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Rigorous treatment of the BCS model of superconductivity

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Abstract. We show that the variational theory of Bardeen–Cooper–Schreifer (BCS) is exact for the BCS reduced Hamiltonian for attractive pair potentials which satisfy reasonable conditions. Specific forms of the pair potential are used for illustrative purposes and to provide explicit proofs of some of the more technical details.

1. Introduction

The Bardeen–Cooper–Schreifer (BCS) theory of superconductivity [1] is arguably one of the most successful and widely known theories in condensed matter physics. The theory is based on the so-called BCS reduced Hamiltonian

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} - \sum_{kl} J_{kl} b_k^\dagger b_l \tag{1.1}$$

where $c_{k\sigma}$ ($c_{k\sigma}^\dagger$) is the destruction (creation) operator for particles with wavevector k, kinetic energy ϵ_k and spin $\sigma = \uparrow$ or $\downarrow$, and

$$b_k \equiv c_{-k\downarrow} c_{k\uparrow} \tag{1.2}$$

is the annihilation operator for a (Cooper) pair of fermions with opposite spin and momentum. The two-body potential J_{kl} is assumed to be attractive (non-negative) and in conventional BCS theory to be mediated by electron–phonon interactions.

In their original paper [1] BCS used standard variational methods to obtain ground state and thermodynamic properties of the model which were subsequently claimed by several authors to be exact in the thermodynamic, or bulk, limit.

Bogoliubov, Zubarev and Tserkovnikov, for example, used thermodynamic perturbation theory [2] and Green function methods [3] in their proof of the validity of BCS theory while Mühlschlegel [4] used a functional integral and saddle-point approach to establish the same result for the special case of a separable potential

$$J_{kl} = v_k v_l . \tag{1.3}$$

The separable case was also considered by Bogoliubov Jr [5] and in all cases the coupling constants were non-negative and satisfied sufficient conditions to guarantee the existence of the thermodynamic limit.

On close scrutiny, however, none of the mentioned proofs of the validity of the BCS theory is strictly valid, from a contemporary statistical-mechanical viewpoint,

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although certain extreme limiting cases such as the strong-coupling limit considered by Thouless [6] and certain ground-state properties discussed by Wada and Fukuda [7], Baumann *et al* [8] and Mattis and Lieb [9] would be classified as rigorous results.

In view of the recent revival of interest in pairing theories as a basis for high-temperature superconductivity [10] it seems timely to re-examine the question of the validity of BCS theory in the context of an exact statistical mechanical treatment of the BCS model with Hamiltonian (1.1).

We make no comment here about possible pairing mechanisms for high-temperature superconductivity, or conventional superconductivity, such as the phonon-mediated electronic attraction in the original BCS theory. We thus make a distinction between BCS theory and the BCS model (1.1), which forms the basis for the present discussion.

In the following section we state our main result and discuss some special cases. The bulk of the proof of our main result is given in sections 3 and 4 where lower and upper bounds, respectively, are obtained for the grand canonical potential. Technical details which show, for example, that the bounds coalesce in the thermodynamic limit, subject to certain conditions on the pairing potential, are given in appendixes. The final section contains a discussion of our results.

2. Statement of the main result

We consider the BCS reduced Hamiltonian (1.1) in a d-dimensional box with volume $V = L^d$, and assume that the matrix J, with pair potentials J_{kl} as entries, is symmetric ($J_{kl} = J_{lk}$), has positive entries ($J_{kl} > 0$), is positive definite (i.e. the eigenvalues of J are positive), and is of *trace class* in the thermodynamic limit.

The grand-canonical partition function $\mathcal{Q}$ is defined by

$$\mathcal{Q} = \operatorname{Tr} \exp\left(-\beta(\mathcal{H} - \mu\mathcal{N})\right) \tag{2.1}$$

where $\beta = (kT)^{-1}$ is the inverse temperature, μ is the chemical potential and

$$\mathcal{N} = \sum_{k\sigma} c_{k\sigma}^{\dagger} c_{k\sigma} \tag{2.2}$$

is the total number operator. The grand-canonical potential is defined by

$$\chi(V, z, T) = V^{-1} \log \mathcal{Q} \tag{2.3}$$

with $z = \exp(\beta\mu)$, the fugacity, determined as a function of the density ρ, by

$$\rho = z\frac{\partial \chi}{\partial z}. \tag{2.4}$$

The BCS expression for χ is [1]

$$\chi_{\mathrm{BCS}} = \log 4z + \frac{2}{V}\sum_{k} \log\cosh\frac{\beta E_k}{2} - \frac{\beta^2}{4V}\sum_{k} \Delta_k^2 h(\beta E_k) \tag{2.5}$$

where

$$E_k = \left[(\epsilon_k - \mu)^2 + \Delta_k^2\right]^{1/2} \tag{2.6}$$

$$h(x) = \frac{2}{x}\tanh\frac{x}{2} \tag{2.7}$$

and Δ_k is a solution of the so-called energy-gap equation

$$\Delta_k = \frac{\beta}{4}\sum_l J_{kl}\Delta_l h(\beta E_l) \tag{2.8}$$

which maximizes χ_{BCS}.

Our main result is expressed as the following

Theorem. For a system of fermions with Hamiltonian (1.1) and pair potential J_{kl} satisfying the above conditions

$$\begin{aligned}\chi(z,T) &= \lim_{V\to\infty}\chi(V,z,T) \\ &= \lim_{V\to\infty}\chi_{\text{BCS}}(V,z,T).\end{aligned} \tag{2.9}$$

In (2.9) it is implicitly assumed that J_{kl} satisfies further conditions to guarantee the existence of the thermodynamic limit.

Specific forms for J_{kl} which satisfy the required conditions and which we use later for illustrative purposes are:

(i) *Translationally invariant*

$$J_{kl} = V^{-1}\tilde{K}\left(2\pi(k-l)L^{-1}\right) \tag{2.10}$$

with $\tilde{K}(\theta)$ the Fourier transform of a positive integrable function K;

(ii) *Separable*

$$J_{kl} = V^{-1}v(2\pi k/L)v(2\pi l/L) \tag{2.11}$$

with $v(\theta)$ a positive, bounded and continuous function;

(iii) *Kac-type*

$$J_{kl} = \gamma^d K(\gamma\|k-l\|) \tag{2.12}$$

where K is positive, continuous and integrable, and γ is a positive constant.

