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APPLICATION OF GEOMETROTHERMODYNAMICS TO THE TWO-DIMENSIONAL SYSTEMS: IDEAL BOSE-GAS AND SYSTEM WITH STRONG INTERACTION

Abstract. In the framework of the method of geometrothermodynamics, in present work, we studied the properties of equilibrium manifolds of the following thermodynamic systems: a two-dimensional Bose gas, a Berezinsky-Kosterlitz-Thouless system. The results are invariant under the Legendre transformations, i.e. independent of the choice of thermodynamic potential. For the systems under consideration, the corresponding metrics and scalar curvatures are calculated, and their properties are also described. Research of two-dimensional quantum thermodynamic systems is becoming more urgent. It is sufficiently to mention that such systems are related to, for example, topological insulators, graphene, systems with quantum Hall effect, etc. Two-dimensional quantum systems may have a statistical distribution different from distributions of Fermi-Dirac and Bose-Einstein. Geometric approaches in research of these thermodynamic systems certainly open the new perspective.

In this paper the thermodynamic properties of two-dimensional Bose-Gas and Berezinsky-Kosterlitz-Thouless system have been studied with the help of geometrothermodynamics. The main objective was to reproduce the Bose-Einstein condensation for the first system and find possible new phase transitions for the second.

In order to study the above mentioned thermodynamic systems, we have consequently calculated the covariant metric tensors of corresponding equilibrium manifolds and their determinants, then counter-variant metric tensors, Christoffel symbols, curvature tensors and corresponding scalar curvatures. Using the thermodynamic potential, we obtained (using the Matlab system) the corresponding geometric values in a wide range of temperature and area.

Explicit formulas were also obtained for each geometric quantity but due to their bulkiness we do not present them in this paper. Examples of calculated scalar curvatures for a certain range of parameters T and S are shown in the figures. The figures also show that despite the significantly different behavior of the curvatures depending on the parameters T and S, both metrics lead to the same General result regarding the location of singularities for the corresponding curvatures.

Next, we used geometric thermodynamics for the system of the Berezinsky-Kosterlitz-Thoules. This is a two-dimensional system of Bose particles with a strong interaction (strong in the sense that topological defects - point vortices-contribute to the thermodynamics of the system) with a complex, not fully studied system of phase transitions. An ideal two-dimensional Bose gas with a finite number of particles and a Berezinsky-Kosterlitz-Thoules system are considered. As thermodynamic potentials for these thermodynamic systems, the chemical potential depending on temperature and area and the Free energy depending on the temperature and size of the system were taken, respectively. The paper also presents 3-dimensional drawings that clearly show at which values of thermodynamic variables scalar curvatures tend to infinity or to zero, which indicates possible phase transitions and possible compensation of interactions by quantum effects, respectively. It is shown that both variants of metrics for an ideal two-dimensional Bose gas lead to the same arrangement of lines, where scalar curvatures become singular. This arrangement of lines is consistent with the region where the phase transition occurs - Bose condensation in a two-dimensional Bose gas. It is also shown that for large values of temperature and area parameters, the curvature is close to zero and this corresponds to a classical ideal two-dimensional gas. When considering the Berezinsky-Kosterlitz-taules system, possible new phase transitions were discovered by the method of geometric thermodynamics. The metric calculation leads to a possible phase transition located below the Berezinsky-Kosterlitz-Taules transition, and the calculation leads to a possible phase transition located above.

Keywords: geometrothermodynamics, Legendre transformations, metric tensor, scalar curvature, two-dimensional Bose gas, Berezinsky-Kosterlitz-Thouless system.

