bcc lattice is lower than that for fcc so that such a structure can exist only at lower temperatures in accord with empirical observations discussed in the Introduction. Next, by going to still lower temperatures we obtain the $\beta'$ phase in coexistence with the $\alpha$ phase. The $\beta'$ phase is made of interpenetrating cubic lattices as depicted in Fig. 3. Such observation, again, is in accord with Table 3 (which tells us that the cubic lattice has still lower free energy than the bcc lattice). The dashed line in this range of concentrations and temperatures represents the line of the second order phase transitions in accord with quotations from Landau and Lifshitz book, Ref.[6], stated above. Exactly the same arguments are applicable to the next, $\beta + L, \beta' - \beta'$ and $(\beta + \gamma') - (\beta' + \gamma')$ portions of the phase diagram so that the dashed line (extending to concentrations just below 60% according to Ref.[6]) is still a line of second order phase transitions where the Lifshitz theory discussed in the Introduction is applicable. Notice that if for such concentrations of Zn we raise the temperature, then we would reach the curved $\beta$ triangle which looks exactly like the curved $\alpha$ triangle but is located strictly below in the temperature range. This is again in complete accord with results of Table 3. Next, notice that the $\gamma$ phase is made essentially of the body-centered cubic-type lattice and in this range of concentrations and temperatures above $700^\circ C$ the situation is analogous to that for the earlier discussed $\alpha$ phase. Below $700^\circ C$ and for concentrations above 68% the diagram exhibits apparent complications as depicted in Fig. 5.

35The lever rule depicted in Fig. 4 can be extended to cover this case by imagining the dashed line in Fig. 1 opening up a little bit initially, thus forming something like an eye, and then, finally closing up. In this case we always would get $C_\beta = C_\alpha = C_0$ and $w_\alpha = w_\beta = 1/2$ in accord with Landau and Lifshitz[6], Chr. 14. Under such conditions the order parameter $\varphi$ is either 0 or 1 in accord with above cited quotations from Ref.[6]. This causes no problems, however, in view of Eq.(1.3).
Although description of these complications lie beyond the scope of Lifshitz theory, we would like to discuss them briefly for the sake of completeness and in view of likely developments in the future.

Since the rest of the phase diagram, Fig.1 (in the range of concentrations above 80% and temperatures below 600°C), is simpler, we would like to discuss it first. Provided that we make formal substitutions of the type: $\alpha \equiv \varepsilon$ and $\beta \equiv \eta$, this portion of the diagram looks exactly the same as the previously discussed portion including $\alpha + L$, $\alpha$, $\alpha + \beta$, $\beta + L$, and $\beta$ phases. This fact should not come as a total surprise in view of the fact that Cu and Zn have different types of lattices. According to the Table 1, they are of fcc and hcp type respectively. Nevertheless, the phase diagram does contain a surprise. It comes from the apparent contradiction between the results of our Table 3 requiring the free energies of fcc and hcp type crystals to be the same and obvious asymmetry of the CuZn phase diagram with respect to temperature axis. Earlier, we noticed that, indeed, the results of computer simulations support the analytical results of our Table 3. To resolve the apparent paradox we have to take into account several additional facts. First, we have to take into account that computer simulations as well as our calculations summarized in Table 3 have been made with account of the fact that the packing fractions (Appendix C) of both hcp and fcc lattices are the same. This is obviously correct for lattices whose vertices contain identical atoms modelled by the hard spheres and arranged in such a way that these spheres touch each other. In reality, however, metals are made
of atoms whose packing behavior may or may not be well modelled by the hard spheres. In particular, the literature data on pure metals, Ref. [88], page 260, indicate that only Li, Na and Sr may form standard (Fig.2, c/a ~ 1.633) hcp lattices. Even for these metals such lattices are not the most common: for Li and Na the most common form is bcc while for Sr is fcc. In our case Cu has a stable fcc lattice while Zn has the elongated (Fig.2, c/a ~ 1.86) fcc lattice. The fact that Li and Na exist in two modifications: bcc and hcp and that, experimentally, the bcc lattice is more stable than hcp, can be used for explanation of the portion of the CuZn phase diagram where the transition from γ + L to γ + δ phase is depicted since γ is of bcc-type lattice while δ is of hcp-type. This fact is in apparent contradiction with the order of appearance of phases of lower symmetry with decreasing temperatures as discussed in the Introduction. Such an order is characteristic only for the phase transitions of the second order however (in accord with Ref.[6]) while a horizontal line between the γ + L and γ + δ phases is characteristic for transitions of the first order as demonstrated experimentally in [7]. Moreover, in comparing our results against experimental data one should keep in mind that the results of Table 3 are for the combination βF while thermodynamically we have to look at F at different temperatures. When it comes to hard spheres, it is clear that the equality β₁Ffcc = β₂Fhcp holds if β₁ = β₂ implying Ffcc = Fhcp in accord with computer simulations [86]. However, for metals such as Cu and Zn, in view of what was said about their crystal structures, it is sufficient to require β₁Ffcc(Cu) = β₂Fhcp(Zn) = N with N being some constant. This leads us to the result:

\[ F_{fcc}(Cu) = \frac{T_1}{T_2} F_{hcp}(Zn). \]

Since the data presented in Fig.1 imply that \( T_1/T_2 > 1 \) this implies that \( F_{fcc}(Cu) > F_{hcp}(Zn) \). This fact formally explains the source of the apparent temperature asymmetry of the phase diagram, Fig.1. Clearly, such an explanation is purely formal and should be replaced by quantum mechanical calculations. This task, however, is beyond the scope of this work.

In looking at the phase diagram, Fig.1 one should keep in mind how such diagram was obtained experimentally (we mentioned this already). That is, experimentally one cannot move horizontally across the diagram. This means that the respective free energies also should be compared with each other only vertically, i.e. temperature changes for the fixed composition.

Now we are ready to provide our final comments regarding Fig.5, i.e. we would like to discuss qualitatively the region of concentrations above 60% but below 80% and temperatures below 700°C. This region contains 3 triple points: two of them, P, at temperature slightly below 700°C, and the third at temperature slightly below 600°C. These triple points are called peritectics. They are interesting because in both cases we have situation when either two phases are transformed into one (γ + L ⇔ δ and δ + L ⇔ ε) or, as in the case of point E (called the eutectic), one phase δ is transformed into two phases γ and ε. Although the Landau theory can be extended, in principle, to describe (locally) situations depicted in Fig.5, attempts to describe the entire phase diagram,
Appendix A. Some facts about lattices, especially 3 dimensional.

A lattice $\Lambda$ is a free abelian group given by

$$\Lambda = \mathbb{Z}v_1 + \ldots + \mathbb{Z}v_n = \{a_1v_1 + \ldots + a_nv_n : a_i \in \mathbb{Z}, i = 1, \ldots, n\}. \quad (A.1)$$

where $v_1, \ldots, v_n$ is a basis in Euclidean space $\mathbb{E}^n$. Hence each lattice is the universal covering space for some $n$-dimensional torus $T^n$. The fundamental parallelotope $P(\Lambda)$ of the lattice $\Lambda$ is given by

$$P(\Lambda) = \{\lambda_1v_1 + \ldots + \lambda_nv_n : 0 \leq \lambda_i \leq 1, i = 1, \ldots, n\}. \quad (A.2)$$