The motivation for considering (2.12) is two-fold. First the BCS theory has a mean-field-like character to it and it is well known that mean-field theories in general become exact for systems with Kac potentials in the limit $\gamma \to 0^+$ (after the thermodynamic limit) [11]. Second, as noted by several people [12], the BCS model is equivalent to a k-space X–Y model with k-dependent transverse magnetic fields so that in a Kac ($\gamma \to 0^+$) limit the BCS theory should reduce to a simple variant of the Curie–Weiss theory of magnetism. We shall see that this is precisely the case in section 5 where the limiting form of the grand-canonical potential, energy gap and critical-temperature equations for the three cases (2.10)–(2.12) are presented and discussed.

3. Lower bound on the grand-canonical potential

In order to obtain a lower bound on the grand-canonical potential we add and subtract c-numbers ψ_k to the pair creation and annihilation operators in (1.1) to obtain

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \tag{3.1}$$

where

$$\mathcal{H}_1 = -\sum_{kl} J_{kl}(b_k^\dagger - \psi_k^*)(b_l - \psi_l) \tag{3.2}$$

and from (1.1) and (1.2)

$$\mathcal{H}_0 - \mu\mathcal{N} = \sum_{k\sigma}(\epsilon_k - \mu)c_{k\sigma}^\dagger c_{k\sigma} - \sum_k(\Delta_k b_k^\dagger + \Delta_k^* b_k) + \sum_k \psi_k^*\Delta_k \tag{3.3}$$

where

$$\Delta_k \equiv \sum_l J_{kl}\psi_l. \tag{3.4}$$

We now apply the Bogoliubov variational principle [13] to obtain a lower bound for the grand-canonical partition function (2.1),

$$\mathcal{Q} \geqslant \mathcal{Q}_0 \exp\left(-\beta\langle\mathcal{H}_1\rangle_0\right) \tag{3.5}$$

where

$$\mathcal{Q}_0 \equiv \mathrm{Tr}\exp\left(-\beta(\mathcal{H}_0 - \mu\mathcal{N})\right) \tag{3.6}$$

and

$$\langle\mathcal{A}\rangle_0 \equiv \mathcal{Q}_0^{-1}\,\mathrm{Tr}\,\mathcal{A}\exp\left(-\beta(\mathcal{H}_0 - \mu\mathcal{N})\right) \tag{3.7}$$

denotes the usual grand-canonical average of $\mathcal{A}$ with respect to the reference system $\mathcal{H}_0$.

The operator $\mathcal{H}_0 - \mu\mathcal{N}$ defined by (3.3) is quadratic in Fermi creation and annihilation operators and can be diagonalized [3] by an appropriate unitary (so-called Bogoliubov–Valatin) transformation. The reference grand-canonical potential is thus found to be

$$\begin{aligned}\chi_0(V,z,T) &= V^{-1}\log\mathcal{Q}_0 - \beta V^{-1}\langle\mathcal{H}_1\rangle_0 \\ &= \log 4z + \frac{2}{V}\sum_k \log\cosh\frac{\beta E_k}{2} - \frac{\beta}{V}\sum_k \psi_k^*\Delta_k \\ &\quad + \frac{\beta}{V}\sum_{kl} J_{kl}\left[\left\langle b_k^\dagger\right\rangle_0 - \psi_k^*\right]\left[\langle b_l\rangle_0 - \psi_l\right] \\ &\quad + \frac{\beta}{4V}\sum_k J_{kk}\left[1 + \frac{\beta(\mu - \epsilon_k)}{2}h(\beta E_k)\right]^2\end{aligned} \tag{3.8}$$

where E_k is defined by (2.6) and h is defined by (2.7). From our assumption that J is of trace class the last term in (3.8) is of order V^{-1} and will be ignored henceforth.

The optimal bound from (3.5) and (3.8) is obtained by choosing

$$\psi_k = \langle b_k \rangle_0 = \tfrac{1}{4}\beta\Delta_k h(\beta E_k) \tag{3.9}$$

which together with (3.4) results in the energy-gap equation (2.8). For this choice of the parameters χ_0 reduces to the BCS expression (2.5) and from (3.5), (3.8) and (2.5) we obtain the lower bound

$$\chi(V,z,T) \geqslant \chi_{\mathrm{BCS}}(V,z,T). \tag{3.10}$$

The result (3.10) and the pair-decoupling manipulation (3.1) are, in fact, quite well known and date back at least to the pioneering work of Bogoliubov [3].

4. Upper bound on the grand-canonical potential

To obtain an upper bound on the grand-canonical potential, we apply the following generalization of the Golden–Thompson inequality [14]

$$\operatorname{Tr} \mathrm{e}^{A+B} \leqslant \operatorname{Tr}(\mathrm{e}^{A/n}\mathrm{e}^{B/n})^n \tag{4.1}$$

which holds for A and B Hermitian operators and $n \geqslant 1$ an integer.

Combining (4.1) with (2.1) and (1.1) we obtain

$$Q \leqslant Q_n \equiv \operatorname{Tr}\left[\exp\left(\frac{1}{n}\sum_k A_k\right)\exp\left(\frac{\beta}{n}\sum_{kl} J_{kl} b_k^\dagger b_l\right)\right]^n \tag{4.2}$$

where

$$A_k \equiv -\beta(\epsilon_k - \mu)(c_{k\uparrow}^\dagger c_{k\uparrow} + c_{-k\downarrow}^\dagger c_{-k\downarrow}). \tag{4.3}$$

We now make use of the following identity [14]

$$\exp\left(\frac{\beta}{n}\sum_{kl} A_{kl} O_k^\dagger O_l\right) = \left(\frac{\beta}{2\pi n}\right)^V \frac{1}{\det A}\int_{\mathbb{R}^{2V}} \prod_k \mathrm{d}^2 z_k \exp\left(-\frac{\beta}{n}\sum_{kl} A_{kl}^{-1} z_k^* z_l\right)$$
$$\times \exp\left(\frac{\beta}{n}\sum_k (z_k^* O_k + z_k O_k^\dagger)\right) \tag{4.4}$$

which holds for any positive definite, real symmetric matrix A, and any set of operators $\{O_k\}$ which commute pairwise and where $\mathrm{d}^2 z_k$ denotes $\mathrm{d}(\operatorname{Re} z)\mathrm{d}(\operatorname{Im} z)$.

