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# Simple Inequality for the Free Energy of Disordered Systems

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It is proved that the free energy of a disordered system described by a quadratic form in Bose or Fermi operators with random coefficients, calculated in the simplest approximation for the associated eigenvalue problem, gives the upper (Bose case) and lower (Fermi case) bounds for the exact free energy.

**KEY WORDS:** Disordered crystal; free energy; ground-state energy; thermodynamic inequalities.

The great variety of excitations in disordered crystals may be described with sufficient accuracy in terms of Hamiltonians which are simply 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 $XY$ chains.[2]

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

In this note we obtain an estimate for the free energy of these systems. The proof is based on the concavity property of the function $A \to \ln \det A$,

$$\sum_i c_i \ln \det A^{(i)} \leqslant \ln \det \sum_i c_i A^{(i)}; \qquad c_i \geqslant 0, \quad \sum_i c_i = 1 \tag{1}$$

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

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

**Lemma.** Let us consider the class of Hamiltonians

$$H_N(S^{(i)}, R^{(i)}) = \sum_{\alpha,\beta} S^{(i)}_{\alpha\beta} a_\alpha{}^+ a_\beta + \tfrac{1}{2} \sum_{\alpha,\beta} (R^{(i)}_{\alpha\beta} a_\alpha{}^+ a_\beta{}^+ + \text{h.c.}), \qquad \alpha, \beta = 1, \ldots, N \tag{2}$$

where $a_\alpha{}^+$ and $a_\alpha$ are Bose and Fermi operators, and $S^{(i)}$ and $R^{(i)}$ are real matrices with obvious symmetry properties:

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

which, for the Bose case, satisfy the additional conditions:

$$S^{(i)} + R^{(i)} \text{ and } S^{(i)} - R^{(i)} \text{ both positive definite, } [S^{(i)}, R^{(i)}] = 0 \tag{4}$$

Then if we introduce some probability distribution on this class and define the mean free energy $F_N$ as

$$F_N \equiv -\beta^{-1}\{\ln \operatorname{Tr} \exp[-\beta H_N(S^{(i)}, R^{(i)})]\}_{\text{AV}}, \qquad \beta = 1/kT \tag{5}$$

where $\{\cdots\}_{\text{AV}}$ is the average with a given distribution function, the following inequalities hold:

$$F_N \leqslant -\tfrac{1}{2} \operatorname{Tr}(S^{(i)})_{\text{AV}} + \beta^{-1} \ln \det 2 \sinh\{\tfrac{1}{2}\beta[(D^{(i)^2})_{\text{AV}}]^{1/2}\} \quad \text{(Bose)} \tag{6}$$

$$F_N \geqslant \tfrac{1}{2} \operatorname{Tr}(S^{(i)})_{\text{AV}} - \beta^{-1} \ln \det 2 \cosh\{\tfrac{1}{2}\beta[(D^{(i)^2})_{\text{AV}}]^{1/2}\} \quad \text{(Fermi)} \tag{7}$$

The matrices $D^{(i)^2} = (S^{(i)} + R^{(i)})(S^{(i)} - R^{(i)})$ in (7) and (8) are at least positive semidefinite for the Fermi case and positive definite for the Bose case and their averages $(D^{(i)^2})_{\text{AV}}$ and quadratic roots have the same properties.

***Proof.*** The above assumptions guarantee that the quadratic forms (2) describe for any $(i)$ the well-defined elementary excitations, i.e., may be transformed by the Bogoliubov canonical $(u, v)$ transformation into

$$H^{(i)}_N = E^{(i)}_{0,N} + \sum_\nu \epsilon^{(i)}_\nu b_\nu{}^+ b_\nu \tag{8}$$

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

$$D^{(i)^2} n^{(i)}_\nu = \epsilon^{(i)^2}_\nu n^{(i)}_\nu \tag{9}$$

and

$$E^{(i)}_{0,N} = -\tfrac{1}{2}\left(\operatorname{Tr} S^{(i)} - \sum_\nu \epsilon^{(i)}_\nu\right) \qquad \text{(Bose case)} \tag{10}$$

$$E^{(i)}_{0,N} = \tfrac{1}{2}\left(\operatorname{Tr} S^{(i)} - \sum_\nu \epsilon^{(i)}_\nu\right) \qquad \text{(Fermi case)} \tag{11}$$

The formula for the ground-state energy $E_{0,N}^{(i)}$ can be obtained simply in the Fermi case from the invariance of the trace under $(u, v)$ transformation. For the Bose case we can obtain it from the standard expression $E_{0,N}^{(i)} = -\sum_{\nu,\alpha} \epsilon_{\alpha}^{(i)} |v_{\alpha\nu}^{(i)}|^2$ (see, e.g., Ref. 4), where $u_{\alpha\nu}$ and $v_{\alpha\nu}$ are the coefficients of the $(u, v)$ transformation, if we derive, taking into account the corresponding orthonormality relations, the following intermediate result:

$$E_{0,N}^{(i)} = \tfrac{1}{2} \sum_{\nu} \epsilon_{\nu}^{(i)} - \tfrac{1}{2} \sum_{\alpha\nu\gamma} (u_{\alpha\nu}^{(i)} S_{\gamma\alpha}^{(i)} u_{\alpha\nu}^{(i)} - v_{\alpha\nu}^{(i)} S_{\gamma\alpha}^{(i)} v_{\alpha\nu}^{(i)}) \tag{12}$$

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

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

$$F_N = -\tfrac{1}{2}(\mathrm{Tr}\, S^{(i)})_{\mathrm{AV}} + \beta^{-1}[\ln \det 2 \sinh(\tfrac{1}{2}\beta D^{(i)})]_{\mathrm{AV}} \qquad \text{(Bose)} \tag{13}$$

$$F_N = \tfrac{1}{2}(\mathrm{Tr}\, S^{(i)})_{\mathrm{AV}} - \beta^{-1}[\ln \det 2 \cosh(\tfrac{1}{2}\beta D^{(i)})]_{\mathrm{AV}} \qquad \text{(Fermi)} \tag{14}$$

where $D^{(i)} = (D^{(i)2})^{1/2}$. Expanding the functions sinh and cosh in (13) and (14) in infinite products and taking the logarithm, we obtain

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

$$\ln \det 2 \cosh \frac{\beta D^{(i)}}{2} = N \ln 2 + \sum_{k=0}^{\infty} \ln \det\left(I + \frac{\beta^2 D^{(i)2}}{(2k+1)^2 \pi^2}\right) \tag{16}$$

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

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

The conditions (4) imposed on Bose systems seem, at first sight, to be very restrictive. However, the corresponding class of Hamiltonians includes, e.g., all disordered phonon Hamiltonians in the harmonic approximation with dynamical matrix equivalent to $D^{(i)2}$.

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

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

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

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

The limit $T = 0$ can be taken in (6) and (7), which gives the corresponding estimates for the ground-state energy.

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

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

and then apply the basic inequality (1).

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