In solid state physics the fundamental parallelotope is known as primitive cell [13]. If the crystal lattice is composed of atoms of several different types, it is required that the atoms of a given type under basic translations are sent to atoms of the same type. Hence a lattice as a whole is a union of primitive lattices (e.g. see Fig.2) so that the symmetry of the crystal lattice as a whole does not in general coincide with that for a specific primitive lattice. To distinguish between primitive lattices the concept of a volume for $P(\Lambda)$ is useful. It is defined by

$$volP(\Lambda) = |\det(v_1, \ldots, v_n)|. \quad (A.3)$$

If the vector basis is changed by the unimodular transformation, $volP(\Lambda)$ remains unchanged. In solid state physics such equivalent lattices (primitive cells) are called Bravis lattices. Since not all Bravis lattices are connected by the unimodular transformation, in 3 dimensions there are 7 different crystal systems and 14 Bravis lattices associated with them. These lattices differ from each other by the length ratios between their edges and by the angles between these edges. The Bravis lattice of any kind has symbol $P$ (for primitive) in solid state physics. The body-centered and the face-centered lattices are not primitive and are denoted by $I$ and $F$ respectively. Let $G_n(\Lambda)$ denote a (crystallographic) group of isometries of $\mathbb{E}^n$ which maps $\Lambda$ to itself. Fedorov, Schoenflies and Barlow [89] have independently established that for $n = 3$ there are 230 such groups of isometries. Bieberbach has looked at the same problem in $n$-dimensions [90]. The 3rd column of Table 1 provides information about the particular catalog number ($\#$) for the space group $G_3(\Lambda)$. Every group $G_3(\Lambda)$ is a composition of some orthogonal transformation $\alpha$ and translation $T$, i.e. $\forall g \in G_3(\Lambda)$. We should have $g = T \circ \alpha$. The orthogonal transformation is called rotation if $\det \alpha = 1$ and rotatory reflection if $\det \alpha = -1$. In general $T \circ \alpha \neq \alpha \circ T$. Clearly, $\alpha$ belongs to a point group $H_3(\Lambda)$ in the sense that for every Bravis lattice $\Lambda_B$ it is a stabilizer, i.e. $\alpha\Lambda_B = \Lambda_B$. As a group, $H_3(\Lambda)$ is finite and each of its finitely many elements is a rotation about some axis going through the (arbitrarily chosen, e.g. coinciding with one of the lattice sites) origin $O$.
by the angle which is an integer multiple of either $\pi/3$ or $\pi/2$. Let $C_n$ be a rotation which corresponds to the angle $2\pi/n$, then a rotatory reflection is given by $S_n = \sigma \circ C_n$, i.e. it is a superposition of a rotation followed by reflection $\sigma$ (rotation by the $\pi$ angle) in the plane perpendicular to the axis of rotation. In particular, the inversion $i = \sigma \circ C_2$, while the reflection itself is given by $\sigma \circ E = E$, where $E$ is the unit element of the cyclic group $C$. The simplest group after the cyclic group $C_n$ is the group $D_n$ consisting of all rotations transforming regular $n$-sided prism into itself. This group has one $n$-th order $C_n$ axis and $n$ second order axes perpendicular to it thus containing altogether $2n$ elements [9]. Next, we need the group $\hat{T}$ which consists of all rotations transforming a tetrahedron to itself. Analogously, the group $\hat{O}$ (the octahedral group) contains all rotations leaving the cube invariant. To bring all these facts to the level at which the symbols of Table 1 can be explained, we need yet a couple more complications. First, we introduce a group $\hat{C}_{nv}$. It is a symmetry group of a regular $n$-gonal pyramid containing one $n$-th order axis $C_n$ coinciding with the height of the pyramid and $n$ vertical reflection planes that pass through $C_n$ axis. Reflections in these planes are elements of $\hat{C}_{nv}$. It can be shown [9] that this group is isomorphic to $\hat{D}_n$. Second, the group $\hat{D}_{nh}$ is the symmetry group of a regular $n$-gonal prism differs from earlier introduced $\hat{D}_n$ by the presence of additional $n$ vertical reflection planes (just like $\hat{C}_{nv}$) causing extra reflections in these planes. Third, the group $\hat{T}_h$ is related to $\hat{T}$ as $S_n$ is related to $C_n$. Lastly, the group $\hat{O}_h$ is related to $\hat{O}$ in the same way as $\hat{T}_h$ to $\hat{T}$.