Since J is real symmetric and positive definite (by assumption) and the b_k-operators commute pairwise, we can apply (4.4) separately to each of n terms in the right-hand side of (4.2) to obtain

$$Q_n = \left(\frac{\beta}{2\pi n}\right)^{nV} (\det J)^{-n} \int_{\mathbb{R}^{2Vn}} \prod_k \prod_{t=1}^n \mathrm{d}^2 z_{kt} \prod_{t=1}^n \exp\left(\frac{\beta}{n}\sum_{kl} J_{kl}^{-1} z_{kt}^* z_{lt}\right)$$
$$\times \operatorname{Tr}\prod_{t=1}^n \left[\exp\left(\frac{1}{n}\sum_k A_k\right)\exp\left(\frac{1}{n}\sum_k B_{kt}\right)\right] \tag{4.5}$$

where

$$B_{kt} \equiv \beta \left(z_{kt}^* b_k + z_{kt} b_k^\dagger \right) . \tag{4.6}$$

In order to bound the trace appearing in (4.5) we use the Hölder trace inequality [15]

$$\left| \mathrm{Tr} \prod_{t=1}^{n} O_t \right| \leqslant \prod_{t=1}^{n} \left[\mathrm{Tr} \left(O_t^\dagger O_t \right)^{n/2} \right]^{1/n} \tag{4.7}$$

with

$$O_t = \exp\left(\frac{1}{n} \sum_k A_k \right) \exp\left(\frac{1}{n} \sum_k B_{kt} \right) \tag{4.8}$$

to obtain the bound

$$\left| \mathrm{Tr} \prod_{t=1}^{n} O_t \right| \leqslant \prod_{t=1}^{n} \left[\prod_k \mathrm{Tr}_k [\exp(2A_k/n) \exp(2B_{kt}/n)]^{n/2} \right]^{1/n} \tag{4.9}$$

where Tr_k denotes a trace over the block

$$H_k \equiv \left\langle |0\rangle , c_{k\uparrow}^\dagger |0\rangle , c_{-k\downarrow}^\dagger |0\rangle , c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger |0\rangle \right\rangle \tag{4.10}$$

of the Hilbert space $H = \bigotimes_k H_k$ on which A_k and B_{kt} act and here and henceforth we assume that n is even.

Next we use the following inequality [14]

$$\left| \mathrm{Tr} \left[\mathrm{e}^{2A/n} \mathrm{e}^{2B/n} \right]^{n/2} \right| \leqslant \left(1 + \frac{4}{n} \mathrm{e}^{3(||A||+||B||)} \right) \left| \mathrm{Tr}\ \mathrm{e}^{A+B} \right| \tag{4.11}$$

where

$$||A|| \equiv \sup_{||\phi||=1} ||A\phi|| \tag{4.12}$$

denotes the norm of the operator A and $||\phi||$ denotes the norm of the vector ϕ. Combining (4.8), (4.9) and (4.11) we obtain

$$\left| \mathrm{Tr} \prod_{t=1}^{n} O_t \right| \leqslant \prod_{t=1}^{n} \left[\prod_k \left\{ \left(1 + \frac{4}{n} \mathrm{e}^{3(||A_k||+||B_{kt}||)} \right) \left| \mathrm{Tr}_k\ \mathrm{e}^{-\beta \mathcal{H}_{kt}} \right| \right\} \right]^{1/n} \tag{4.13}$$

where

$$-\beta \mathcal{H}_{kt} \equiv A_k + B_{kt} . \tag{4.14}$$

From (4.3) and (4.6) it will be noted that $\mathcal{H}_{kt}$ is quadratic in Fermi operators and hence can be diagonalized by a Bogoliubov–Valatin transformation. The traces in (4.13) are thus readily evaluated and on combining (4.2), (4.5) and (4.13) we obtain

$$\mathcal{Q} \leqslant q_n^n \tag{4.15}$$

where

$$q_n \equiv \left(\frac{\beta}{2\pi n}\right)^V \frac{1}{\det J} \int_{\mathbb{R}^{2V}} \prod_k \mathrm{d}^2 z_k \exp\left(-\frac{\beta}{n}\sum_{kl} J_{kl}^{-1} z_k^* z_l\right)$$
$$\times \left[\prod_k \left\{\left(1+\frac{4}{n}\mathrm{e}^{6\beta(|\epsilon_k-\mu|+|z_k|)}\right) 4z \cosh^2 \frac{\beta\sqrt{(\epsilon_k-\mu)^2+|z_k|^2}}{2}\right\}\right]^{1/n} \tag{4.16}$$

and in the final simplification we have factored the $(2Vn)$-dimensional integral into a product of n identical $(2V)$-dimensional integrals and used the elementary bounds

$$||A_k|| \leqslant 2\beta\,|\epsilon_k-\mu| \qquad ||B_{kt}|| \leqslant 2\beta\,|z_{kt}| \tag{4.17}$$

which follows easily from (4.3), (4.6) and (4.12).