1. Introduction. Interactions in thermodynamic systems in geometrothermodynamics (GTD) developed by H. Quevedo (described in detail by him and his co-authors, for example, in papers [1-8]) are determined using the scalar curvature of equilibrium manifolds. This curvature, in turn, is invariant relatively to Legendre transformations. In thermodynamics, the physical properties of the system also do not depend on the choice of thermodynamic potentials using which this system is described. Transition from one set of thermodynamic potentials to another is carried out with the help of Legendre transformations, and in this sense the thermodynamics is invariant relatively to Legendre transformations. In GTD, for example, as it is shown in [1], the ideal gas, which particles do not interact with each other, corresponds to manifold with zero curvature. In the case of interacting systems with nontrivial structure of phase transitions, the curvature, as shown in [2-5], reproduces the behavior of the system near the points where phase transitions occur. So, for example, near the phase transitions in gases of Van der Waals, Bose - Einstein, etc., the scalar curvature of the corresponding equilibrium manifolds tends to infinity, i.e. becomes singular. This circumstance can be used for searching unknown phase transitions in insufficiently studied thermodynamic systems. Research of two-dimensional quantum thermodynamic systems is becoming more urgent. It is sufficiently to mention that such systems are related to, for example, topological insulators, graphene, systems with quantum Hall effect, etc. Two-dimensional quantum systems may have a statistical distribution different from distributions of Fermi-Dirac and Bose-Einstein. Geometric approaches in research of these thermodynamic systems certainly open the new perspectives. In this paper the thermodynamic properties of two-dimensional Bose-Gas and Berezinsky-Kosterlitz-Thouless (BKT) system have been studied with the help of GTD. The main objective was to reproduce the Bose-Einstein condensation for the first system and find possible new phase transitions for the second.

2. Formalism of GTD method. In order to study the above mentioned thermodynamic systems, we have consequently calculated the covariant metric tensors of corresponding equilibrium manifolds and their determinants, then counter-variant metric tensors, Christoffel symbols, curvature tensors and corresponding scalar curvatures.

For calculating metrics and corresponding metric tensors we used the following formulas [1]:

$$dl^2 = E_a \frac{\partial\Phi}{\partial E^a}\delta_{ab}\frac{\partial^2\Phi}{\partial E^b\partial E^c}dE^a E^c \tag{1}$$

$$dl^2 = E_a \frac{\partial\Phi}{\partial E^a}\eta_{ab}\frac{\partial^2\Phi}{\partial E^b\partial E^c}dE^a E^c \tag{2}$$

where l^2 - square of thermodynamic length, $\Phi \equiv \Phi(E^a)$ – thermodynamic potential, which obviously depends on other thermodynamic potentials - E^a (a = 1,….,n), n – number of thermodynamic potentials, from which Φ depends $\delta_{a,b} = diag(1,1,\ldots,1)$ and $\eta_{a,b} = diag(1,-1,\ldots,-1)$. Both relations (1) and (2) are invariant with respect to Legendre transformations [1].

The expression for the curvature tensor has the general form:

$$R_{abcd} = \frac{1}{2}\left(\frac{\partial^2 g_{ad}}{\partial E^b\partial E^c} + \frac{\partial^2 g_{bc}}{\partial E^a\partial E^d} - \frac{\partial^2 g_{ac}}{\partial E^b\partial E^d} - \frac{\partial^2 g_{bd}}{\partial E^a\partial E^c}\right) + g_{np}\left(\Gamma^n_{bc}\Gamma^p_{ad} - \Gamma^n_{bd}\Gamma^p_{ac}\right) \tag{3}$$

where $g^{nm}(g_{ad})$ – metric tensor, $\Gamma^n_{bc} = \frac{1}{2}g^{nm}\left(\frac{\partial g_{mb}}{\partial E^c} + \frac{\partial g_{mc}}{\partial E^b} - \frac{\partial g_{bc}}{\partial E^m}\right)$ – Christoffel symbols. Further, the scalar curvature is calculated by formula: $R = g^{ac}g^{bd}R_{abcd}$.

Since in the future we deal with systems which depend only on two thermodynamic potentials, the expression for scalar curvature is simplified to:

$$R = \frac{2P_{1212}}{\det(g)}, \tag{4}$$

where det(g) – determinant of two-dimensional metric tensor.