Since each of 230 lattice space groups is made the same way as some composition of the point group symmetry followed by translational symmetry, one can arrange these groups either in ascending or descending level of symmetry. In particular, to explain the data in Table 1 we need only lattices with point groups associated with cubic and hexagonal symmetries. The needed information can be arranged for instance in the following way

| The Bravis lattice | The point symmetry | The crystallographic symbol |
|-------------------|--------------------|---------------------------|
| Cubic (P, I)      | $O_h, T_d, O, T_h, T$ | m3m, 43m, 432, m3, 23 |
| Hexagonal (P)     | $D_{6h}, D_{3h}, C_{6v}, D_6, C_{6h}, C_{3h}, C_6$ | 6/mmm, 6m2, 6mm, 622, 6/m, 6, 6 |

Here the elements of point group symmetry are arranged from left to right in descending order (with the leftmost being the most symmetric). The crystallographic nomenclature symbols follow the ordering of point symmetry groups.

All that was said about the direct lattice can be said also about its dual. To this purpose let $x = (x_1, \ldots, x_n)$ and $y = (y_1, \ldots, y_n)$ be two vectors of $E^n$ such that their scalar product $x \cdot y = x_1y_1 + \ldots + x_ny_n$. Then, the dual (or reciprocal) lattice $\Lambda^*$ in $E^n$ is defined by

$$\Lambda^* = \{ x \in E^n : x \cdot y \in \mathbb{Z} \ \forall y \in \Lambda \}. \quad (A.4)$$

36This can be easily understood using two dimensional plane $\mathbb{R}^2$ as an example. In Section 5 we have mentioned that in case of Euclidean geometry such plane can be tesselated either by squares or by triangles. The three dimensional space can then be viewed as $\mathbb{R}^2 \times \mathbb{R}$. 

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The dual basis $v_1^*, ..., v_n^*$ is defined in such way that $v_i^* \cdot v_j = \delta_{ij}$ so that the dual lattice can also be presented as

$$\Lambda^* = Zv_1^* + ... + Zv_n^*$$  \hspace{1cm} (A.5)

In solid state physics [13] instead of the requirement $x \cdot y \in \mathbb{Z}$ in Eq.(A4) the alternative requirement $x \cdot y = 2\pi Z$ is used. It is motivated by the Fourier analysis and the Bloch theorem [11]. It can be easily demonstrated that $vol(\Lambda) \cdot vol(\Lambda^*) = 1$ while in the solid state physics one gets accordingly: $vol(\Lambda) \cdot vol(\Lambda^*) = (2\pi)^n$. A lattice $\Lambda$ is called integral if $\Lambda \subseteq \Lambda^*$. This means that $\forall x, y \in \Lambda$ one has $x \cdot y \in \mathbb{Z}$. If $v_1, ..., v_n$ is the basis of such integral lattice, then the matrix $A_{ij} = v_i \cdot v_j$ is an integral matrix. In this case the discriminant of lattice $\Lambda$ is defined by

$$disc(\Lambda) = det(A).$$  \hspace{1cm} (A.6)

But $[vol(\Lambda)]^2 = det A$ and, therefore, $[vol(\Lambda)]^2 = disc(\Lambda) = \frac{vol(\Lambda)}{vol(\Lambda^*)}$. Again this result should be amended in the case of solid state physics where we have instead $disc(\Lambda) = (2\pi)^n \frac{vol(\Lambda)}{vol(\Lambda^*)}$. From the definition of the matrix $A_{ij}$ it follows that each vector $v_i$ has its own decomposition : $v_i = (v_{i1}, ..., v_{in})$. Accordingly, for the integral lattice any vector $x$ of such a lattice is made of matrix products of the type: $x = \xi M$ with $\xi$ being a vector with integer coefficients: $\xi = (\xi_1, ..., \xi_n)$ and $M$ being a matrix: $M = M_{ij} = \{v_{ij}\}$. Let $M^T$ be a transposed matrix. Then, the earlier defined matrix $A$ (called the Gram matrix [52]) is made of $M$ and $M^T$ according to the rule:

$$A = MM^T$$  \hspace{1cm} (A.7)