For $0<\epsilon<1$ we now define a set of positive quantities

$$\zeta_k = 4[(1-\epsilon)\beta h(\beta E_k)]^{-1} \tag{4.18}$$

and a corresponding diagonal matrix ζ with entries ζ_k where E_k is defined by (2.6). Adding and subtracting a diagonal term to the exponent in (4.16) we obtain

$$q_n = \left(\frac{\beta}{2\pi n}\right)^V \frac{1}{\det J} \int_{\mathbb{R}^{2V}} \prod_k \mathrm{d}^2 z_k \exp\left(-\frac{\beta}{n}\sum_{kl}(J_{kl}^{-1}-\zeta_k^{-1}\delta_{kl}) z_k^* z_l\right)\mathrm{e}^{V\chi\{z\}/n} \tag{4.19}$$

where

$$\chi\{z\} = \log 4z + \frac{2}{V}\sum_k \log\cosh\frac{\beta\sqrt{(\mu-\epsilon_k)^2+|z_k|^2}}{2}$$
$$+\frac{1}{V}\sum_k \log\left(1+\frac{4}{n}\mathrm{e}^{6\beta(|\epsilon_k-\mu|+|z_k|)}\right) - \frac{\beta}{V}\sum_k \frac{|z_k|^2}{\zeta_k}. \tag{4.20}$$

It then follows that

$$q_n \leqslant \frac{\mathrm{e}^{Vn^{-1}\chi_{\max}}}{\det(I-J\zeta^{-1})} \tag{4.21}$$

where

$$\chi_{\max} \equiv \max_{\{z\}} \chi\{z\} \tag{4.22}$$

and in obtaining (4.21), we have used (4.4), assuming that $J^{-1}-\zeta^{-1}$ is positive definite. The proof of this assumption is given in appendix A.1.

Combining (2.3), (4.15) and (4.21) we then have

$$\chi \leqslant \chi_{\mathrm{FI}} \tag{4.23}$$

where

$$\chi_{\rm FI} \equiv \chi_{\max} - \frac{n}{V} \log\det(I - J\zeta^{-1}). \tag{4.24}$$

By differentiating (4.20) with respect to z_k it is easily established that $\chi\{z\}$ is maximized when

$$|z_k| = \Delta_k + O(\epsilon) + O(n^{-1}). \tag{4.25}$$

Combining (2.5), (2.6), (4.18), (4.20), (4.22), (4.24) and (4.25) it then follows that

$$\chi_{\rm FI} = \chi_{\rm BCS} - \frac{n}{V} \log\det(I - J\zeta^{-1}) + O(\epsilon) + O(n^{-1}) \tag{4.26}$$

where $\chi_{\rm BCS}$ is defined by (2.5). The subdominant terms in (4.26) are uniformly bounded over V.

Finally, in order to establish our main result (2.9), we need to show, from (3.10), (4.23) and (4.26), that

$$\lim_{V\to\infty} V^{-1} \log\det(I - J\zeta^{-1}) = 0. \tag{4.27}$$

In appendix B we show that (4.27) holds for several choices of the pair potential mentioned in section 2.

5. Summary and discussion

In this paper we have shown that the variational theory of BCS is exact for the BCS reduced Hamiltonian in the thermodynamic limit, provided the pair potential satisfies reasonable conditions, stated in section 2. Specific forms for the potential were used for illustrative purposes and to provide explicit proofs for some of the more technical details.

The grand-canonical potential in the thermodynamic limit is given, in general, by

$$\lim_{V\to\infty} \chi(V, z, T) = \log 4z - \frac{\beta^2}{4(2\pi)^d} \int_{[0,2\pi]^d} (\Delta(\theta))^2 h(\beta E(\theta))\, \mathcal{D}\theta + \frac{2}{(2\pi)^d} \int_{[0,2\pi]^d} \log\cosh \frac{\beta E(\theta)}{2} \mathcal{D}\theta \tag{5.1}$$

where

$$E(\theta) = \left[(\mu - \epsilon(\theta))^2 + (\Delta(\theta))^2\right]^{1/2}. \tag{5.2}$$

The energy-gap equation (2.8) in the thermodynamic limit reduces in the translationally invariant case (2.10) to

$$\Delta(\theta) = \frac{\beta}{4(2\pi)^d} \int_{[0,2\pi]^d} \tilde{K}(\theta - \phi)\Delta(\phi) h(\beta E(\phi))\mathcal{D}\phi. \tag{5.3}$$

In the separable case (2.11) $\Delta(\theta) = av(\theta)$ and a is the solution of the scalar gap equation

$$a = \frac{\beta a}{4(2\pi)^d} \int_{[0,2\pi]^d} (v(\theta))^2 h\left(\beta\sqrt{(\mu-\epsilon(\theta))^2 + (av(\theta))^2}\right) \mathcal{D}\theta. \quad (5.4)$$

In the case of the Kac potential (2.12) we show in appendix B.3 that (2.8) completely decouples in the Kac limit ($\gamma \to 0^+$) (after the thermodynamic limit) yielding

$$\Delta(\theta) h\left(\beta E(\theta)\right) = \frac{4\Delta(\theta)}{\alpha\beta} \quad (5.5)$$

where

$$\alpha \equiv \int_{\mathbb{R}^d} K(||r||)\mathcal{D}r. \quad (5.6)$$

The result (5.5) is not, surprisingly, equivalent to mean-field theory for the X–Y model [16] and is to be compared with the usual Ising model Curie–Weiss theory [11] which in the present notation has equation of state

$$h\left(\beta m_0\right) = 4/\alpha\beta \quad (5.7)$$

where m_0 is the spontaneous magnetization.

In the more general BCS setting the energy gap plays the role of an order parameter and by analogy with the magnetic case, the energy gap vanishes above the critical temperature T_c. The equation determining T_c is given in appendix A.2 where we show that there exists a non-trivial solution to the gap equation if and only if $T < T_c$ and that the non-trivial solution must be taken in order to obtain the correct grand-canonical potential.