3. Two-dimensional ideal Bose gas. First consider the well-known system - two-dimensional ideal Bose-gas particles with mass *m*. As a thermodynamic potential we take the chemical potential μ, which depends on temperature T and area S (two-dimensional volume) with a fixed number of particles N (see for example [9]):

$$\mu(T,S) = T\ln\left(1 - e^{-\frac{2\pi\hbar^2 N}{SmT}}\right) \tag{5}$$

To simplify the formula, let's assume a constant $\frac{2\pi\hbar^2 N}{m}$ is equal to one and rewrite the expression (5) in the form:

$$\mu(T,S) = T\ln\left(1 - e^{-\frac{1}{ST}}\right) \tag{6}$$

Figure 1 shows a graph (6) for certain range of parameters T and S. Using (1 - 4) and thermodynamic potential (6) we have obtained (using the Matlab system) corresponding geometric values in a wide range of temperature and area. For each geometric value we have also obtained explicit formulas, but due to their extensionality we do not show them in this paper. Examples of calculated scalar curvatures for certain range of parameters T and S are shown in Figures 2a and 2b for metrics (1) and (2) respectively.

From calculations and figure 2a and (2b) it can be seen, that curvature tends to plus (minus) infinities when approaching zero of temperature at finite value of parameter of the area, that is just corresponds to Bose condensation for two-dimensional Bose-gas (see for example [10]). Also from these calculations and figure 2a and (2b) it is seen, that the curvature tends to plus (minus) infinities when approaching infinity of density at finite value of temperature. At large values of parameters T and S the curvatures are close to zero and it corresponds to classical ideal gas.

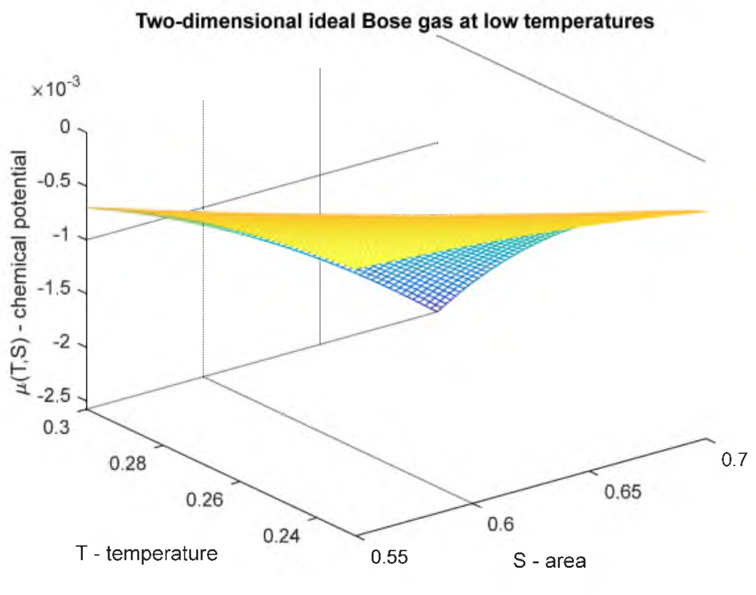
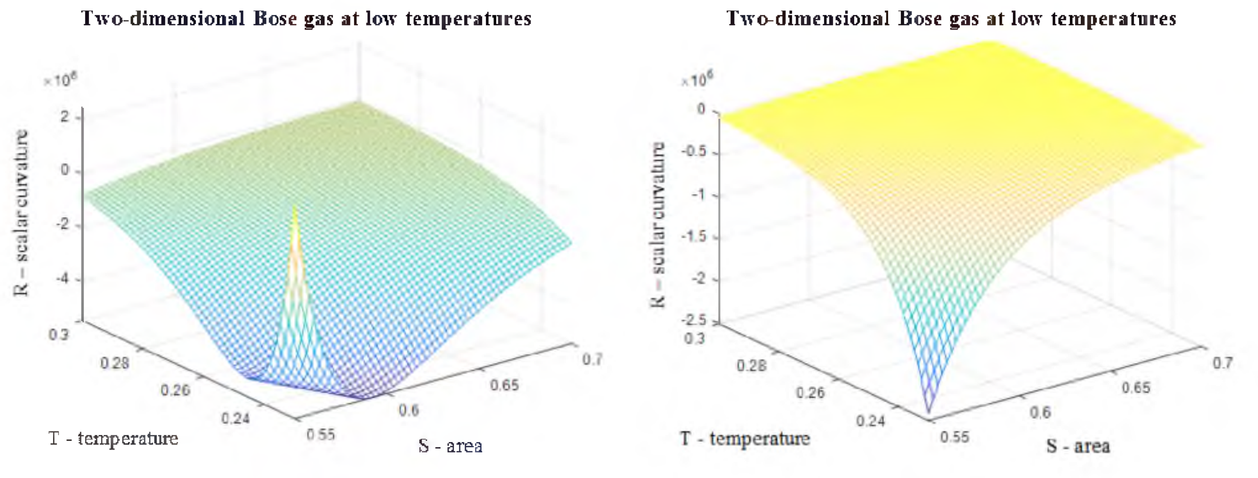