Based on this definition, the norm $N(x)$ of the vector $x$ can be defined as:

$$N_A(x) = x \cdot x = \xi A \xi.$$  \hspace{1cm} (A.8)

Appendix B. Number-theoretic aspects of lattices.

Based on the information presented in the Appendix A, we consider generalization of CM, discussed in Section 5, to multidimensional lattices. To this purpose consider the following eigenvalue equation

$$\begin{align*}
x v_1 &= a_{11} v_1 + ... + a_{1n} v_n \\
x v_2 &= a_{21} v_1 + ... + a_{2n} v_n \\
&\vdots \\
x v_n &= a_{n1} v_1 + ... + a_{nn} v_n
\end{align*}$$  \hspace{1cm} (B.1)
where the matrix elements $a_{ij} \in \mathbb{Z}$. This equation can be looked upon from different directions. For instance, if we consider it as an eigenvalue equation, i.e.

$$\det(xI - A) = 0 \quad (B.2)$$

then, written explicitly, we obtain an $n$-th order algebraic equation

$$x^n + a_{n-1}x^{n-1} + ... + a_0 = 0 \quad (B.3)$$

with integer coefficients. By definition, $n$ solutions $\{x_i\}$ of such equation are algebraic integers $[91, 92]$. For instance, $\pm 1, \pm i$ (the Gaussian integers discussed in Section 5) are solutions of the equation $x^4 = 1$ while $j = \frac{1}{2}(-1 + \sqrt{-3})$ (also discussed in Section 5) is one of the solutions of the equation $x^3 = 1$. In both cases solutions are roots of unity $\zeta(n)_k = \exp(\pm ik\frac{2\pi}{n})$, $k = 0, ..., n-1$ (for $n = 4$ and 3 respectively). Solutions $\zeta(n)_k$ by construction are independent of each other and can be considered as basis vectors (instead of $v_1, ..., v_n$) in some vector space. This analogy can be made more precise. Let $x_i$ be one of the solutions of Eq.(B.3). Substitute it into Eq.(B.3) and rewrite the result as

$$-a_0 = x_i a_1 + ... + x_i^a a_n \quad (B.4)$$

(Perhaps, with $a_n = 1$). Then, the analogy with Eq.(A.1) becomes complete if we identify $(x_1, ..., x_n)$ with $(v_1, ..., v_n)$. From this analogy, the norm, the trace and the discriminant can be defined as well. There are some differences though connected with the Galois group symmetry. Since these topics are not immediately connected with results of the main text, the interested reader can look up these things in number theory literature. What is important for us, however, is the fact that only for quadratic number fields does the norm, Eq.(A.8), coincide with that defined in number theory. For higher order fields this is no longer true $[92]$. Therefore, two dimensional results presented in Section 5 are not immediately generalizable to higher dimensions.

Fortunately, there is an alternative approach bypassing the difficulty just described, which we would like to describe now. We begin with defining the Epstein zeta function $Z(A,s)$ is defined as

$$Z(A,s) = \frac{1}{2} \sum_{\xi \in \mathbb{Z}^n \setminus 0} |N_A(x)|^{-s} \quad (B.5)$$

where $N_A(x)$ is defined by Eq.(A.8).