The critical temperature in the bulk limit is given in the translationally invariant case (i) (2.10) by

$$0 = \max_{||y||=1} \left\{ \frac{1}{(2\pi)^d} \int_{[0,2\pi]^d} \mathcal{D}\theta \int_{[0,2\pi]^d} \mathcal{D}\phi \, y(\theta) y(\phi) \tilde{K}(\theta-\phi) - \frac{4}{\beta_c(2\pi)^d} \int_{[0,2\pi]^d} \frac{(y(\theta))^2}{h(\beta_c(\mu-\epsilon(\theta)))} \mathcal{D}\theta \right\} \quad (5.8)$$

where

$$||y|| \equiv \frac{1}{(2\pi)^d} \int_{[0,2\pi]^d} (y(\theta))^2 \mathcal{D}\theta.$$

In case (ii) (2.11) we have

$$1 = \frac{\beta_c}{4(2\pi)^d} \int_{[0,2\pi]^d} (v(\theta))^2 h(\beta_c(\mu-\epsilon(\theta)))\mathcal{D}\theta \quad (5.10)$$

and in case (iii) (2.12) we have

$$1 = \frac{\alpha\beta_c}{4} \max_{\theta} h(\beta_c(\mu-\epsilon(\theta))). \quad (5.11)$$

Finally, in the separable and Kac cases it is clear from (5.4) and (5.5) that a unique non-trivial solution exists to the gap equation below T_c while in case (i) it is clear *a posteriori* from our main result that if (5.3) has more than one non-trivial solution then they must yield the same grand-canonical potentials (5.1).

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Appendix A. Proof that the matrix $J^{-1} - \zeta^{-1}$ is positive definite and the critical temperature

A1. Proof that the matrix $J^{-1} - \zeta^{-1}$ is positive definite

In this appendix we show that the matrix $J^{-1} - \zeta^{-1}$ is positive definite, where J satisfies the requirements stated in section 2 and ζ is defined in section 4.

Now $J^{-1} - \zeta^{-1}$ is congruent to $\zeta^{1/2} J^{-1} \zeta^{1/2} - I$ so it suffices to show that all of the eigenvalues of $\zeta^{-1/2} J \zeta^{-1/2}$ are bounded below and away from 1. We, in fact, show that the maximum eigenvalue is not greater than $1 - \epsilon$.

In doing so we require the following result [17].

Theorem A.1. (Perron–Frobenious.) If A is a square matrix with positive entries $(A_{ij} > 0)$ then the eigenvalue of A which is greatest in magnitude is real and positive. It is also simple and the corresponding eigenvector can be chosen so that all components are positive. Further, A can have no other eigenvector with all components non-negative.

We note that using (4.18), (2.8) may be written

$$\zeta^{-1/2} J \zeta^{-1/2} \xi = (1 - \epsilon) \xi \tag{A.1}$$

where

$$\xi \equiv \zeta^{-1/2} \Delta \geqslant 0 \tag{A.2}$$

and Δ denotes the vector with components Δ_k.

We also require some properties of the function χ_0. Ignoring the last term in (3.8) and assuming Δ to be real, we can use (3.4) to obtain

$$\chi_0 \equiv \log 4z + \frac{2}{V} \sum_k \log \cosh \frac{\beta E_k}{2} - \frac{\beta^2}{2V} \sum_k \Delta_k^2 h(\beta E_k) + \frac{\beta^3}{16V} \sum_{kl} J_{kl} \Delta_k \Delta_l h(\beta E_k) h(\beta E_l). \tag{A.3}$$

Differentiating we get

$$\frac{\partial \chi_0}{\partial \Delta_k} = \frac{2\beta \nu_k}{V} \left[\frac{\beta}{4} \sum_l J_{kl} \Delta_l h(\beta E_l) - \Delta_k \right] \tag{A.4}$$

where

$$\nu_k \equiv \frac{\beta}{4} \left[h(\beta E_k) + \frac{\beta \Delta^2}{E_k} h'(\beta E_k) \right] \tag{A.5}$$

$$= \frac{\beta}{4} \left[\operatorname{sech}^2 \frac{\beta E_k}{2} - \frac{(\mu - \epsilon_k)^2}{E_k} h'(\beta E_k) \right] \tag{A.6}$$

$$> 0 \tag{A.7}$$

the last inequality being due to the fact that $h'(x) < 0$ for $x > 0$.

χ_0 is bounded above, is decreasing in $||\Delta||$ if $||\Delta||$ is sufficiently large and the stationary points of χ_0 are the solution of (2.8). Now, χ_0 clearly does not decrease if we replace the Δ_k by their absolute values (J is assumed to have positive entries). It follows that there is a non-negative solution of (2.8) at which χ_0 attains its global maximum.

The Hessian matrix corresponding to a stationary point of χ_0 is

$$H = \frac{2\beta}{V}\nu^{1/2}\left[\nu^{1/2}J\nu^{1/2} - I\right]\nu^{1/2} \tag{A.8}$$

where ν is the diagonal matrix with entries ν_k.

Suppose that (2.8) has a non-negative, non-zero solution. Then from (A.1) and (A.2) ξ is a non-negative eigenvector of $\zeta^{-1/2}J\zeta^{-1/2}$ with eigenvalue $1-\epsilon$. $\zeta^{-1/2}J\zeta^{-1/2}$ has positive entries, however, so from theorem A.1 the maximum eigenvalue of $\zeta^{-1/2}J\zeta^{-1/2}$ is $1-\epsilon$.

Next we suppose that (2.8) does not have a non-negative, non-zero solution. We take $\Delta = 0$ and so using (4.18) and (2.6) we have

$$\zeta_k = \frac{4}{\beta(1-\epsilon)h\left(\beta\left(\mu-\epsilon_k\right)\right)}. \tag{A.9}$$

We consider the Hessian matrix H_0 corresponding to $\Delta = 0$ namely

$$H_0 = \frac{2\beta}{V}\nu_0^{1/2}\left[\nu_0^{1/2}J\nu_0^{1/2} - I\right]\nu_0^{1/2} \tag{A.10}$$

where $\nu_0 \equiv \nu(\Delta = 0)$. Now using (A.9), (A.5) and (2.6) we obtain

$$(\nu_0)_k = \frac{\zeta_k^{-1}}{1-\epsilon} \tag{A.11}$$

so from (A.10) H_0 is congruent to $\zeta^{1/2}J\zeta^{1/2} - (1-\epsilon)I$. But from our assumption that (2.8) has no non-negative, non-zero solution and the properties of χ_0, χ_0 must take on its global maximum at $\Delta = 0$ and H_0 and therefore $\zeta^{1/2}J\zeta^{1/2} - (1-\epsilon)I$ must be semi-negative definite.