Figure 1: Chemical potential (6) depending on the temperature and area of two-dimensional ideal Bose-gas at low temperatures [9]



A b

Figure 2 - Dependence of scalar curvature on temperature and area: a) metrics calculated using formula (1), b) metrics calculated using formula (2).

Figures 2a and 2b also show that despite the significantly different behavior of the curvatures depending on the T and S parameters, both metrics (1) and (2) lead to one common result related to the location of singularities for the corresponding curvatures.

4. BKT system. Then we applied GTD to BKT system (see for example [11-15]). This is a two-dimensional Bose system of particles with strong interaction (strong in the sense that the contribution to the thermodynamics of the system is made by topological defects - point vortices) with a complicated, not fully understood system of phase transitions [16-20]. Consider free energy as a thermodynamic potential [20]:

$$F(T,L)=(J\pi-2k_BT)\ln\left(\frac{L}{a}\right) \tag{7}$$

where T – temperature, L – system size, a – vortices size, k_B - Boltzmann constant, J – certain constant. Formula (7) makes sense at $L > a$, and near the BKT transition at $T=T_c=\frac{J\pi}{2k_B}$ when the appearance of a free vortex becomes energetically favorable. At lower temperatures in the system there is a vortex - anti vortex bound pair and the phase transition is interpreted as a process of dissociation of this pair.

To simplify the following calculations, we assume $J\pi=k_B=a=1$. Then

$$F(T,L)=(1-2T)\ln(L) \tag{8}$$

Figure 3 shows the graph (8) for certain range of parameters T and L. Applying the formula (1) to expression for metrics (8) we obtain the metric tensor:

$$g(T,L)=\begin{bmatrix} 0 & \frac{2(T+T\ln(L)-0.5)}{L} \\ \frac{2(T+T\ln(L)-0.5)}{L} & -\frac{(2T-1)^2}{L^2} \end{bmatrix} \tag{9}$$

Determinat of this tensor:

$$\det(g)=-\frac{4(T+T\ln(L)-0.5)^2}{L^2} \tag{10}$$

and the scalar curvature (4):

$$R=\frac{L^2\left(\frac{4(\ln(L)+1)}{L^2}-\frac{12}{L^2}+\frac{(\ln(L)+1)(\frac{8T-4}{L^2}-\frac{T+T\ln(L)-0.5}{L^2}+\frac{T}{L^2})}{4(T+T\ln(L)-0.5)}\right)}{4(T+T\ln(L)-0.5)^2} \quad (11)$$

Applying the formula for the metrics (2) to the expression (6), we obtain:

$$g_1(T,L)=\begin{bmatrix} 0 & \frac{2(T\ln(L)-T+0.5)}{L} \\ \frac{2(T\ln(L)-T+0.5)}{L} & \frac{(2T-1)^2}{L^2} \end{bmatrix} \quad (12)$$