Using the known identity

$$x^{-s} \Gamma(s, x) = \int_0^\infty dyy^{s-1}\exp(-xy) \quad (B.6)$$

we can rewrite Eq.(B.5) as

$$\Lambda(A,s) = \frac{1}{2} \int_0^\infty dyy^{s-1}(\Theta(A; y) - 1) \quad (B.7)$$
where $\Lambda(A, s) = \pi^{-s} \Gamma(s) Z(A, s)$. The theta function

$$\Theta(A; y) = \sum_{\xi \in \mathbb{Z}^n} \exp(-\pi N_A(x)y)$$  \hspace{1cm} (B.8)$$
can be represented alternatively as follows

$$\Theta(A; y) = \sum_{n=0}^{\infty} a(n) q^n,$$  \hspace{1cm} (B.9)$$
where $q = \exp(-\pi ny)$ and $a(n)$ is the number of integer solutions of the equation $N_A(x) = n$. These results are used in Section 6.

Appendix C. Exterema of the positive definite quadratic forms and the problem of closest packing of spheres.

Although methods discussed in Section 5 are capable of providing (indirectly) the information about the best (closest) possible packing of hard discs, they are not immediately generalizable to higher dimensions. Because of this, we sketch here an alternative approach. To this purpose, let us consider a positive definite quadratic form

$$f(\xi_1, \xi_2) = a_{11} \xi_1^2 + 2a_{12} \xi_1 \xi_2 + a_{22} \xi_2^2 \equiv \xi A \xi$$  \hspace{1cm} (C.1)$$
whose determinant $D = a_{11}a_{22} - a_{12}^2$. Consider now a subset $R$ of the $\xi$-plane such that $f(\xi_1, \xi_2) \leq K$ with $K$ being some positive number. Following Cassels, Ref.[93], we would like to demonstrate that, provided that, $K \geq (4D/3)^{\frac{1}{2}}$, the subset $R$ contains some point $(\xi_1, \xi_2)$, other than the origin $(0,0)$, with integer coordinates. This result can be understood based on the following chain of arguments. First, let us assume that $\inf f(u_1, u_2) = a_{11}$ with $u_1, u_2$ being integers not both equal to 0. Clearly, every quadratic form can be rewritten as

$$f(\xi_1, \xi_2) = a_{11} (\xi_1 + \frac{a_{12}}{a_{11}} \xi_2)^2 + \frac{D}{a_{11}} \xi_2^2,$$  \hspace{1cm} (C.2)$$
so that by construction, $f(u_1, u_2) \geq a_{11}$. Second, without loss of generality, we can demand that $f(u_1, 1) \geq a_{11}$. If, in addition, we assume that $\left| u_1 + \frac{a_{12}}{a_{11}} \right| \leq \frac{1}{2}$ then, we obtain the following chain of inequalities

$$a_{11} \leq f(u_1, 1) \leq \frac{a_{11}}{4} + \frac{D}{a_{11}}$$  \hspace{1cm} (C.3)$$
leading to

$$a_{11}^2 \leq \frac{4D}{3}$$  \hspace{1cm} (C.4)$$
In $d$-dimensions the proof of this fact is known as the Minkowski theorem. It plays a major role in geometric number theory and the theory of polytopes and oriented matroids.
and, finally, to
\[
\inf f(\xi_1, \xi_2) \leq \sqrt{\frac{4D}{3}}. \tag{C.5}
\]
Consider a special case of the quadratic form \( f(\xi_1, \xi_2) = m (\xi_1^2 + \xi_1 \xi_2 + \xi_2^2) \). It has determinant \( D = \frac{3m^2}{4} \). So that inequality (C.5) is reduced to the identity \( : m = m \). For any other quadratic form the sign \( \leq \) in (C.5) should be replaced by \( < \). The quadratic form \( \xi_1^2 + \xi_1 \xi_2 + \xi_2^2 \) corresponds to the hexagonal lattice \([52,94]\) whose matrix \( M \) is given by
\[
M = \begin{pmatrix}
1 & 0
\frac{1}{2} & \frac{1}{2}\sqrt{3}
\end{pmatrix}
\tag{C.6}
\]
This matrix gives rise to the matrix \( A = MM^T \). Two of such matrices are equivalent if they are connected by the unimodular transformation made of matrix \( U \) with integer entries whose determinant is one, i.e. \( A' = UAU^T \). This observation permits us to use as well the matrix \([52]\), page 43,
\[
M = \begin{pmatrix}
1 & 0
\frac{1}{2} & \frac{1}{2}\sqrt{3}
\end{pmatrix}
\tag{C.7}
\]
made of two basis vectors (ideals) as discussed in Section 5.

