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SIMPLE INEQUALITY FOR THE FREE ENERGY OF DISORDERED SYSTEMS

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A great variety of excitations in disordered crystals may be described with sufficient accuracy in terms of Hamiltonians which are **simply** the quadratic forms in Bose or Fermi operators with random coefficients. To this class there belong electron systems, phonons, excitons and magnons as well as some one-dimensional magnetic systems such as random XY chain *).

In spite of apparent simplicity of these Hamiltonians, the spectral problems caused by randomness are by no means trivial and were intensively investigated by many authors (see, e.g., a comprehensive review [2]).

In this note we give some estimation for the free energy of these systems. The proof is based on the concavity property of the function $A \longrightarrow \ln\det A$

$$\sum c_i \ln\det A^{(i)} \leq \ln\det \sum c_i A^{(i)}\,; \quad c_i \geq 0\,,\ \sum c_i = 1, \qquad (1)$$

where $A^{(i)}$ are the positive definite $N \times N$ matrices. The inequality (1) follows directly from the Minkowski inequality for determinants [3] .

<u>Lemma</u>

Let us consider the class of Hamiltonians

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*) With spin Hamiltonian unitarily equivalent (Jordan-Wigner transformation) to some quadratic form in Fermi operators [1] .

$$H_N(S^{(i)},R^{(i)})=\sum S^{(i)}_{\alpha\beta}a^+_\alpha a_\beta + \frac{1}{2}\sum(R^{(i)}_{\alpha\beta}a^+_\alpha a^+_\beta + h.c.), \quad (\alpha,\beta=1,\dots,N), \qquad (2)$$

where a^+_α, a_α are Bose or Fermi operators, and $S^{(i)}$, $R^{(i)}$ are real random matrices with a given probability distribution and with obvious symmetry properties

$$S^{(i)}_{\alpha\beta}=S^{(i)}_{\beta\alpha} \qquad R_{\alpha\beta}=\begin{cases} R_{\beta\alpha} & \text{(Bose case)} \\ -R_{\beta\alpha} & \text{(Fermi case)}\end{cases} \qquad (3)$$

Then if we introduce the matrix

$$D^{(i)2}:=(S^{(i)}+R^{(i)})(S^{(i)}-R^{(i)}) \qquad (4)$$

assume its positive definiteness, and define the mean free energy F_H of the system as

$$F_N:=-\beta^{-1}\left(\ln Tr\, exp(-\beta H_N(S^{(i)},R^{(i)}))\right)_{Av}, \quad (\beta:=\frac{1}{\kappa T}) \qquad (5)$$

the following inequalities

$$F_N \leqslant -\frac{1}{2}Tr(S^{(i)})_{Av} + \beta^{-1}\ln\det 2\sinh\frac{\beta}{2}((D^{(i)2})_{Av})^{1/2} \quad \text{(B.c.)}, \qquad (6)$$

$$F_N \geqslant \frac{1}{2}Tr(S^{(i)})_{Av} - \beta^{-1}\ln\det 2\cosh\frac{\beta}{2}((D^{(i)2})_{Av})^{1/2} \quad \text{(F.c.)} \qquad (7)$$

hold.

Here $(\dots)_{Av}$ denotes the average with a given distribution function and $((D^{(i)2})_{Av})^{1/2}$ is the positive definite quadratic root of $(D^{(i)2})_{Av}$.

Proof

As is well known, under the above assumptions the quadratic form (2) may by the Bogolubov's canonical (u,v) transformation be transformed to

$$H_N = E^{(i)}_{0,N} + \sum_\nu \varepsilon^{(i)}_\nu b^+_\nu b_\nu, \qquad (8)$$

where $\varepsilon^{(i)}_\nu > 0$ are determined from the eigenvalue problem

$$D^{(i)2}n^{(i)}_\nu = \varepsilon^{(i)2}_\nu n^{(i)}_\nu \qquad (9)$$

and

$$E^{(i)}_{0,N} = -\frac{1}{2}(Tr S^{(i)} - \sum_\nu \varepsilon^{(i)}_\nu) \qquad \text{(B.c.)}, (10)$$

$$E^{(i)}_{0,N} = \frac{1}{2}(Tr S^{(i)} - \sum_\nu \varepsilon^{(i)}_\nu) \qquad \text{(F.c.)}. (11)$$