Determinant of this tensor:

$$\det(g_1)=-\frac{4(T\ln(L)-T+0.5)^2}{L^2} \quad (13)$$

And scalar curvature:

$$R_1=\frac{L^2\left(\frac{4(\ln(L)-1)}{L^2}+\frac{4}{L^2}-\frac{(\ln(L)-1)(\frac{8T-4}{L^2}-\frac{T-T\ln(L)-0.5}{L^2}-\frac{T}{L^2})}{4(T+T\ln(L)-0.5)}\right)}{4(T\ln(L)-T+0.5)^2} \quad (14)$$

Examples of calculated scalar curvatures for a certain range of parameters T and L are shown in the figures 4a and 4b for the metrics (1) and (2), respectively.

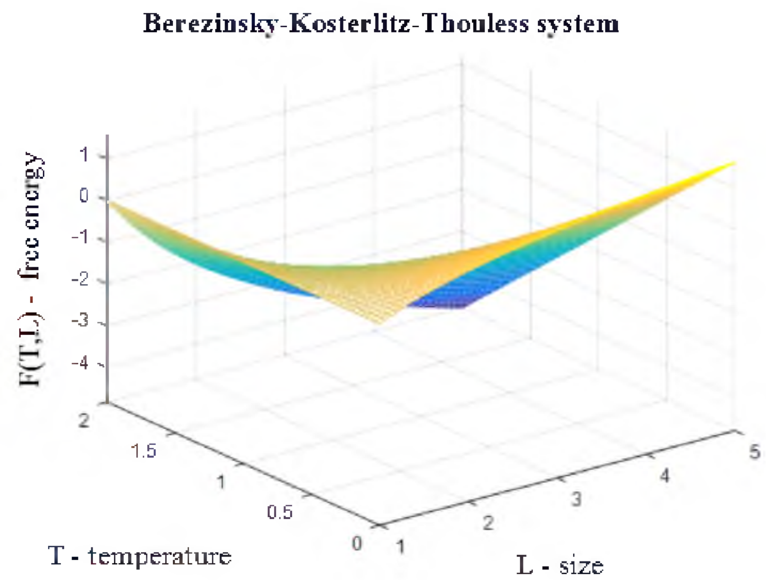


Figure 3 - Free energy (8) depending on temperature and system size [20]