Consider the obtained results from a slightly different angle. Let (in any dimension)
\[
a = \inf \xi A\xi \tag{C.8}
\]
for \( \xi \in \mathbb{Z}^n \setminus \{0\} \). Let each lattice point be filled with a sphere of radius \( r \) and let the radius \( r \) be such that spheres at nearby points touch each other. Then, \( 2r \leq \sqrt{a} \). In view of Eq.(A.6), the volume of the fundamental parallelootope, \( \text{vol}(A) = \sqrt{\det A} \). If the volume \( V_n \) of the \( n \) dimensional sphere is given by \( V_n = \frac{\pi^\frac{n}{2}}{\Gamma(1 + \frac{n}{2})} r^n \equiv \sigma_n r^n \), then the most optimal packing fraction \( q_n \) can be defined as
\[
\frac{V_n}{\sqrt{\det A}} = \frac{\sigma_n}{2^n} \frac{a^\frac{n}{2}}{\sqrt{\det A}} \leq \frac{\sigma_n}{2^n} \gamma_n \equiv q_n \tag{C.9}
\]
where the constant \( \gamma_n \) is defined by the following inequality
\[
a \leq \gamma_n (\det A)^{\frac{n}{2}}. \tag{C.10}
\]
According to Eq.(C.5) we obtained in two dimensions : \( \gamma_2 = \frac{2}{\sqrt{3}} \). This produces at once \( q_2 = \frac{2}{\sqrt{3}} \cdot \frac{\pi}{2} = \frac{\pi}{\sqrt{12}} = 0.9069 \) in accord with Ref.[52], page 110. In the case of 3 dimensions, the analog of the hexagonal two dimensional lattice is the face centered cubic lattice \([52]\) (fcc) whose quadratic form is known to be
\[
f(\xi_1, \xi_2, \xi_3) = \xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_1 \xi_2 + \xi_2 \xi_3 + \xi_3 \xi_1. \tag{C.11}
\]
Calculations similar to those leading to inequality (C.5) were made originally by Gauss and can be found in Ref. [61,93,94]. They now lead to the following inequality
\[
a \leq (2 \det A)^\frac{n}{2}. \tag{C.12}
\]
thus yielding $\gamma_3 = 2^{\frac{1}{3}}$ and $q_3 = \frac{4h}{3\sqrt{3}}\sqrt{2} = \frac{\pi}{\sqrt{2}} = 0.7405$. This value is not unique, however, since the hexagonal closed packed (hcp) lattice also possesses the same value for $q_3$.

**Appendix D. Representative calculation of determinant without zeta function regularization**

The quantum harmonic oscillator is a benchmark example of quantum mechanical calculations in any course of quantum mechanics. Its eigenvalue spectrum is known to be: $E_n = \hbar\omega(n + \frac{1}{2})$, where $\omega$ is the classical frequency of the oscillator and $\hbar$ is Planck’s constant. Given this result, the partition function $Z(\beta)$ at temperature $\beta^{-1}$ is obtained in a standard way as

$$Z(\beta) = \sum_{n=0}^{\infty} \exp(-\beta E_n) = \frac{1 - \exp(-\beta\hbar\omega)}{1 - \exp(-\beta\hbar)}.$$  \hspace{2cm} (D.1)