The formula for the ground state energy $E^{(i)}_{0,N}$ may be obtained simply in Fermi case from the invariance of trace H_N under (u,v) transformation. For the Bose case we may obtain it from the standard expression

$$E^{(i)}_{0,N} = -\sum_{\nu,\alpha}\varepsilon^{(i)}_\alpha |v^{(i)}_{\alpha\nu}|^2$$

(see, e.g., [4]) where $U_{\alpha\nu}$, $V_{\alpha\nu}$ are the coefficients of the (u,v) transformation, if we derive, taking into account the orthonormality relations, the following intermediate result

$$E^{(i)}_{0,N} = \frac{1}{2}\sum_\nu \varepsilon^{(i)}_\nu - \frac{1}{2}\sum_{\alpha\nu\gamma}\left(U^{(i)}_{\alpha\nu}S^{(i)}_{\gamma\alpha}U^{(i)}_{\alpha\nu} - V^{(i)}_{\alpha\nu}S^{(i)}_{\gamma\alpha}V^{(i)}_{\alpha\nu}\right). \qquad (12)$$

For diagonal $S^{(i)}$ formula (10) is then obvious and holds in general due to the invariance of the orthonormality relations under orthogonal transformations diagonalizing the symmetric matrix $S^{(i)}$.

Now, after simple algebra, we may write the exact free energy in the form

$$F_N = -\frac{1}{2}(Tr\, S^{(i)})_{AV} + \beta^{-1}(\ln\det 2\sinh\frac{\beta D^{(i)}}{2})_{AV} \qquad \text{(B.c.)}, \qquad (13)$$

$$F_N = \frac{1}{2}(Tr\, S^{(i)})_{AV} - \beta^{-1}(\ln\det 2\cosh\frac{\beta D^{(i)}}{2})_{AV} \qquad \text{(F.c)}, \qquad (14)$$

where $D^{(i)} = (D^{(i)2})^{1/2}$, $D^{(i)}$ is positive definite.

Expanding the functions sinh and cosh in (13) and (14) in infinite products and taking the logarithm we obtain

$$\ln\det 2\sinh\frac{\beta D^{(i)}}{2} = \frac{1}{2}\ln\beta^2\det D^{(i)2} + \sum_{k=1}^{\infty}\ln\det\left(I + \frac{\beta^2 D^{(i)2}}{4\pi^2 k^2}\right), \qquad (15)$$

$$\ln\det 2\cosh\frac{\beta D^{(i)}}{2} = N\ln 2 + \sum_{k=1}^{\infty}\ln\det\left(I + \frac{\beta^2 D^{(i)2}}{(2k+1)^2\pi^2}\right). \qquad (16)$$

Finally, applying the inequality (1) term by term to the above expansions we complete the proof of (6) and (7) .

Comments

The obtained bounds correspond to the simplest approximation in the eigenvalue problem, when we replace $D^{(i)2}$ by $(D^{(i)2})_{AV}$. In practice, this matrix can be easily calculated and diagonalized (as a rule, after averaging we restore the crystal symmetry).

For Fermi systems, when H_N is a bounded operator, the upper bound for the free energy can be easily obtained taking into account the convexity property of the function $A \longrightarrow \ln Tr\, e^A$ [5] which leads to

$$F_N \leqslant F_N[H_N((S^{(i)})_{AV}, (R^{(i)})_{AV})] \qquad (17)$$

and corresponds to the so-called "virtual crystal approximation" in the theory of disordered systems.

The similar argument cannot be applied to the Bose systems when H_N is unbounded. Instead, we have our upper bound (6) .

The limit $T \to 0$ can be taken in (6) and (7) which gives the corresponding estimations for the ground state energy.

On the other hand, the same result may be obtained directly if we exploit the known integral identity

$$Tr[(D^{(i)2})^{1/2}] = \frac{1}{2\pi}\int_0^{\infty} dx\, x^{-3/2}\ln\det(I + xD^{(i)2}) \qquad (18)$$

and then apply the basic inequality (1) .

References:

[1]. E.Lieb, T.Schultz, D.Mattis. Ann.Phys., 16, 407 (1961).

[2]. E.J.Elliot, J.A.Krumhansl, P.L.Leath. Rev.Mod.Phys., 46, 465 (1974).

[3]. M.Marcus, H.Minc. A Survey of the Matrix Theory and Matrix Inequalities, Allyn and Bacon, Inc., Boston (1964).

[4]. С.В.Тябликов. Методы квантовой теории магнетизма, Наука, Москва (1975).

[5]. D.Ruelle. Statistical Mechanics, Rigorous Results, W.A. Benjamin Inc., New York- Amsterdam (1969).

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