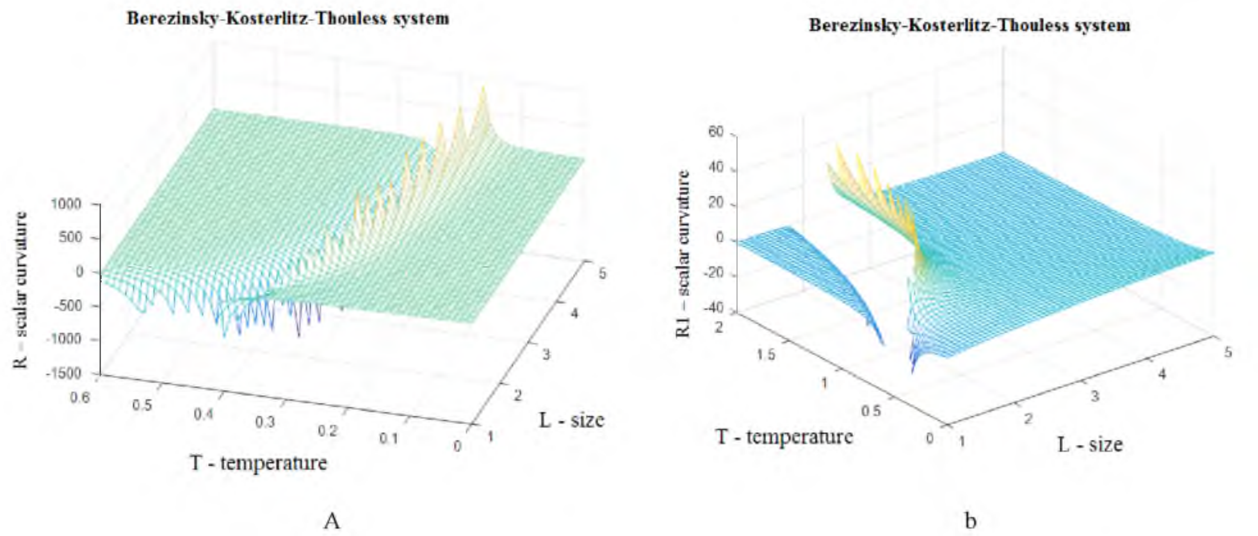


Figure 4 - Dependence of the scalar curvature on temperature and size of the system:
a) metrics calculated by formula (1), b) metrics calculated by formula (2)

Formulas (11) and (14), as well as Figures 4a and 4b show that the scalar curvatures for metrics (1) and (2) become singular at $T_1(L) = \frac{1}{2(1+\ln(L))}$ and $T_2(L) = \frac{1}{2(1-\ln(L))}$ respectively. At these values of T and L parameters, GTD predicts possible phase transitions. Moreover, if using the metrics (1), then the phase transition is located below the BKT transition (in given units $T_c = \frac{1}{2}$), and if using (2), then above. At larger values of parameter T the curvatures, and thus the intensity of the interaction between the particles of the system (both for metrics (1) and for (2)) are close to zero.

5. Conclusion. Using GTD method in this work, the metric tensors and scalar curvatures are calculated for equilibrium manifolds of two-dimensional quantum systems.

The ideal two-dimensional Bose-gas with a finite number of particles and BKT system are considered. Chemical potential depending on temperature and area and the free energy depending on temperature and size of the system were taken as thermodynamic potentials for these thermodynamic systems, respectively.

The paper also presents 3-dimensional figures which clearly show at which values of thermodynamic variables the scalar curvatures tend to infinity or to zero that indicates possible phase transitions and possible compensation of interactions by quantum effects.

It is shown that both versions of metrics (1) and (2) for an ideal two-dimensional Bose-gas lead to the same location of the lines where the scalar curvatures become singular. This location of the lines consistents with the region in which the phase transition occurs (the Bose condensation in the two-dimensional ideal Bose gas). It is also shown that for large values of the temperature and area the curvatures are close to zero and this corresponds to the classical ideal two-dimensional gas.

When considering BKT system using GTD method, possible new phase transitions (calculations based on metrics (1) and (2)) have been found. Calculation by metrics (1) leads to a possible phase transition located below the BKT transition, while calculation by metrics (2) leads to a possible phase transition located above. For large values of the temperature the curvatures, and hence the interactions between particles of the system (both for metric (1) and for (2)) are small.

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ГЕОМЕТРОТЕРМОДИНАМИКАНЫ ЕКІӨЛШЕМДІ ЖҮЙЕГЕ ҚОЛДАНУ: ИДЕАЛДЫ БОЗЕ ГАЗ ЖӘНЕ КҮШТІ ӨЗАРА ӘСЕРЛЕСУ ЖҮЙЕСІ

Аннотация. Жұмыста Березин-Костерлиц-Таулес жүйесі мен екіөлшемді идеалды Бозе-газ термодинамикалық жүйесі бойынша тепе-теңдіктің көптүрлілік қасиеті геометротермодинамика әдісі арқылы зерттелді. Термодинамикалық потенциалды есепке алмай Лежандр түрлендіруіне қатысты инвариантты нәтижелер алынды. Қарастырып отырган жүйелерге сәйкес өлшемдер мен скалярлық қисықтық есептелді және қасиеттері сипатталды.

Екіөлшемді кванттық термодинамикалық жүйелерді зерттеу қазіргі кезде өзекті саналады. Мұндай жүйелерге мысалы, топологиялық оқшаулагыш, графен, Холлдың кванттық эффектісі бар жүйелер және т.б. жүйелер жатады. Бозе-Эйнштейн және Ферми Дирак үлестірулерінен өзгеше екіөлшемді кванттық жүйеде статистикалық үлестіру болуы мүмкін. Осы термодинамикалық жүйелерді геометротермодинамика әдісі арқылы зерттеу барысында жаңа нәтижелер алынды.