Using this result the free energy $F$ is obtained as

$$\beta F = -\ln Z(\beta) = \beta\frac{\hbar\omega}{2} + \ln(1 - \exp(-\beta\hbar\omega)).$$  \hspace{2cm} (D.2)

We would like to reproduce this simple result now using Feynman’s path integral approach to quantum and statistical mechanics. To this purpose, following Feynman [95], we write for the free energy the following path integral ($\hbar = 1$)

$$\exp(-\beta F) = \int_{q(0)=q(\beta)} D[q(\tau)] \exp\left(-\frac{1}{2} \int_0^\beta d\tau(q^2 + \omega^2 q^2)\right)$$  \hspace{2cm} (D.3)

where $\dot{q} = \frac{d}{d\tau}q(\tau)$. Since for given boundary conditions for $q(\tau)$ we can write

$$\int_0^\beta d\tau q^2 = -\int_0^\beta d\tau q\left(\frac{d^2}{d\tau^2}\right)q$$  \hspace{2cm} (D.4)

this fact allows us to rewrite the path integral, Eq.(D.3), in the following equivalent form

$$\exp(-\beta F) = \int_{q(0)=q(1)} D[q(\tau)] \exp\left(-\frac{1}{2} \int_0^1 d\tau \int_0^1 d\tau' qA(\tau, \tau')q\right)$$  \hspace{2cm} (D.5)

where the operator $A(\tau, \tau') = \left(-\frac{d^2}{d\tau^2} + \omega^2 \beta^2\right)\delta(\tau - \tau')$. By expanding $q(\tau)$ in Fourier series with basis made of eigenfunctions of such operator the calculation
of the path integral is reduced to the calculation of the Gaussian path integrals
of the standard type
\[ \int_{-\infty}^{\infty} dx \exp(-\frac{a_n}{2} x^2) = \sqrt{\frac{2\pi}{a_n}} \]  
where \( a_n = 4\pi^2 n^2 + \omega^2 \beta^2, n = 0, \pm 1, \pm 2, \ldots \) Thus, we obtain
\[ \det A = \prod_{-\infty}^{\infty} a_n \]  
and, therefore, the free energy is formally given by
\[ \beta F = \frac{1}{2} \ln \det A + \text{const} \]  
where the actual value of \( \text{const} \) is unimportant to us since it is temperature-

independent and can be dropped since the free energy \( F \) is always defined with

respect to some reference. To calculate the free energy we follow the method

described in our earlier work [82]. To this purpose, we let \( \omega^2 \beta^2 = x^2 \) and consider
\[ \frac{d}{dx} \ln \det A = \frac{1}{x^2} + 2 \sum_{n=1}^{\infty} \frac{1}{4\pi^2 n^2 + x^2}. \] 
Then, formally we obtain
\[ \ln \det A = \int \frac{dx^2}{x^2} \left[ \frac{1}{x^2} + 2 \sum_{n=1}^{\infty} \frac{1}{4\pi^2 n^2 + x^2} \right], \]  
where the lower limit of integration will be carefully chosen. By noticing that
\[ \coth \pi x = \frac{1}{\pi x} + \frac{2x}{\pi} \sum_{n=1}^{\infty} \frac{1}{n^2 + x^2}, \] 
we obtain
\[ \frac{d}{dx^2} \ln \det A = \frac{1}{2x} \coth \frac{x}{2} \]  
and, accordingly,
\[ \frac{\ln \det A(\omega \beta)}{\det A(0)} = \int_0^{\omega \beta} dx \coth \frac{x}{2} = \omega \beta + 2 \ln(1 - \exp(-\beta \omega)) \]  
Finally, taking into account Eq.(D.8) we obtain \( \hbar = 1 \)
\[ \beta F = \frac{\omega \beta}{2} + \ln(1 - \exp(-\beta \omega)) \]  
in accord with Eq.(D.2).
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