In either case then the maximum eigenvalue of $\zeta^{-1/2}J\zeta^{-1/2}$ is not greater than $1-\epsilon$ as required as long as we define Δ to be the non-zero, non-negative solution of (2.8) if one exists and zero otherwise.

A2. The critical temperature and the existence of non-trivial solutions to the gap equation

The argument in the previous section leads naturally to the critical temperature $T_c = 1/k\beta_c$ below which the system is ordered (the energy gap is non-zero). We showed that if (2.8) has no non-zero, non-negative solution, then H_0 (or equivalently $\nu_0^{1/2}J\nu_0^{1/2} - I$) is semi-negative definite. We now show the converse, i.e. if $\nu_0^{1/2}J\nu_0^{1/2} - I$ is semi-negative definite then (2.8) has no non-zero, non-negative solutions. Contrapositively, (2.8) has a non-negative, non-zero solution if and only if $\nu_0^{1/2}J\nu_0^{1/2} - I$ has a positive eigenvalue.

To establish this, we can use (A.6) and properties of h to deduce that

$$\nu_k \leqslant (\nu_0)_k \,. \tag{A.12}$$

It follows from Courant's principle [17] and (A.8) that if H_0 is semi-negative definite then all the stationary points of χ_0 are maxima (i.e. they all have semi-negative definite Hessian matrices). But then χ_0 can only have one stationary point—a maximum at $\Delta = 0$. The required result thus follows.

We next note that from Rayleigh's principle, the maximum eigenvalue of $\nu_0^{1/2} J \nu_0^{1/2} - I$ is

$$\lambda_{\max} = \max_{||x||=1} x^\dagger \left(\nu_0^{1/2} J \nu_0^{1/2} - I \right) x \tag{A.13}$$

$(\nu_0)_k$ is easily seen to be a strictly monotone decreasing function of β. A simple monotonicity argument then establishes that $\lambda_{\max}$ is a strictly increasing function of β. Also $\lambda_{\max} \to -\infty$ as $\beta \to 0$ and $\lambda_{\max} > 0$ if β is sufficiently large. The critical temperature is therefore defined by

$$\lambda_{\max}(\beta = \beta_c) = 0 \tag{A.14}$$

Appendix B. Proof that $\lim_{V\to\infty} V^{-1} \log\det(I - J\zeta^{-1}) = 0$

In this appendix we show that $V^{-1} \log\det\left(I - J\zeta^{-1}\right) = 0$ vanishes in the thermodynamic limit. We consider, in turn, each of the three cases mentioned in section 2.

B1. Translationally invariant potential

We consider the potential form (2.10). For the sake of simplicity we restrict our derivation to the $d = 1$ case. The extension to higher dimensions is straightforward. In one dimension we have

$$\tilde{K}(\theta) = \sum_{r=-V/2+1}^{V/2} K(|r|) \mathrm{e}^{\mathrm{i}r\theta} \tag{B.1}$$

where K is a positive, continuous function. We assume that there exist positive constants b and M such that

$$K(x) < \frac{1}{x^{1+b}} \qquad \text{for } x > M. \tag{B.2}$$

This ensures the existence of the limiting form of (B.1). We assume, again for simplicity, that K is monotone decreasing.

Now J is cyclic and can be diagonalized by the unitary matrix S where

$$S_{kl} \equiv \frac{\mathrm{e}^{2\pi \mathrm{i} kl/L}}{\sqrt{V}}. \tag{B.3}$$

That is

$$S^\dagger JS = \text{diag}\{K(1), K(2), \ldots, K(\tfrac{1}{2}V-1), K(\tfrac{1}{2}V), K(\tfrac{1}{2}V-1), \ldots, K(1), K(0)\}. \tag{B.4}$$

We let P denote the permutation matrix that transforms $S^\dagger JS$ into a diagonal matrix R with progressively increasing diagonal elements, i.e.

$$R = P^{-1}S^\dagger JSP = \text{diag}\{f_1, \ldots, f_V\} \tag{B.5}$$

where

$$\begin{aligned} f_1 &= K(V/2) \\ f_2 &= f_3 = K(V/2-1) \\ f_4 &= f_5 = K(V/2-2) \\ &\vdots \\ f_{V-2} &= f_{V-1} = K(1) \\ f_V &= K(0). \end{aligned} \tag{B.6}$$

Now

$$\left(S^\dagger \zeta^{-1} S\right)_{kl} = \frac{1}{V}\sum_m \zeta_m^{-1} e^{2\pi i m(k-l)/V} \tag{B.7}$$

so we can use (4.18) and the fact that $0 \leqslant h \leqslant 1$ to obtain

$$\begin{aligned} \left|\left(S^\dagger \zeta^{-1} S\right)_{kl}\right| &\leqslant \frac{\beta}{4V}\sum_m h(\beta E_m) \\ &\leqslant \tfrac{1}{4}\beta. \end{aligned} \tag{B.8}$$

We make the definition

$$Q = P^{-1}S^\dagger \zeta^{-1} SP. \tag{B.9}$$

The matrix elements of Q are those of $S^\dagger\zeta^{-1}S$ rearranged so

$$|Q_{kl}| \leqslant \tfrac{1}{4}\beta. \tag{B.10}$$

Next we note that

$$\log\det\left[I - J\zeta^{-1}\right] = \log\det\left[I - A\right] \tag{B.11}$$

where

$$A \equiv R^{1/2} Q R^{1/2}. \tag{B.12}$$

A is Hermitian and is similar to $\zeta^{-1/2}J\zeta^{-1/2}$ which is obviously positive definite. We show in appendix A1 that the maximum eigenvalue of $\zeta^{-1/2}J\zeta^{-1/2}$ is not greater than $1-\epsilon$. The eigenvalues of A which we denote by $\{\alpha_k\}$ can, therefore, be ordered so that

$$1-\epsilon \geqslant \alpha_1 \geqslant \alpha_2 \geqslant \cdots \geqslant \alpha_{V-1} \geqslant \alpha_V \geqslant 0 \tag{B.13}$$

so applying (B.12) we see that

$$\begin{aligned} 0 &\leqslant -\frac{1}{V}\log\det\left[I - J\zeta^{-1}\right] \\ &= -\frac{1}{V}\sum_{k=1}^{V}\log(1-\alpha_k). \end{aligned} \tag{B.14}$$

We now require some results from matrix theory [17].