Зерттеу барысында геометротермодинамиканы қолдана отырып, екіөлшемді идеалды Бозе газының және Березин-Костерлиц-Таулес жүйесінің термодинамикалық қасиеттерін қарастырдық. Зерттеу барысында негізгі мақсатымыз – бірінші кезеңге қатысты Бозе-Эйнштейн конденсациясын көбейту және екінші кезеңге сәйкес ықтимал жаңа фазалық ауысуды іздестіру. Жогарыда аталган термодинамикалық жүйелерді зерттеу үшін сәйкес тепе-теңдіктің көптүрлілігіне қатысты ковариантты метрикалық тензорды, детерминанттарды, Кристофел символын, қисықтық тензоры және сәйкес скалярлық қисықтықты есептедік.

Термодинамикалық потенциалды пайдаланып, температура мен ауданның кең аумагына сәйкес геометриялық шамаларды Matlab жүйесін қолдана отырып қарастырдық. Әрбір геометриялық шамалар үшін нақты формулалар алынды. T және S параметрлерінің белгілі бір диапазонына есептелген скалярлық қисықтардың мысалы суретте көрсетілді. Суреттен T және S параметрлеріне байланысты қисықтардың әртүрлі болуына қарамастан екі метрикаға сәйкес қисықтарга арналған сингулярлардың орналасуына қатысты жалпы ортақ нәтиже беретінін көруге болады.

Арықарай Березин-Костерлиц-Таулес жүйесіне геометротермодинамика әдісін қолдандық. Бұл екіөлшемді жүйе Бозе жүйесіне қатысты күшті әрекеттесетін бөлшектерді қарастырады. Осы жүйедегі фазалық ауысулар толық зерттелмеген. Сондықтан бұл жерде бөлшектердің соңгы саны және БКТ жүйесі бар идеалды екіөлшемді Бозе – газ қарастырылган. Термодинамикалық жүйенің термодинамикалық потенциалы болгандықтан, сәйкесінше жүйенің өлшемі және температураға тәуелділігі, еркіндік энергиясы, аудан мен температурага тәуелділігі, химиялық потенциалы есептелді.

Сондай-ақ үшөлшемді сызбалар берілген, олар термодинамикалық айнымалылардың қандай шамалары шексіздікке немесе нөлге ұмтылатындыгын көрсетеді, бұл фазалардың ауысуы мен кванттық әсер арқылы өзара әрекеттесудің ықтималдыгын көрсетеді. Идеалды екіөлшемді Бозе газына арналган метриканың екі нұсқасы да скалярық қисықтың сингуляр болып бір сызықтың бойында орналасқаны көрсетілген. Бұл орналасқан сызықтар екіөлшемді Бозе газындагы фазалық ауысулар жүретін аймаққа сәйкес келеді. Сонымен қатар, температура мен ауданның үлкен мәні нөлге ұмтылатындықтан классикалық идеалды екіөлшемді газга сәйкес келеді.

Березин-Костерлиц Таулес жүйесіне геометротермодинамика әдісін қолдану барысында жаңа фазалық ауысу анықталды. Метрика бойынша есептегенде ықтимал фазалық ауысу Березин-Костерлиц-Таулес ауысуынан төмен орналасқан фазалық көшуге, ал есептеу барысында жогарыда орналасқан ықтимал фазалық ауысуга әкеледі.

Түйін сөздер: геометротермодинамика, Лежандр түрлендіруі, метрикалық тензор, скалярлық қисық, екіөлшемді Бозе-газ, Березин-Костерлиц-Таулес жүйесі.

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ПРИМЕНЕНИЕ ГЕОМЕТРОТЕРМОДИНАМИКИ К ДВУМЕРНЫМ СИСТЕМАМ: ИДЕАЛЬНОМУ БОЗЕ-ГАЗУ И СИСТЕМЕ С СИЛЬНЫМ ВЗАИМОДЕЙСТВИЕМ

Аннотация. Методом геометротермодинамики в настоящей работе исследованы свойства равновесных многообразий следующих термодинамических систем: двумерного идеального Бозе-газа и системы Березинского-Костерлица-Таулеса. Получены результаты, инвариантные относительно преобразований Лежандра, т.е. независимые от выбора термодинамического потенциала. Для рассматриваемых систем рассчитаны соответствующие метрики и скалярные кривизны, а также описаны их свойства.

Изучение двумерных квантовых термодинамических систем в настоящее время является актуальным. Достаточно упомянуть, что к таким системам относятся, например, топологические изоляторы, графен, системы с квантовым эффектом Холла и т.д. Двумерные квантовые системы могут иметь статистическое распределение, отличное от распределений Ферми-Дирака и Бозе-Эйнштейна. Геометрические подходы в изучении этих термодинамических систем, безусловно, открывают новые перспективы.

В настоящей работе с помощью геометротермодинамики было проведено исследование термодинамических свойств идеального двумерного Бозе-газа и системы Березинского-Костерлица-Таулеса. Основной целью было воспроизведение конденсации Бозе-Эйнштейна для первой системы и поиск возможных новых фазовых переходов для второй.

Для изучения вышеназванных термодинамических систем мы вычисляли последовательно ковариантные метрические тензоры соответствующих равновесных многообразий, их детерминанты, далее контравариантные метрические тензоры, символы Кристофеля, тензоры кривизны и соответствующие скалярные кривизны.

Используя термодинамический потенциал, нами были получены (с помощью системы Matlab) соответствующие геометрические величины в широком диапазоне температуры и площади. Для каждой геометрической величины также были получены явные формулы, но ввиду громоздкости в настоящей работе мы их не приводим. Примеры вычисленных скалярных кривизн для некоторого диапазона параметров T и S показаны на рисунках. Из рисунков также видно, что несмотря на существенно различное поведение кривизн в зависимости от параметров T и S обе метрики приводят к одному общему результату относительно расположения сингулярностей для соответствующих кривизн.

Далее мы применили геометротермодинамики для системы Березинского-Костерлица-Таулеса. Это двумерная система Бозе – частиц с сильным взаимодействием (сильным в том смысле что вклад в термодинамику системы вносят топологические дефекты - точечные вихри) со сложной, до конца не изученой системой фазовых переходов. Рассмотрены идеальный двумерный Бозе-газ с конечным числом частиц и система БКТ. В качестве термодинамических потенциалов для этих термодинамических систем брались, соответственно, химический потенциал, зависящий от температуры и площади и свободная энергия, зависящая от температуры и размера системы.

В работе также приведены 3-мерные рисунки, на которых хорошо видно, при каких значениях термодинамических переменных скалярные кривизны стремятся к бесконечности или к нулю, что указывает на возможные фазовые переходы и на возможную компенсацию взаимодействий квантовыми эффектами соответственно.

Показано, что оба варианта метрик для идеального двумерного Бозе-газа приводят к одному и тому же расположению линий, где скалярные кривизны становятся сингулярными. Это расположение линий согласуется с областью, в которой происходит фазовый переход - Бозе конденсация в двумерном Бозе-газе. Также показано, что при больших значениях параметров температуры и площади кривизны близки к нулю и это соответствует классическому идеальному двумерному газу.

При рассмотрении системы Березинского-Костерлица-Таулеса методом геометротермодинамики были обнаружены возможные новые фазовые переходы. Расчет по метрике приводит к возможному фазовому переходу расположенному ниже перехода Березинского-Костерлица-Таулеса, а расчет приводит к возможному фазовому переходу расположенному выше.

Ключевые слова: геометротермодинамика, преобразования Лежандра, метрический тензор, скалярная кривизна, двумерный Бозе-газ, система Березинского-Костерлица-Таулеса.

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