Theorem B.1. (The inclusion principle.) Let A be a $V \times V$ Hermitian matrix with eigenvalues

$$\alpha_1 \geqslant \alpha_2 \geqslant \cdots \geqslant \alpha_V$$

and let B denote the $(V-1) \times (V-1)$ matrix obtained by striking out the last row and column of A. If B has eigenvalues

$$\beta_1 \geqslant \beta_2 \geqslant \cdots \geqslant \beta_{V-1}$$

then

$$\alpha_1 \geqslant \beta_1 \geqslant \alpha_2 \geqslant \beta_2 \geqslant \cdots \geqslant \alpha_{V-1} \geqslant \beta_{V-1} \geqslant \alpha_V . \tag{B.15}$$

We extend the principle to obtain the following result.

Corollary B.2. Let A be a $V \times V$ Hermitian matrix with eigenvalues

$$\alpha_1 \geqslant \alpha_2 \geqslant \cdots \geqslant \alpha_V .$$

For each $k = 1, \ldots, V$, we let $A^{(k)}$ denote the $k \times k$ matrix obtained by striking out the last $V - k$ rows and columns of A. Then α_j is bounded above by the maximum eigenvalue of $A^{(V-j+1)}$ for each $j = 1, \ldots, V$.

To prove the corollary we denote the eigenvalues of $A^{(k)}$ by

$$\alpha_1^{(k)} \geqslant \alpha_2^{(k)} \geqslant \cdots \geqslant \alpha_k^{(k)} .$$

Appying the inclusion principle to $A^{(k)}$, we arrive at

$$\alpha_j^{(k)} \leqslant \alpha_{j-1}^{(k-1)} \qquad \text{for } j = 2, \ldots, k. \tag{B.16}$$

Iterating this, we get

$$\alpha_j \equiv \alpha_j^{(V)} \leqslant \alpha_{j-1}^{(V-1)} \leqslant \alpha_{j-2}^{(V-2)} \leqslant \cdots \leqslant \alpha_1^{(V-j+1)} \tag{B.17}$$

thus establishing the result.

Theorem B.3. (Gershgorin) If B is a $k \times k$ matrix, then each of its eigenvalues, λ satisfies one of the following set of inequalities

$$|\lambda - B_{ii}| \leqslant \sum_{j \neq i} |B_{ij}| \qquad i = 1, \ldots, k. \tag{B.18}$$

A simple consequence of this result is that the maximum eigenvalue $\lambda_{\max}$ of a $k \times k$ Hermitian matrix, B satisfies

$$\lambda_{\max} \leqslant k \max_{ij} |B_{ij}| . \tag{B.19}$$

Now $A_{ij} = f_i^{1/2} Q_{ij} f_j^{1/2}$ so applying (B.10) and using the fact that $f_1 \leqslant f_2 \leqslant f_3 \leqslant \cdots \leqslant f_V$, we obtain a bound on the elements of $A^{(k)}$, the $k \times k$ submatrix of A, namely

$$\left|A_{ij}^{(k)}\right| \leqslant \frac{\beta}{4} K\left(\frac{V-k}{2}\right). \tag{B.20}$$

It follows from (B.19) that the maximum eigenvalue of $A^{(k)}$ is bounded above by $\frac{1}{4}k\beta K[(V-k)/2)]$. It thus follows, using the corollary to the inclusion principle, that

$$\alpha_k \leqslant \frac{V\beta}{4} K\left(\frac{k-1}{2}\right). \tag{B.21}$$

We now make the definition

$$0 < c \equiv \frac{1+b/2}{1+b} < 1 \tag{B.22}$$

and set

$$V \geqslant \max\left\{M^{1/c}, \left(\frac{\beta}{2}\right)^{2/b}\right\}. \tag{B.23}$$

If $k > 1 + 2V^c$ then $(k-1)/2 > V^c > M$ and so applying (B.2) and (B.22) we have

$$\begin{aligned}
\frac{V\beta}{4} K(\tfrac{1}{2}k - 1) &< \frac{V\beta}{4(\frac{1}{2}(k-1))^{(1+b)}} \\
&< \frac{V\beta}{4V^{c(1+b)}} \\
&= \frac{\beta}{4V^{b/2}} \\
&< \tfrac{1}{2}
\end{aligned} \tag{B.24}$$

where use has been made of (B.23). It follows using (B.21) and (B.24) that

$$\begin{aligned}
-\log(1-\alpha_k) &\leqslant -\log\left[1 - \frac{V\beta}{4} K\left(\frac{k-1}{2}\right)\right] \\
&= \log\left[1 + \frac{V\beta}{4} K\left(\frac{k-1}{2}\right)\left[1 - \frac{V\beta}{4} K\left(\frac{k-1}{2}\right)\right]^{-1}\right] \\
&\leqslant \log\left[1 + \frac{V\beta}{2} K\left(\frac{k-1}{2}\right)\right] \\
&\leqslant \frac{V\beta}{2} K\left(\frac{k-1}{2}\right)
\end{aligned} \tag{B.25}$$

where in performing the last step we make use of the fact that $\log(1+x) < x$.

Combining (B.25) with (B.13) and (B.14), we achieve

$$\begin{aligned}
0 &\leqslant -\frac{1}{V}\log\det\left[I - J\zeta^{-1}\right] \\
&= -\frac{1}{V}\sum_{k=1}^{1+2V^c}\log(1-\alpha_k) - \frac{1}{V}\sum_{k=1+2V^c}^{V}\log(1-\alpha_k) \\
&\leqslant -\frac{1+2V^c}{V}\log\epsilon + \frac{1}{V}\frac{V\beta}{2}\sum_{k=1+2V^c}^{V} K\left(\frac{k-1}{2}\right) \\
&= -\left(V^{-1} + 2V^{-b/2(1+b)}\right)\log\epsilon + \frac{\beta}{2}\sum_{k=1+2V^c}^{\infty} K\left(\frac{k-1}{2}\right).
\end{aligned} \tag{B.26}$$

The second term is a tail of a convergent series and so the required result follows.

B2. Separable potential

We next examine the separable potential form (2.11).

The matrix J in this case is a projection matrix, i.e.

$$J = \eta^2 u_1 u_1^\dagger \tag{B.27}$$

where

$$\eta \equiv \left[V^{-1}\sum_k v_k^2\right]^{1/2} \tag{B.28}$$

and u_1 is the unit vector with components

$$(u_1)_k \equiv \frac{v_k}{\eta\sqrt{V}}. \tag{B.29}$$

We let $u_2, \ldots, u_V$ denote an orthonormal basis for the kernal of J (i.e. the subspace orthogonal to u_1). $\{\zeta u_2, \ldots, \zeta u_V\}$ is then a linearly independent set of $V-1$ eigenvectors for $I - J\zeta^{-1}$, each with eigenvalue 1. We let λ_1 denote the other eigenvalue of $I - J\zeta^{-1}$. Now $J\zeta^{-1}$ is similar to $\zeta^{-1/2}J\zeta^{-1/2}$ and it is shown in appendix A1 that the maximum eigenvalue of $\zeta^{-1/2}J\zeta^{-1/2}$ is not greater than $1-\epsilon$ so $\lambda_1 \geqslant \epsilon$.

Combining these results, we obtain

$$\begin{aligned}
0 &\leqslant -\frac{1}{V}\log\det\left(I - J\zeta^{-1}\right) \\
&= -\frac{\log\lambda_1}{V} \\
&< -\frac{\log\epsilon}{V}
\end{aligned} \tag{B.30}$$

from which the required result follows.

B3. Kac potential

We consider the Kac form (2.12).

In this case (2.8) then completely decouples in the Kac limit ($\gamma \to 0^+$) (after the thermodynamic limit). That is, for large k and V with k/V fixed, Δ_k approaches a limit $\Delta\,(2\pi k_1/L, \ldots, 2\pi k_d/L)$ and

$$\begin{aligned}\Delta_k &= \frac{\beta}{4}\sum_l J_{kl}\Delta_l h\,(\beta E_l)\\ &= \frac{\beta\gamma^d}{4}\sum_l K(\gamma\|k-l\|)\Delta_l h\,(\beta E_l)\\ &\approx \frac{\beta\Delta_k h\,(\beta E_k)}{4}\sum_l \gamma^d K(\gamma\|l\|)\\ &\approx \frac{\alpha\beta\Delta_k h\,(\beta E_k)}{4}\end{aligned} \tag{B.31}$$

where

$$\alpha \equiv \int_{\mathbb{R}^d} K(\|r\|)\mathcal{D}r. \tag{B.32}$$

$\Delta(\theta)$ is therefore determined by

$$\Delta(\theta)h\,(\beta E(\theta)) = 4\Delta(\theta)/\alpha\beta \tag{B.33}$$

and we choose the non-trivial solution if one exists. That is, using the fact that the function $h\left(\beta\sqrt{(\mu-\epsilon(\theta))^2+x^2}\right)$ is positive and monotone decreasing in $x \geqslant 0$, $\Delta(\theta) = 0$ if $h(\beta(\mu-\epsilon(\theta))) < 4/\alpha\beta$ and is the positive solution of

$$h(\beta E(\theta)) = 4/\alpha\beta \tag{B.34}$$

otherwise where

$$E(\theta) \equiv \sqrt{(\epsilon(\theta)-\mu)^2 + (\Delta(\theta))^2}. \tag{B.35}$$

$\Delta(\theta)$ is continuous and $\Delta_k - \Delta\,(2\pi k_1/L, \ldots, 2\pi k_d/L)$ vanishes to zeroth order in γ and $1/V$, the correction terms being uniformly bounded over k. Applying the previously mentioned properties of $\Delta(\theta)$, (4.18) and the continuity and monotonicity of h we arrive at

$$\zeta_k^{-1} \approx \frac{\beta(1-\epsilon)}{4} h\left(\beta E\left(\frac{2\pi k_1}{L}, \ldots, \frac{2\pi k_d}{L}\right)\right) \tag{B.36}$$

so

$$\zeta_k^{-1} \leqslant \frac{1-\epsilon/2}{\alpha} \tag{B.37}$$

as long as γ and $1/V$ are sufficiently small, the requirements being uniform over k.

J is cyclic and is diagonalized by the matrix S where

$$S_{kl} = \frac{1}{\sqrt{V}} e^{2\pi i k \cdot l / L} \tag{B.38}$$

having eigenvalues

$$\lambda_k = \gamma^d \sum_r K(\gamma ||r||) e^{-2\pi i k \cdot r / L}. \tag{B.39}$$

Using (B.37) and (B.39) then, we obtain

$$\begin{aligned}
0 \leqslant -\frac{1}{V} \log \det \, [I - J\zeta^{-1}] \\
&= -\frac{1}{V} \log \det \left[I - \zeta^{-1/2} J \zeta^{-1/2} \right] \\
&\leqslant -\frac{1}{V} \log \det \left[I - \frac{(1-\epsilon/2)}{\alpha} J \right] \\
&= -\frac{1}{V} \sum_k \log \left[1 - \frac{(1-\epsilon/2)\gamma^d}{\alpha} \sum_r K(\gamma ||r||) e^{2\pi i k \cdot r / L} \right] \\
&\to -\frac{1}{(2\pi)^d} \int_{[0,2\pi]^d} \left[1 - \frac{(1-\epsilon/2)\gamma^d}{\alpha} \sum_r K(\gamma ||r||) e^{i\theta \cdot r} \right] \mathcal{D}\theta \quad \text{as } V \to \infty \\
&\to 0 \qquad \text{as } \gamma \to 0^+
\end{aligned} \tag{B.40}$$

and hence the required result. The last step relies on the Reimann–Lebesgue lemma, namely

$$\gamma^d \sum_r K(\gamma ||r||) e^{i\theta \cdot r} \to 0 \qquad \text{as } \gamma \to 0^+ \text{ if } \theta \neq 0 \tag{B.41}$$

and was established by Thompson and Silver [18].

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